

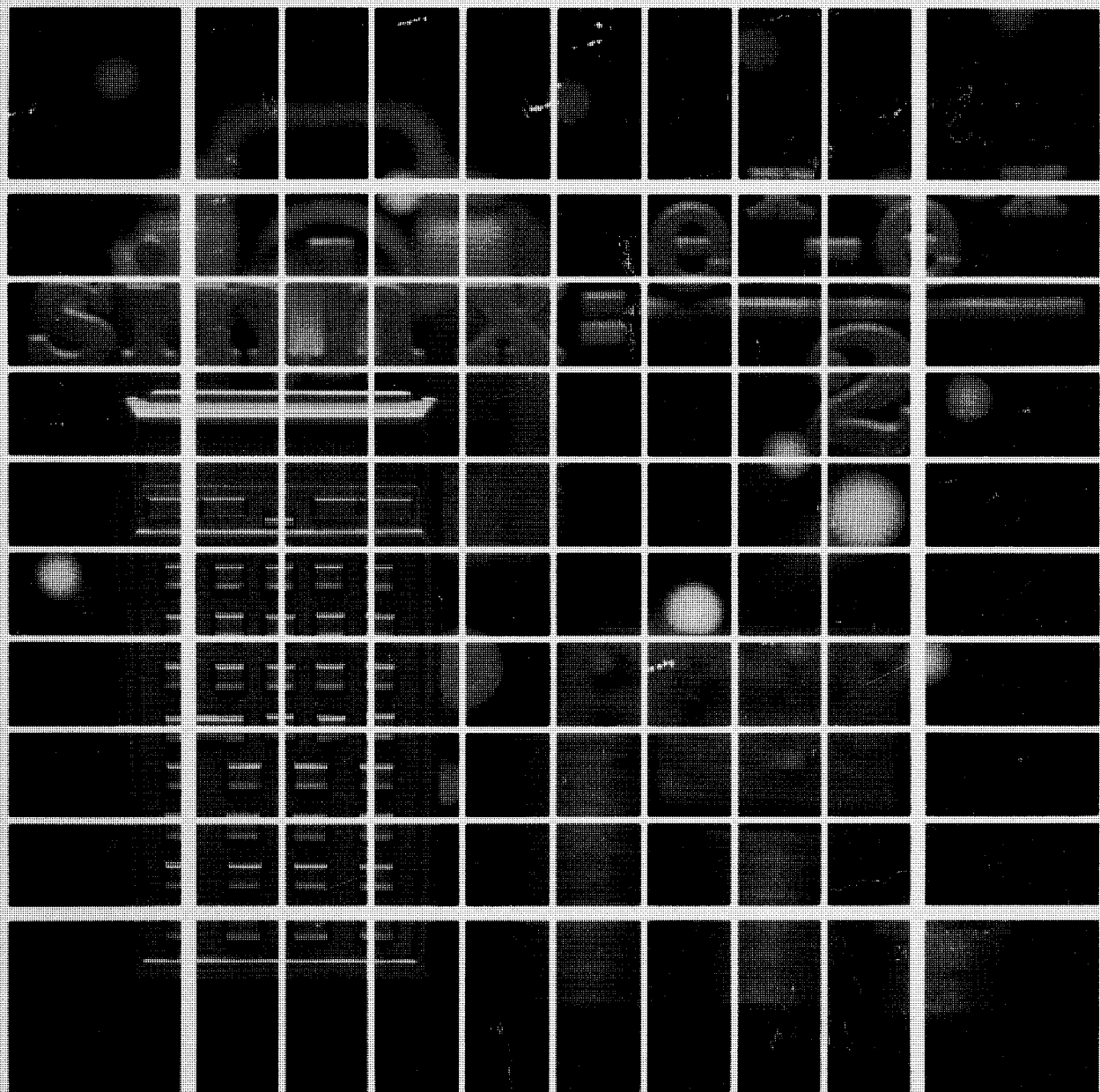
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HEWLETT-PACKARD

HP-41

USERS' LIBRARY SOLUTIONS

Chemistry



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## INTRODUCTION

This HP-41C Solutions book was written to help you get the most from your calculator. The programs were chosen to provide useful calculations for many of the common problems encountered.

They will provide you with immediate capabilities in your everyday calculations and you will find them useful as guides to programming techniques for writing your own customized software. The comments on each program listing describe the approach used to reach the solution and help you follow the programmer's logic as you become and expert on your HP calculator.

## KEYING A PROGRAM INTO THE HP-41C

There are several things that you should keep in mind while you are keying in programs from the program listings provided in this book. The output from the HP 82143A printer provides a convenient way of listing and an easily understood method of keying in programs without showing every keystroke. This type of output is what appears in this handbook. Once you understand the procedure for keying programs in from the printed listings, you will find this method simple and fast. Here is the procedure:

1. At the end of each program listing is a listing of status information required to properly execute that program. Included is the SIZE allocation required. Before you begin keying in the program, press **XEQ** **ALPHA** **SIZE** **ALPHA** and specify the allocation (three digits; e.g., 10 should be specified as 010).

Also included in the status information is the display format and status of flags important to the program. To ensure proper execution, check to see that the display status of the HP-41C is set as specified and check to see that all applicable flags are set or clear as specified.

2. Set the HP-41C to PRGM mode (press the **PRGM** key) and press **■** **GTO** **■** **■** to prepare the calculator for the new program.
3. Begin keying in the program. Following is a list of hints that will help you when you key in your programs from the program listings in this handbook.
  - a. When you see " (quote marks) around a character or group of characters in the program listing, those characters are ALPHA. To key them in, simply press **ALPHA**, key in the characters, then press **ALPHA** again. So "SAMPLE" would be keyed in as **ALPHA** "SAMPLE" **ALPHA**.
  - b. The diamond in front of each LBL instruction is only a visual aid to help you locate labels in the program listings. When you key in a program, ignore the diamond.
  - c. The printer indication of divide sign is /. When you see / in the program listing, press **÷**.
  - d. The printer indication of the multiply sign is \*. When you see \* in the program listing, press **×**.
  - e. The † character in the program listing is an indication of the **APPEND** function. When you see †, press **■** **APPEND** in ALPHA mode (press **■** and the K key).
  - f. All operations requiring register addresses accept those addresses in these forms:

nn (a two-digit number)

IND nn (INDIRECT: **■**, followed by a two-digit number)

X, Y, Z, T, or L (a STACK address: **■** followed by X, Y, Z, T, or L)

IND X, Y, Z, T or L (INDIRECT stack: **■** **■** followed by X, Y, Z, T, or L)

Indirect addresses are specified by pressing **■** and then the indirect address. Stack addresses are specified by pressing **■** followed by X, Y, Z, T, or L. Indirect stack addresses are specified by pressing **■** **■** and X, Y, Z, T, or L.

### Printer Listing

```

01 ♦ LBL "SAM
PLE"
02 "THIS IS
A "
03 "†SAMPLE
"
04 AVIEW
05 6
06 ENTER†
07 -2
08 /
09 ABS
10 STO IND
L
11 "R3="
12 ARCL 03
13 AVIEW
14 RTN

```

### Keystrokes

```

■ LBL ALPHA SAMPLE ALPHA
ALPHA THIS IS A ALPHA
ALPHA ■ APPEND SAMPLE
■ AVIEW ALPHA
6
ENTER*
2 CHS
÷
XEQ ALPHA ABS ALPHA
STO ■ L
ALPHA R3= ■ ARCL 03
■ AVIEW
ALPHA
■ RTN

```

### Display

```

01 LBLT SAMPLE
02T THIS IS A
03T † SAMPLE
04 AVIEW
05 6
06 ENTER†
07 -2
08 /
09 ABS
10 STO IND L
11T R3=
12 ARCL 03
13 AVIEW
14 RTN

```

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| *   | REQUIRES ONE MEMORY MODULE                                                                                                                                                                                              |    |

## pH OF WEAK ACID OR BASE SOLUTIONS

This program calculates the pH of a weak acid or base in aqueous solution by Newton-Raphson iteration of:

$$f(x) = x^3 + Kx^2 - (KC + K_w)x - KK_w = 0$$

where  $x$ ,  $K$  and  $C$  are  $[H^+]$ ,  $K_a$ , and  $C_a$ , respectively, for weak acid solutions and  $[OH^-]$ ,  $K_b$  and  $C_b$  for weak base solutions. The first estimate of  $x$  in the iteration is:

$$x = (KC + K_w)^{1/2}$$

An error term,  $f(x)/f'(x)$ , is also calculated.

The program is designed to be totally compatible with the HP-82143A peripheral printer, but will run equally well without. It is not compatible with any mass storage devices, and requires one standard memory module for operation.

Reference: J. N. Butler, *Ionic Equilibrium, A Mathematical Approach*, Addison-Wesley, Reading, MA, 1964.

Example 1: (without the printer) Find the pH of  $1.0 \times 10^{-4}M$  acetic acid if its  $K_a$  is  $1.8 \times 10^{-5}$ .

Keystrokes:

Display:

[XEQ] [ALPHA] SIZE [ALPHA] 011

[///] [FIX] 2

[XEQ] [ALPHA] PH [ALPHA]

ACID/BASE?

[<-]

ACID (Default)

[R/S]

CONC. ACID?

[EEX] [CHS] 4 [R/S]

$K_a, PK_a, K_b, PK_b$

1.8 [EEX] [CHS] 5 [A]

PH=4.46

[R/S]

$K_a=1.80E-5$

[R/S]

$<H^+>=3.45E-5$

[R/S]

ERR.=1.10E-7

Example 2: (with the printer) Calculate the pH of .002 molar KCN.  
 $pK_a = 9.32$ .

Keystrokes:

[XEQ] [ALPHA] PH [ALPHA]

BASE [R/S]

.002 [R/S]

9.32 [D]

[<-]

Display:

(Prints title)

ACID/BASE?

CONC. BASE?

(Prints base concentration)

Kb,PKb,Ka,PKa

(Prints pKa, pOH, Kb, [OH-]  
 and the error term)

ACID/BASE?

BASE (Note that default is  
 now base)

Sample printer output:

pH Calculations

[BASE]=2.00E-3 M

pKa=9.32

pOH=3.71

Kb=2.09E-5

[OH-]=1.95E-4

ERR.=6.98E-7

# User Instructions

|      |                                                        |       |                | SIZE: 011     |
|------|--------------------------------------------------------|-------|----------------|---------------|
| STEP | INSTRUCTIONS                                           | INPUT | FUNCTION       | DISPLAY       |
| 1    | Load the program.                                      |       |                |               |
| 2    | Set size and display format.                           |       | [XEQ] SIZE 011 |               |
|      |                                                        |       | [////] [FIX] 2 |               |
| 3    | Execute the program.                                   |       | [XEQ] PH       |               |
|      | If printer is attached, the paper is                   |       |                |               |
|      | advanced "pH Calculations" is printed                  |       |                |               |
|      | and the paper is advanced again.                       |       |                | ACID/BASE?    |
| 4    | Choose ACID or BASE mode.                              |       |                |               |
|      | Initial Default mode is ACID, but default              |       |                |               |
|      | mode is always the mode of the last                    |       |                |               |
|      | calculation. Default mode can always be                |       |                |               |
|      | checked by pressing [ $\leftarrow$ ] when "ACID/BASE?" |       |                |               |
|      | is in the display to view the alpha                    |       |                |               |
|      | register.                                              |       |                |               |
|      |                                                        |       | "ACID" [R/S]   | CONC. ACID?   |
|      |                                                        | or    | "BASE" [R/S]   | COND. BASE?   |
| 5    | In put the molar concentration of acid                 |       |                |               |
|      | or base. The concentration used in the                 |       |                |               |
|      | last calculation is in the X-register and              |       |                |               |
|      | may be viewed and/or used by pressing                  |       |                |               |
|      | [ $\leftarrow$ ] and/or [R/S] respectively. If the     | C     | [R/S]          |               |
|      | printer is attached, [ACID]= or [BASE]=,               |       |                |               |
|      | the input concentration, and the symbol                |       |                |               |
|      | M (for mode) will be printed.                          |       | (in ACID mode) | Ka,PKa,kb,PKb |
|      |                                                        |       | (in BASE mode) | Kb,PKb,Ka,PKa |
| 6    | Choose the equilibrium constant represen-              |       |                |               |
|      | tation. The display indicated the                      |       |                |               |

# User Instructions

|      |                                                 |        |          | SIZE:      |
|------|-------------------------------------------------|--------|----------|------------|
| STEP | INSTRUCTIONS                                    | INPUT  | FUNCTION | DISPLAY    |
|      | functions of the first four, top-row keys.      |        |          |            |
|      | In ACID mode:                                   | $K_a$  | [A]      |            |
|      |                                                 | $pK_a$ | [B]      |            |
|      |                                                 | $K_b$  | [C]      |            |
|      |                                                 | $pK_b$ | [D]      |            |
|      | In BASE mode:                                   | $K_b$  | [A]      |            |
|      |                                                 | $pK_b$ | [B]      |            |
|      |                                                 | $K_a$  | [C]      |            |
|      |                                                 | $pK_a$ | [D]      |            |
|      | In all cases, if the printer is                 |        |          |            |
|      | attached, the input name and values are         |        |          |            |
|      | printed.                                        |        |          |            |
| 7    | View the output.                                |        |          |            |
|      | In ACID mode:                                   |        |          | PH=( )     |
|      |                                                 |        |          | $K_a$ =( ) |
|      |                                                 |        |          | <H+>=( )   |
|      |                                                 |        |          | ERR.=( )   |
|      | In BASE mode:                                   |        |          | POH=( )    |
|      |                                                 |        |          | $K_b$ =( ) |
|      |                                                 |        |          | <OH->=( )  |
|      |                                                 |        |          | ERR.=( )   |
|      | In either mode, the previous $K_a$ or $K_b$ is  |        |          |            |
|      | recalled into the X-register and may be         |        |          |            |
|      | viewed and/or used by pressing [ $\leftarrow$ ] |        |          |            |
|      | and/or [R/S] respectively.                      |        |          |            |
|      | In either mode, if the printer is               |        |          |            |
|      | attached, all values are printed out            |        |          |            |

# User Instructions

|      |                                           |       |           | SIZE :     |
|------|-------------------------------------------|-------|-----------|------------|
| STEP | INSTRUCTIONS                              | INPUT | FUNCTION  | DISPLAY    |
|      | after a paper advance to separate them    |       |           |            |
|      | from input values. In this case, the      |       |           |            |
|      | P's are lower case and <>'s are replaced  |       |           |            |
|      | by [ ]'s. A paper advance is executed     |       |           |            |
|      | and execution goes immediately to step 4. |       |           |            |
| 8    | To change output to alternate mode.       |       |           |            |
|      | In ACID mode:                             |       | [E]       | POH=( )    |
|      |                                           |       |           | Kb=( )     |
|      |                                           |       |           | <OH->=( )  |
|      |                                           |       |           | ERR.=( )   |
|      | In BASE mode:                             |       | [E]       | PH=( )     |
|      |                                           |       |           | Ka=( )     |
|      |                                           |       |           | <H+>=( )   |
|      |                                           |       |           | ERR.=( )   |
|      | If printer is attached, the calculator    |       |           |            |
|      | must be taken out of ALPHA mode before    |       |           |            |
|      | [E] is pressed. The values are output     |       |           |            |
|      | as in step 7, and execution goes          |       |           |            |
|      | immediately to step 4.                    |       |           |            |
| 9    | To start a new problem or re-input        |       |           |            |
|      | concentration:                            |       | [///] [a] | ACID/BASE? |
|      | Execution is transferred to step 4. If    |       |           |            |
|      | the printer is attached, an additional    |       |           |            |
|      | advance is executed to help separate      |       |           |            |
|      | problems.                                 |       |           |            |
|      |                                           |       |           |            |
|      |                                           |       |           |            |

# Program Listings

|             |                           |             |                                 |
|-------------|---------------------------|-------------|---------------------------------|
| 01♦LBL "PH" | Enable printer            | 51 RCL 06   |                                 |
| 02 SF 21    |                           | 52 STO 10   |                                 |
| 03 SF 27    | Set USER mode             | 53 "CONC. " |                                 |
| 04 "ACID"   |                           | 54 ARCL 10  |                                 |
| 05 ASTO 05  |                           | 55 "F?"     | Prompt for concentration        |
| 06 ASTO 10  | Store default             | 56 RCL 09   |                                 |
| 07 "BASE"   |                           | 57 PROMPT   |                                 |
| 08 ASTO 06  |                           | 58 STO 09   |                                 |
| 09 ADV      |                           | 59 FC? 55   |                                 |
| 10 FC? 55   | No printer? Go to line 29 | 60 GTO 00   | No printer? Go to line 74       |
| 11 GTO 00   |                           | 61 ASTO 08  |                                 |
| 12 SF 13    |                           | 62 CLA      |                                 |
| 13 CF 12    |                           | 63 91       |                                 |
| 14 4        |                           | 64 ACCHR    |                                 |
| 15 SKPCHR   |                           | 65 ARCL 10  | Print concentration             |
| 16 "P"      |                           | 66 ACA      |                                 |
| 17 ACA      |                           | 67 93       |                                 |
| 18 CF 13    | Print title               | 68 ACCHR    |                                 |
| 19 "H C"    |                           | 69 "="      |                                 |
| 20 ACA      |                           | 70 ARCL 09  |                                 |
| 21 SF 13    |                           | 71 "F M"    |                                 |
| 22 "ALCULAT |                           | 72 ACA      |                                 |
| IONS"       |                           | 73 PRBUF    |                                 |
| 23 ACA      |                           | 74♦LBL 00   |                                 |
| 24 PRBUF    |                           | 75 "K"      |                                 |
| 25♦LBL a    |                           | 76 XEQ 09   | Prompt for equilibrium constant |
| 26 CF 06    | Initialize                | 77 "F,PK"   |                                 |
| 27 CF 13    |                           | 78 XEQ 09   |                                 |
| 28 ADV      |                           | 79 "F,K"    |                                 |
| 29♦LBL 00   |                           | 80 XEQ 08   |                                 |
| 30 CLA      |                           | 81 "F,PK"   |                                 |
| 31 ARCL 05  |                           | 82 XEQ 08   |                                 |
| 32 "F/"     |                           | 83 PROMPT   |                                 |
| 33 ARCL 06  | Prompt for mode           | 84♦LBL 10   |                                 |
| 34 "F?"     |                           | 85 "F="     |                                 |
| 35 CF 21    |                           | 86 ARCL X   |                                 |
| 36 AVIEW    |                           | 87 ACA      | Common output routine           |
| 37 SF 21    |                           | 88 PRBUF    |                                 |
| 38 CLA      |                           | 89 RTN      |                                 |
| 39 ARCL 10  |                           | 90♦LBL B    |                                 |
| 40 AON      |                           | 91 SF 06    |                                 |
| 41 STOP     |                           | 92♦LBL D    |                                 |
| 42 AOFF     |                           | 93 SF 13    |                                 |
| 43 ASTO X   |                           | 94 "P"      | Input and print pK's            |
| 44 RCL 05   |                           | 95 FS? 55   |                                 |
| 45 X=Y?     | Store indicated mode      | 96 ACA      |                                 |
| 46 SF 00    |                           | 97 CF 13    |                                 |
| 47 X=Y?     |                           | 98 "K"      |                                 |
| 48 CF 00    |                           | 99 FC? 06   |                                 |
| 49 RCL 05   |                           | 100 XEQ 08  |                                 |
| 50 FS? 00   |                           | 101 FS? 06  |                                 |

# Program Listings

|                       |                                                 |            |                   |
|-----------------------|-------------------------------------------------|------------|-------------------|
| 102 XEQ 09            |                                                 | 153 XEQ 01 |                   |
| 103 FS? 55            |                                                 | 154*LBL 11 |                   |
| 104 XEQ 10            |                                                 | 155 STO 01 |                   |
| 105 CHS               |                                                 | 156 RCL 09 |                   |
| 106 10↑X              |                                                 | 157 *      |                   |
| 107 FC? 06            |                                                 | 158 1 E-14 |                   |
| 108 1 E14             |                                                 | 159 +      |                   |
| 109 FC? 06            |                                                 | 160 STO 03 | First             |
| 110 *                 |                                                 | 161 LASTX  | approximation     |
| 111 FC?C 06           |                                                 | 162 RCL 01 |                   |
| 112 1/X               |                                                 | 163 *      |                   |
| 113 GTO 11            |                                                 | 164 STO 04 |                   |
| 114*LBL 01            | Go to calculation routine                       | 165 RCL 03 |                   |
| 115 1 E14             |                                                 | 166 SQRT   |                   |
| 116 *                 |                                                 | 167 STO 02 |                   |
| 117 1/X               | K <sub>a</sub> to K <sub>b</sub> and vice versa | 168*LBL 04 |                   |
| 118 RTN               |                                                 | 169 RCL 02 |                   |
| 119*LBL 08            |                                                 | 170 RCL 01 |                   |
| 120 FS? 00            |                                                 | 171 +      |                   |
| 121 "H <sub>a</sub> " |                                                 | 172 RCL 02 |                   |
| 122 FC? 00            | Common prompt and output format routine         | 173 *      |                   |
| 123 "H <sub>b</sub> " |                                                 | 174 RCL 03 |                   |
| 124 RTN               |                                                 | 175 -      |                   |
| 125*LBL 09            |                                                 | 176 RCL 02 |                   |
| 126 FC? 00            |                                                 | 177 *      |                   |
| 127 "H <sub>a</sub> " |                                                 | 178 RCL 04 |                   |
| 128 FS? 00            | Common prompt and output format routine         | 179 -      |                   |
| 129 "H <sub>b</sub> " |                                                 | 180 RCL 02 |                   |
| 130 RTN               |                                                 | 181 3      |                   |
| 131*LBL E             |                                                 | 182 *      | Iterative routine |
| 132 RCL 01            |                                                 | 183 RCL 01 |                   |
| 133 XEQ 01            | Output mode conversion routine                  | 184 2      |                   |
| 134 STO 01            |                                                 | 185 *      |                   |
| 135 RCL 02            |                                                 | 186 +      |                   |
| 136 XEQ 01            |                                                 | 187 RCL 02 |                   |
| 137 STO 02            |                                                 | 188 *      |                   |
| 138 FS?C 00           |                                                 | 189 RCL 03 |                   |
| 139 GTO 05            |                                                 | 190 -      |                   |
| 140 SF 00             |                                                 | 191 /      |                   |
| 141 GTO 05            |                                                 | 192 STO 00 |                   |
| 142*LBL C             |                                                 | 193 ABS    |                   |
| 143 SF 06             |                                                 | 194 RCL 02 |                   |
| 144*LBL A             |                                                 | 195 99     |                   |
| 145 "K"               | Input and print K'a                             | 196 /      |                   |
| 146 FC? 06            |                                                 | 197 X<>Y   |                   |
| 147 XEQ 09            |                                                 | 198 X<=Y?  |                   |
| 148 FS? 06            |                                                 | 199 GTO 05 |                   |
| 149 XEQ 08            |                                                 | 200 RCL 00 |                   |
| 150 FS? 55            |                                                 | 201 ST- 02 |                   |
| 151 XEQ 10            |                                                 | 202 GTO 04 |                   |
| 152 FS?C 06           |                                                 | 203*LBL 05 |                   |

# Program Listings

|              |                                                   |            |                          |
|--------------|---------------------------------------------------|------------|--------------------------|
| 204 RCL 02   | Output pH or<br>pOH                               | 255 ACA    | Common output<br>routine |
| 205 LOG      |                                                   | 256 FS? 55 |                          |
| 206 CHS      |                                                   | 257 PRBUF  |                          |
| 207 STO 07   |                                                   | 258 FC? 55 |                          |
| 208 ADV      |                                                   | 259 AVIEW  |                          |
| 209 SF 13    |                                                   | 260 .END.  |                          |
| 210 "P"      |                                                   |            |                          |
| 211 FS? 55   |                                                   |            |                          |
| 212 ACA      |                                                   |            |                          |
| 213 CF 13    |                                                   | 60         |                          |
| 214 FS? 55   | Output K <sub>a</sub> or K <sub>b</sub>           |            |                          |
| 215 CLA      |                                                   |            |                          |
| 216 FS? 00   |                                                   |            |                          |
| 217 "H="     |                                                   |            |                          |
| 218 "H="     |                                                   |            |                          |
| 219 ARCL X   |                                                   |            |                          |
| 220 XEQ 07   |                                                   |            |                          |
| 221 "K"      |                                                   |            |                          |
| 222 XEQ 09   |                                                   |            |                          |
| 223 "H="     |                                                   | 70         |                          |
| 224 ARCL 01  | Output [H <sup>+</sup> ] or<br>[OH <sup>-</sup> ] |            |                          |
| 225 XEQ 07   |                                                   |            |                          |
| 226 CLA      |                                                   |            |                          |
| 227 FC? 55   |                                                   |            |                          |
| 228 "<"      |                                                   |            |                          |
| 229 91       |                                                   |            |                          |
| 230 FS? 55   |                                                   |            |                          |
| 231 ACCHR    |                                                   |            |                          |
| 232 FS? 00   |                                                   |            |                          |
| 233 "H-OH="  |                                                   | 80         |                          |
| 234 FC? 00   | Output Error<br>term.                             |            |                          |
| 235 "H+ "    |                                                   |            |                          |
| 236 FS? 55   |                                                   |            |                          |
| 237 ACA      |                                                   |            |                          |
| 238 FC? 55   |                                                   |            |                          |
| 239 "H>"     |                                                   |            |                          |
| 240 93       |                                                   |            |                          |
| 241 FS? 55   |                                                   |            |                          |
| 242 ACCHR    |                                                   |            |                          |
| 243 FS? 55   |                                                   |            |                          |
| 244 CLA      |                                                   | 90         |                          |
| 245 "H="     |                                                   |            |                          |
| 246 ARCL 02  |                                                   |            |                          |
| 247 XEQ 07   |                                                   |            |                          |
| 248 "ERR. =" |                                                   |            |                          |
| 249 ARCL 00  |                                                   |            |                          |
| 250 XEQ 07   |                                                   |            |                          |
| 251 ADV      |                                                   |            |                          |
| 252 GTO a    |                                                   |            |                          |
| 253 LBL 07   |                                                   |            |                          |
| 254 FS? 55   |                                                   | 00         |                          |

# REGISTERS, STATUS, FLAGS, ASSIGNMENTS

| DATA REGISTERS |                                                                             | STATUS                |              |                        |                         |
|----------------|-----------------------------------------------------------------------------|-----------------------|--------------|------------------------|-------------------------|
| 00             | f(x)/f' (x)<br>K<br>[H+] or [OH-]<br>CK + K <sub>w</sub><br>KK <sub>w</sub> | SIZE 011              | TOT. REG. 84 | USER MODE              |                         |
|                |                                                                             | ENG                   | FIX          | SCI                    | ON X OFF                |
|                |                                                                             | DEG                   | RAD          | GRAD                   |                         |
| 05             | "ACID"<br>"BASE"<br>pH<br>Temp. Alpha Storage<br>Concentration              | FLAGS                 |              |                        |                         |
| 10             | "ACID" or "BASE"                                                            | #                     | INIT S/C     | SET INDICATES          | CLEAR INDICATES         |
|                |                                                                             | 00                    |              | Base                   | Acid                    |
|                |                                                                             | 06                    |              | Subroutine B or C      | Any other location      |
|                |                                                                             | 12                    |              | Double wide characters | Single width characters |
|                |                                                                             | 13                    |              | Lower case characters  | Upper case characters   |
|                |                                                                             | 21                    |              | Printer enabled        | Printer disabled        |
|                |                                                                             | 27                    |              | User mode ON           | User mode OFF           |
|                |                                                                             | 55                    |              | Printer exists         | Printer doesn't exist   |
|                |                                                                             | ASSIGNMENTS           |              |                        |                         |
|                |                                                                             | ACID mode             |              | BASE Mode              |                         |
|                |                                                                             | FUNCTION              | KEY          | FUNCTION               | KEY                     |
|                |                                                                             | Ka                    | A            | Kb                     | A                       |
|                |                                                                             | pKa                   | B            | pKb                    | B                       |
|                |                                                                             | Kb                    | C            | Ka                     | C                       |
|                |                                                                             | pKb                   | D            | pKa                    | D                       |
|                |                                                                             | output alter mode     | E            | output alter mode      | E                       |
|                |                                                                             | Reinput concentration |              |                        | a                       |

pH OF WEAK ACID BASE SOLUTIONS

PROGRAM REGISTERS NEEDED: 73

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 1 (1 : 4)



ROW 2 (4 : 8)



ROW 3 (9 : 16)



ROW 4 (16 : 21)



ROW 5 (22 : 23)



ROW 6 (23 : 31)



ROW 7 (31 : 37)



ROW 8 (37 : 46)



ROW 9 (47 : 53)



ROW 10 (53 : 60)



ROW 11 (60 : 67)



ROW 12 (67 : 72)



ROW 13 (73 : 77)



ROW 14 (78 : 81)



ROW 15 (81 : 87)



ROW 16 (87 : 94)



ROW 17 (94 : 100)



ROW 18 (100 : 106)



ROW 19 (107 : 113)



ROW 20 (113 : 121)



ROW 21 (121 : 127)



ROW 22 (127 : 133)



ROW 23 (134 : 141)



ROW 24 (141 : 147)



ROW 25 (147 : 152)



ROW 26 (153 : 159)



ROW 27 (160 : 172)



ROW 28 (173 : 185)



ROW 29 (186 : 197)



ROW 30 (198 : 207)



ROW 31 (208 : 214)



ROW 32 (215 : 220)



ROW 33 (220 : 225)



ROW 34 (225 : 231)



ROW 35 (232 : 235)



ROW 36 (236 : 241)



## pH OF WEAK ACID BASE SOLUTIONS

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 37 (242 : 247)



ROW 38 (248 : 252)



ROW 39 (252 : 258)



ROW 40 (259 : 260)



## ACID-BASE EQUILIBRIUM (DIPROTIC)

Program determines  $[H^+]$  of pH of a solution of a dibasic acid and/or its salts. Required input are:

$K_1$  and  $K_2$ : First and second equilibrium constants of the acid.

$C_a$ : Initial conc. of the acid ( $H_2A$ ).

$C_{s,1}$ : Initial conc. of the first salt ( $NaHA$ ).

$C_{s,2}$ : Initial conc. of the second salt ( $Na_2A$ ).

$$K_w = 1 \cdot 10^{-14}$$

The following equations are used: ( $x = [H_3O^+]$ )

| Mixture of (in $H_2O$ ) | Equation                                                                                                           |
|-------------------------|--------------------------------------------------------------------------------------------------------------------|
| 1. $H_2A$               | $x^4 + K_1x^3 + (K_1K_2 - K_w - K_1C_a)x^2 - (K_wK_1 + 2K_1K_2C_a)x - K_wK_1K_2 = 0$                               |
| 2. $H_2A + NaHA$        | $x^4 + (C_{s,1} + K_1)x^3 + (K_1K_2 - K_w - K_1C_a)x^2 - (K_wK_1 + 2K_1K_2C_a + K_1K_2C_{s,1})x - K_wK_1K_2 = 0$   |
| 3. $NaHA$               | $x^4 + (C_{s,1} + K_1)x^3 + (K_1K_2 - K_w)x^2 - (K_wK_1 + K_1K_2C_{s,1})x - K_wK_1K_2 = 0$                         |
| 4. $NaHA + Na_2A$       | $x^4 + (C_{s,1} + 2C_{s,2} + K_1)x^3 + (K_1K_2 - K_w + K_1C_{s,2})x^2 - (K_wK_1 + K_1K_2C_{s,1})x - K_wK_1K_2 = 0$ |
| 5. $Na_2A$              | $x^4 + (2C_{s,2} + K_1)x^3 + (K_1K_2 - K_w + K_1C_{s,2})x^2 - K_wK_1x - K_wK_1K_2 = 0$                             |

Approximate values (used as starting values for the iterative solution) are:

1.  $x \doteq (K_1C_a)^{1/2}$
2.  $x \doteq K_1C_a/C_{s,1}$
3.  $x \doteq (K_1K_2)^{1/2}$
4.  $x \doteq K_2C_{s,1}/C_{s,2}$
5.  $x \doteq (K_wK_2/C_{s,2})^{1/2}$

NOTE: The representations  $H_2A$ ,  $NaHA$ , etc. are used in a general sense and do not refer to any particular substance.

Reference: J.G. Dick, *Analytical Chemistry*, McGraw-Hill Book Co., 1973.

Example: What is the  $[H_3O^+]$  of a solution containing 0.05 M sodium hydrogen oxalate and 0.01 M oxalic acid? What pH is this?

$$K_1 = 5.9 \times 10^{-2}$$

$$K_2 = 6.5 \times 10^{-5}$$

$$C_a = 0.01 \text{ M}$$

$$C_{S,1} = 0.05 \text{ M}$$

Keystrokes:

Display:

[XEQ] [ALPHA] SIZE [ALPHA] 015

[XEQ] [ALPHA] EQUIL [ALPHA]

K1?

5.9 [EEX] [CHS] 2 [R/S]

K2?

6.4 [EEX] [CHS] 5 [R/S]

Ca?

.01 [R/S]

CS,1?

.05 [R/S]

CS,2?

[R/S]

<H3O+>=5.54E-3

[R/S]\*

PH-2.26

\* [R/S] is omitted if printer is present.

# User Instructions

|      |                                                 |           |             | SIZE: 015            |
|------|-------------------------------------------------|-----------|-------------|----------------------|
| STEP | INSTRUCTIONS                                    | INPUT     | FUNCTION    | DISPLAY              |
| 1    | Load the program.                               |           |             |                      |
| 2    | Initialize.                                     |           | [XEQ] EQUIL | K1=?                 |
| 3    | Input $K_1$ .                                   | $K_1$     | [R/S]       | K2=?                 |
|      | The value of $K_1$ used in the last problem     |           |             |                      |
|      | may be viewed and/or reused by pressing         |           |             |                      |
|      | [←] and/or [R/S] respectively.                  |           |             |                      |
| 4    | Input $K_2$ .                                   | $K_2$     | [R/S]       | Ca=?                 |
|      | You have the same option as in step 3.          |           |             |                      |
| 5    | Input $C_a$ .                                   | $C_a$     | [R/S]       | CS,1=?               |
|      | The value of $C_a$ used in the last problem     |           |             |                      |
|      | is in the Y-register while 0 is in the          |           |             |                      |
|      | X-register. Thus, you have the option           |           |             |                      |
|      | of keying in a new $C_a$ , pressing [R/S] to    |           |             |                      |
|      | store zero (if there is no acid in the          |           |             |                      |
|      | system) or pressing [R↓] [R/S] to reuse         |           |             |                      |
|      | the last value of $C_a$ . Go to step 9 if       |           |             |                      |
|      | there are no other components.                  |           |             |                      |
| 6    | Input $C_{s,1}$ .                               | $C_{s,1}$ | [R/S]       | CS,2=?               |
|      | You have the same options as in step 5.         |           |             |                      |
| 7    | Input $C_{s,2}$ .                               | $C_{s,2}$ | [R/S]       | <H3O+>=( )           |
|      | You have the same options as in step 5.         |           | [R/S]*      | PH=( )               |
| 8    | For a new problem:                              |           | [A]         | K1=?                 |
| 9    | To calculate pH and $[H_3O^+]$ based on the     |           | [B]         |                      |
|      | current input values:                           |           | [B]         |                      |
| 10   | To change pH and $[H_3O^+]$ to pOH and $[OH^-]$ |           |             |                      |
|      | and back:                                       |           | [D]         | <H3O+>= or<br><OH->= |
|      | Each mode is maintained until the next          |           | [R/S]*      | PH= or POH=          |

[illegible]

# Program Listings

|                    |                  |            |                      |
|--------------------|------------------|------------|----------------------|
| 01*LBL "EQU<br>IL" |                  | 49 RTN     |                      |
| 02 SF 27           |                  | 50*LBL D   |                      |
| 03 CF 00           |                  | 51 FC?C 00 | Mode toggle          |
| 04 CLRG            | Initialize       | 52 SF 00   |                      |
| 05*LBL A           |                  | 53 GTO C   |                      |
| 06 9.013           |                  | 54*LBL 09  |                      |
| 07 STO 07          |                  | 55 RCL 09  |                      |
| 08 1 E-14          |                  | 56 STO 03  |                      |
| 09 STO 08          |                  | 57 RCL 10  |                      |
| 10 CF 05           |                  | 58 *       |                      |
| 11 "K1"            |                  | 59 STO 02  |                      |
| 12 XEQ 00          | Input parameters | 60 STO 00  |                      |
| 13 "K2"            |                  | 61 RCL 08  | First                |
| 14 XEQ 00          |                  | 62 CHS     | approximation        |
| 15 "Ca"            |                  | 63 ST+ 02  | routine              |
| 16 SF 05           |                  | 64 ST* 00  |                      |
| 17 XEQ 00          |                  | 65 RCL 10  |                      |
| 18 "CS,1"          |                  | 66 *       |                      |
| 19 XEQ 00          |                  | 67 STO 01  |                      |
| 20 "CS,2"          |                  | 68 RCL 12  |                      |
| 21*LBL 00          |                  | 69 ST+ 03  |                      |
| 22 RCL IND         |                  | 70 RCL 13  |                      |
| 07                 |                  | 71 ST+ 03  |                      |
| 23 FS? 05          | Common input     | 72 ST+ 03  |                      |
| 24 0               | routine          | 73 XEQ IND |                      |
| 25 "I=?"           |                  | 05         |                      |
| 26 PROMPT          |                  | 74 STO 04  |                      |
| 27 STO IND         |                  | 75 STO 06  |                      |
| 07                 |                  | 76 FIX 8   |                      |
| 28 ISG 07          |                  | 77*LBL 10  |                      |
| 29 RTN             |                  | 78 RCL 04  |                      |
| 30*LBL B           |                  | 79 RCL 03  |                      |
| 31 CF 05           | Pointer          | 80 +       |                      |
| 32 0               | initializing     | 81 RCL 04  |                      |
| 33 STO 05          | routine          | 82 *       |                      |
| 34 1               |                  | 83 RCL 02  |                      |
| 35 RCL 11          |                  | 84 +       |                      |
| 36 XEQ 08          |                  | 85 RCL 04  |                      |
| 37 2               |                  | 86 *       |                      |
| 38 RCL 12          |                  | 87 RCL 01  |                      |
| 39 XEQ 08          |                  | 88 +       |                      |
| 40 4               |                  | 89 RCL 04  |                      |
| 41 RCL 13          |                  | 90 *       |                      |
| 42 XEQ 08          |                  | 91 RCL 00  |                      |
| 43 GTO 09          |                  | 92 +       |                      |
| 44*LBL 08          |                  | 93 RCL 04  |                      |
| 45 X=0?            |                  | 94 4       |                      |
| 46 RTN             |                  | 95 *       |                      |
| 47 RDN             | Common pointer   | 96 RCL 03  |                      |
| 48 ST+ 05          | routine          | 97 3       |                      |
|                    |                  | 98 *       |                      |
|                    |                  |            | Iterative<br>routine |

# Program Listings

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                             |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------|
| <pre> 99 + 100 RCL 04 101 * 102 RCL 02 103 ST+ X 104 + 105 RCL 04 106 * 107 RCL 01 108 + 109 / 110 RCL 04 111 X&lt;&gt;Y 112 ST- 04 113 CLX 114 RCL 04 115 - 116 RND 117 X≠0? 118 GTO 10 119♦LBL C 120 SF 21 121 SCI 2 122 RCL 04 123 FC? 00 124 GTO 11 125 RCL 08 126 / 127 1/X 128♦LBL 11 129 "&lt;" 130 FC? 00 131 "FH30+" 132 FS? 00 133 "FOH-" 134 "F&gt;=" 135 ARCL X 136 AVIEW 137 LOG 138 CHS 139 FIX 2 140 "P" 141 FS? 00 142 "FO" 143 "FH=" 144 ARCL X 145 AVIEW 146 RTN 147♦LBL 01 148 XEQ 05 149 RCL 09 </pre> | Output routine | <pre> 150 RCL 11 151 * 152 ST- 02 153 STO 14 154 SQRT 155 RTN 156♦LBL 02 157 XEQ 07 158 LASTX 159 SQRT 160 RTN 161♦LBL 03 162 XEQ 05 163 XEQ 07 164 RCL 09 165 RCL 11 166 * 167 ST- 02 168 RCL 12 169 / 170 RTN 171♦LBL 04 172 SF 05 173♦LBL 06 174 FC? 05 175 XEQ 07 176 RCL 09 177 RCL 13 178 * 179 ST+ 02 180 FS? 05 181 RCL 08 182 FC? 05 183 RCL 12 184 RCL 10 185 * 186 RCL 13 187 / 188 FS?C 05 189 SQRT 190 RTN 191♦LBL 07 192 RCL 12 193 GTO 07 194♦LBL 05 195 RCL 11 196 ST+ X 197♦LBL 07 198 RCL 10 199 RCL 09 200 * </pre> | Initial guess<br>subroutine |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------|

# Program Listings

|            |  |    |  |
|------------|--|----|--|
| 201 *      |  | 51 |  |
| 202 ST- 01 |  |    |  |
| 203 RTN    |  |    |  |
| 204 END    |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
| 10         |  | 60 |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
| 20         |  | 70 |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
| 30         |  | 80 |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
| 40         |  | 90 |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
| 50         |  | 00 |  |

[illegible]

ACID-BASE EQUILIBRIUM  
(DIPROTIC)  
PROGRAM REGISTERS NEEDED: 49

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 1 (1 : 2)



ROW 2 (3 : 8)



ROW 3 (8 : 13)



ROW 4 (13 : 17)



ROW 5 (18 : 20)



ROW 6 (21 : 27)



ROW 7 (28 : 36)



ROW 8 (36 : 43)



ROW 9 (44 : 52)



ROW 10 (53 : 63)



ROW 11 (63 : 72)



ROW 12 (72 : 82)



ROW 13 (83 : 95)



ROW 14 (96 : 107)



ROW 15 (108 : 118)



ROW 16 (119 : 123)



ROW 17 (123 : 131)



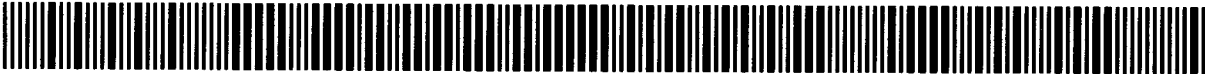
ROW 18 (131 : 134)



ACID-BASE EQUILIBRIUM  
(DIPROTIC)

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 19 (134 : 141)



ROW 20 (142 : 148)



ROW 21 (148 : 157)



ROW 22 (157 : 165)



ROW 23 (166 : 175)



ROW 24 (175 : 183)



ROW 25 (184 : 194)



ROW 26 (195 : 203)



ROW 27 (204 : 204)



## WEAK ACID/BASE TITRATION CURVE

THIS PROGRAM REQUIRES 1 ADDITIONAL MEMORY MODULE

This program concerns the titration of weak acids  $H_4A$ ,  $H_3A$ ,  $H_2A$  and  $HA$ , and weak bases  $A(OH)_4$ ,  $A(OH)_3$ ,  $A(OH)_2$  and  $AOH$ . Given the dissociation constants  $K_n$ , and the beginning volume and molarity ( $V$  and  $M$ ) of the acid or base being titrated, and the normality ( $N$ ) of the titrant, the pH of the solution can be calculated for different volumes of titrant added. Since an iterative technique is being used, an initial guess for pH must be supplied. If it is a base that is being titrated then the main routine calculates pOH; however, pOH is converted to pH for display.

### References:

Breneman, G.L., "A General Acid-Base Titration Curve Computer Program," Journal of Chemical Education; vol. 51, pp. 812-813.

### Example:

For phosphoric acid,  $H_3PO_4$ ,  $K_1 = 7.5 \times 10^{-3}$ ,  $K_2 = 6.2 \times 10^{-8}$  and  $K_3 = 1 \times 10^{-12}$ . Plot a titration curve from 0 to 75 ml of 0.500 N NaOH added to 50.00 ml of 0.200 M  $H_2PO_4$ .

Solution(s): For a complete solution for purposes of a plot, calculations of the pH at approximately 45 different titrant volumes are required. For purposes of illustration the following 15 calculations will suffice:

### Keystrokes:

### Display:

|                                |                 |
|--------------------------------|-----------------|
| [USER]                         | (set USER mode) |
| [XEQ] [ALPHA] SIZE [ALPHA] 026 |                 |
| [XEQ] [ALPHA] A/B [ALPHA]      | ACID Y/N        |
| Y [R/S]                        | K?              |
| 7.5 [EEX] [CHS] 3 [R/S]        | K?              |
| 6.2 [EEX] [CHS] 8 [R/S]        | K?              |
| [EEX] [CHS] 12 [R/S]           | K?              |
| [A]                            | V?              |
| 50 [R/S]                       | M?              |
| .2 [R/S]                       | N?              |
| .5 [R/S]                       | INIT. GUESS     |
| [R/S]                          | VOLUME ADDED    |
| 0 [R/S]                        | PH=1.454        |

Keystrokes:

[R/S]  
10 [R/S]  
[R/S]  
15 [R/S]  
[R/S]  
19.4 [R/S]  
[R/S]  
20 [R/S]  
[R/S]  
20.4 [R/S]  
[R/S]  
21 [R/S]  
[R/S]  
25 [R/S]  
[R/S]  
35 [R/S]  
[R/S]  
39 [R/S]  
[R/S]  
39.8 [R/S]  
[R/S]  
40.1 [R/S]  
[R/S]  
40.8 [R/S]  
[R/S]  
45 [R/S]  
[R/S]  
75 [R/S]

Display:

VOLUME ADDED  
PH=2.192  
VOLUME ADDED  
PH=2.637  
VOLUME ADDED  
PH=3.654  
VOLUME ADDED  
PH=4.677  
VOLUME ADDED  
PH=5.527  
VOLUME ADDED  
PH=5.930  
VOLUME ADDED  
PH=6.731  
VOLUME ADDED  
PH=7.685  
VOLUME ADDED  
PH=8.483  
VOLUME ADDED  
PH=9.142  
VOLUME ADDED  
PH=9.832  
VOLUME ADDED  
PH=10.584  
VOLUME ADDED  
PH=11.457  
VOLUME ADDED  
PH=12.845

# User Instructions

|      |                                                 |          |           | SIZE: 026    |
|------|-------------------------------------------------|----------|-----------|--------------|
| STEP | INSTRUCTIONS                                    | INPUT    | FUNCTION  | DISPLAY      |
| 1    | Load program and set USER mode                  |          | [USER]    |              |
| 2    | Begin execution:                                |          | [XEQ] A/B | ACID Y/N     |
|      | if acid                                         | Y        | [R/S]     | K?           |
|      | if base                                         | N        | [R/S]     | K?           |
| 3    | Input $K_1$ , $K_2$ , $K_3$ and $K_4$ as needed | $K_1$    | [R/S]     | K?           |
|      |                                                 | $K_2$    | [R/S]     | K?           |
|      |                                                 | $K_3$    | [R/S]     | K?           |
|      |                                                 | $K_4$    | [R/S]     | K?           |
| 4    | When all K's are input, continue                |          | [A]       | V?           |
|      |                                                 | V        | [R/S]     | M?           |
|      |                                                 | <u>M</u> | [R/S]     | N?           |
|      |                                                 | <u>N</u> | [R/S]     | INIT. GUESS  |
| 5    | Begin calculations:                             |          |           |              |
|      | input guess for pH*                             | pHest    | [R/S]     | VOLUME ADDED |
|      | input volume of titrant added                   | V        | [R/S]     | PH =         |
| 6    | Repeat step 5                                   |          |           |              |
|      |                                                 |          |           |              |
|      |                                                 |          |           |              |
| *    | A guess for pH need not be entered IF:          |          |           |              |
|      | 1) The volume of titrate is going to be         |          |           |              |
|      | zero                                            |          |           |              |
|      | OR                                              |          |           |              |
|      | 2) The pH in the display left over from         |          |           |              |
|      | the last problem is suitable.                   |          |           |              |
|      |                                                 |          |           |              |
|      |                                                 |          |           |              |
|      |                                                 |          |           |              |

# Program Listings

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                              |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|
| <pre> 01*LBL "A/B " 02 FIX 3 03 "ACID Y/ N" 04 AON 05 PROMPT 06 AOFF 07 ASTO X 08 "Y" 09 ASTO Y 10 CF 00 11 X=Y? 12 SF 00 13 CLRG 14*LBL E 15 1 16 ST+ 25 17 "K?" 18 PROMPT 19 STO IND 25 20 GTO E 21*LBL A 22 "V?" 23 PROMPT 24 STO 23 25 "M?" 26 PROMPT 27 * 28 STO 24 29 "N?" 30 PROMPT 31 STO 21 32 RCL 25 33 1 34 + 35 STO 00 36 "INIT. G UESS" 37 PROMPT 38*LBL B 39 "VOLUME ADDED" 40 PROMPT 41 CF 02 42 X=0? 43 SF 02 44 RCL 21 45 X&lt;&gt;Y 46 * </pre> | <pre> Initialization </pre> <hr/> <pre> Initialize for coefficients </pre> | <pre> 47 LASTX 48 RCL 23 49 + 50 / 51 STO 20 52 RCL 24 53 LASTX 54 / 55 STO 22 56 R↑ 57 STO 00 58 RCL 00 59 STO 07 60*LBL c 61 RCL 07 62 .5 63 + 64 STO 25 65 ISG 25 66 RCL IND 25 67 RCL 20 68 + 69 .5 70 ST- 25 71 RDN 72 DSE 25 73 RCL 25 74 RCL 22 75 * 76 - 77 RCL IND 25 78 * 79 E-14 80 - 81*LBL b 82 DSE 25 83 GTO 00 84 RCL 07 85 X&lt;&gt; 25 86 X&lt;&gt;Y 87 RCL 25 88 10 89 + 90 RDN 91 STO IND T 92 DSE 07 93 GTO c 94 RCL 00 </pre> | <pre> ----- [Na<sup>+</sup>] → R<sub>20</sub> ----- c → R<sub>22</sub> pH<sub>est</sub> → R<sub>08</sub> ----- Calculate coefficients </pre> |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|

# Program Listings

|             |                          |             |                 |
|-------------|--------------------------|-------------|-----------------|
| 95 STO 25   |                          | 144 RCL 14  |                 |
| 96 RCL 01   |                          | 145 XEQ 07  |                 |
| 97 RCL 20   |                          | 146 RCL 15  |                 |
| 98 +        |                          | 147♦LBL 09  |                 |
| 99 STO 10   |                          | 148 +       |                 |
| 100 RCL 01  |                          | 149 RCL 16  |                 |
| 101 RCL 22  |                          | 150 /       |                 |
| 102 *       |                          | 151 -       |                 |
| 103 SQRT    |                          | 152 X<0?    |                 |
| 104 FS?C 02 |                          | 153 GTO a   |                 |
| 105 GTO 01  |                          | 154 STO 09  |                 |
| 106 GTO B   |                          | 155 %CH     |                 |
| 107♦LBL 00  |                          | 156 ABS     |                 |
| 108 RCL IND |                          | 157 1       |                 |
| 25          |                          | 158 X<=Y?   |                 |
| 109 *       |                          | 159 SF 02   |                 |
| 110 GTO b   |                          | 160 RCL 09  |                 |
| 111♦LBL a   | -----                    | 161 FS?C 02 |                 |
| 112 2       | Change pH <sub>est</sub> | 162 GTO 01  |                 |
| 113 FS? 00  | by ± 2                   | 163 LOG     |                 |
| 114 CHS     |                          | 164 CHS     |                 |
| 115 ST+ 00  |                          | 165 XEQ d   | -----           |
| 116♦LBL B   |                          | 166 "PH="   | Display         |
| 117 RCL 00  |                          | 167 ARCL %  |                 |
| 118 XEQ d   |                          | 168 RVIEW   |                 |
| 119 CHS     |                          | 169 STOP    |                 |
| 120 10↑X    |                          | 170 GTO B   |                 |
| 121♦LBL 01  |                          | 171♦LBL d   | -----           |
| 122 ENTER↑  |                          | 172 FS? 00  | Convert to base |
| 123 ENTER↑  |                          | 173 RTN     |                 |
| 124 GTO IND |                          | 174 14      |                 |
| 25          |                          | 175 X<>Y    |                 |
| 125♦LBL 05  | -----                    | 176 -       |                 |
| 126 6       | start forming            | 177 RTN     |                 |
| 127 *       | f'([H <sup>+</sup> ])    | 178♦LBL 06  | -----           |
| 128 RCL 10  |                          | 179 *       | Common routine  |
| 129 5       |                          | 180♦LBL 07  |                 |
| 130 XEQ 06  |                          | 181 +       |                 |
| 131 RCL 11  |                          | 182 *       |                 |
| 132 4       |                          | 183 RTN     |                 |
| 133 XEQ 06  |                          | 184♦LBL 08  |                 |
| 134 RCL 12  |                          | 185 +       |                 |
| 135 3       |                          | 186 STO 16  |                 |
| 136 XEQ 06  |                          | 187 CLX     |                 |
| 137 RCL 13  |                          | 188 RCL 10  |                 |
| 138 2       |                          | 189 XEQ 07  |                 |
| 139 XEQ 06  |                          | 190 RCL 11  |                 |
| 140 RCL 14  |                          | 191 XEQ 07  |                 |
| 141 XEQ 08  |                          | 192 RCL 12  |                 |
| 142 RCL 13  |                          | 193 FS?C 02 |                 |
| 143 XEQ 07  |                          | 194 GTO 09  |                 |

|     |      |    |                       |    |  |
|-----|------|----|-----------------------|----|--|
| 195 | GTO  | 07 | f'[(H <sup>+</sup> )] | 51 |  |
| 196 | ♦LBL | 04 |                       |    |  |
| 197 | 5    |    |                       |    |  |
| 198 | *    |    |                       |    |  |
| 199 | RCL  | 10 |                       |    |  |
| 200 | 4    |    |                       |    |  |
| 201 | XEQ  | 06 |                       |    |  |
| 202 | RCL  | 11 |                       |    |  |
| 203 | 3    |    |                       |    |  |
| 204 | XEQ  | 06 |                       | 60 |  |
| 205 | RCL  | 12 |                       |    |  |
| 206 | 2    |    |                       |    |  |
| 207 | XEQ  | 06 |                       |    |  |
| 208 | RCL  | 13 |                       |    |  |
| 209 | XEQ  | 08 |                       |    |  |
| 210 | RCL  | 13 |                       |    |  |
| 211 | XEQ  | 07 |                       |    |  |
| 212 | RCL  | 14 |                       |    |  |
| 213 | GTO  | 09 |                       |    |  |
| 214 | ♦LBL | 03 |                       | 70 |  |
| 215 | 4    |    |                       |    |  |
| 216 | *    |    |                       |    |  |
| 217 | RCL  | 10 |                       |    |  |
| 218 | 3    |    |                       |    |  |
| 219 | XEQ  | 06 |                       |    |  |
| 220 | RCL  | 11 |                       |    |  |
| 221 | 2    |    |                       |    |  |
| 222 | XEQ  | 06 |                       |    |  |
| 223 | RCL  | 12 |                       |    |  |
| 224 | XEQ  | 08 |                       | 80 |  |
| 225 | RCL  | 13 |                       |    |  |
| 226 | GTO  | 09 |                       |    |  |
| 227 | ♦LBL | 02 |                       |    |  |
| 228 | 3    |    |                       |    |  |
| 229 | *    |    |                       |    |  |
| 230 | RCL  | 10 |                       |    |  |
| 231 | 2    |    |                       |    |  |
| 232 | XEQ  | 06 |                       |    |  |
| 233 | RCL  | 11 |                       |    |  |
| 234 | SF   | 02 |                       | 90 |  |
| 235 | GTO  | 08 |                       |    |  |
| 236 | END  |    |                       |    |  |
|     |      |    |                       |    |  |
|     |      |    |                       |    |  |
|     |      |    |                       |    |  |
|     |      |    |                       |    |  |
|     |      |    |                       |    |  |
|     |      |    |                       |    |  |
| 50  |      |    |                       | 00 |  |

[illegible]

WEAK ACID/BASE TITRATION CURVE

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

PROGRAM REGISTERS NEEDED: 59

ROW 1 (1 - 3)

ROW 2 (3 - 9)

ROW 3 (9 - 17)

ROW 4 (17 - 22)

ROW 5 (23 - 29)

ROW 6 (30 - 36)

ROW 7 (36 - 39)

ROW 8 (39 - 41)

ROW 9 (42 - 51)

ROW 10 (51 - 60)

ROW 11 (61 - 68)

ROW 12 (69 - 76)

ROW 13 (77 - 83)

ROW 14 (83 - 91)

ROW 15 (92 - 99)

ROW 16 (100 - 107)

ROW 17 (108 - 115)

ROW 18 (115 - 124)

## WEAK ACID/BASE TITRATION CURVE

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 19 (124 - 133)



ROW 20 (133 - 141)



ROW 21 (141 - 148)



ROW 22 (149 - 158)



ROW 23 (159 - 166)



ROW 24 (166 - 172)



ROW 25 (172 - 183)



ROW 26 (184 - 191)



ROW 27 (192 - 201)



ROW 28 (201 - 208)



ROW 29 (209 - 216)



ROW 30 (217 - 224)



ROW 31 (224 - 233)



ROW 32 (234 - 236)



## EQUATIONS OF STATE

This program provides both ideal gas and Redlich-Kwong equations of state. Given four of the five state variables, the fifth is calculated. For the Redlich-Kwong solution, the critical pressure and temperature of the gas must be known. They are not needed for ideal gas solutions.

Values of the Universal Gas Constants

| Value of R | Units of R                      | Units of P       | Units of V               | Units of T |
|------------|---------------------------------|------------------|--------------------------|------------|
| 8.314      | N-m/g mole-K                    | N/m <sup>2</sup> | m <sup>3</sup> /g mole   | K          |
| 83.14      | cm <sup>3</sup> -bar/g mole-K   | bar              | cm <sup>3</sup> /g mole  | K          |
| 82.05      | cm <sup>3</sup> -atm/g mole-K   | atm              | cm <sup>3</sup> /g mole  | K          |
| 0.7302     | atm-ft <sup>3</sup> /lb mole-°R | atm              | ft <sup>3</sup> /lb mole | °R         |
| 10.73      | psi-ft <sup>3</sup> /lb mole-°R | psi              | ft <sup>3</sup> /lb mole | °R         |
| 1545       | psf-ft <sup>3</sup> /lb mole-°R | psf              | ft <sup>3</sup> /lb mole | °R         |

Critical Temperatures and Pressures

| Substance               | T <sub>c</sub> , K | T <sub>c</sub> , °R | P <sub>c</sub> , ATM |
|-------------------------|--------------------|---------------------|----------------------|
| Ammonia                 | 405.6              | 730.1               | 112.5                |
| Argon                   | 151                | 272                 | 48.0                 |
| Carbon dioxide          | 304.2              | 547.6               | 72.9                 |
| Carbon monoxide         | 133                | 239                 | 34.5                 |
| Chlorine                | 417                | 751                 | 76.1                 |
| Helium                  | 5.3                | 9.5                 | 2.26                 |
| Hydrogen                | 33.3               | 59.9                | 12.8                 |
| Nitrogen                | 126.2              | 227.2               | 33.5                 |
| Oxygen                  | 154.8              | 278.6               | 50.1                 |
| Water                   | 647.3              | 1165.1              | 218.2                |
| Dichlorodifluoromethane | 384.7              | 692.5               | 39.6                 |
| Dichlorofluoromethane   | 451.7              | 813.1               | 51.0                 |
| Ethane                  | 305.5              | 549.9               | 48.2                 |
| Ethanol                 | 516.3              | 929.3               | 63                   |
| Methanol                | 513.2              | 923.8               | 78.5                 |
| n-Butane                | 425.2              | 765.4               | 37.5                 |
| n-Haxane                | 507.9              | 914.2               | 29.9                 |
| n-Pentane               | 469.5              | 845.1               | 33.3                 |
| n-Octane                | 568.6              | 1023.5              | 24.6                 |
| Trichlorofluoromethane  | 471.2              | 848.1               | 43.2                 |

Equations:

Ideal gas:  $PV = nRT$

Redlich-Kwong: 
$$P = \frac{nRT}{(V - b)} - \frac{a}{T^{1/2} V (V + b)}$$

$$a = 4.934 b nRT_c^{1.5}$$

$$b = 0.0867 \frac{nRT_c}{P_c}$$

where:

P is the absolute pressure;

V is the volume;

n is the number of moles present;

R is the universal gas constant;

T is the absolute temperature;

$T_c$  is the critical temperature;

$P_c$  is the critical pressure.

Remarks:

P, V, n and T must have units compatible with R.

At low temperatures or high pressures, the ideal gas law does not represent the behavior of real gases.

No equation of state is valid for all substances or over an infinite range of conditions. The Redlich-Kwong equation gives moderate to good accuracy for a variety of substances over a wide range of conditions. Results should be used with caution and tempered by experience.

Solutions for V, n, R and T, using the Redlich-Kwong equation, require an iterative technique. Newton's method is employed using the ideal gas law to generate the initial guess. Iteration time is generally a function of the amount of deviation from ideal gas behavior. For extreme cases, the routine may fail to converge entirely, resulting in "DATA ERROR".

## Example 1:

0.63 g moles of air are enclosed in a 25,000 cm<sup>3</sup> space at 1200 K. What is the pressure in bars? Assume ideal gas behavior.

Keystrokes:

Display:

[XEQ] [ALPHA] SIZE [ALPHA] 015

[XEQ] [ALPHA] ID [ALPHA]

P?

0 [R/S]

V?

25000 [R/S]

N?

0.63 [R/S]

R?

83.14 [R/S]

T?

1200 [R/S]

P=2.51

## Example 2:

The specific volume of a gas in a container is 800 cm<sup>3</sup>/g mole. The temperature will reach 400 K. What will the pressure be, according to the Redlich-Kwong relation?

$$P_c = 48.2 \text{ atm}$$

$$T_c = 305.5 \text{ K}$$

$$R = 82.05 \text{ cm}^3 - \text{atm/g mole-K}$$

Keystrokes:

Display:

[XEQ] [ALPHA] RK [ALPHA]

TC?

305.5 [R/S]

PC?

48.2 [R/S]

P?

0 [R/S]

V?

800 [R/S]

N?

1 [R/S]

R?

82.05 [R/S]

T?

400 [R/S]

P=36.29



# Program Listings

|             |                |            |           |
|-------------|----------------|------------|-----------|
| 01*LBL "ID" | Initialization | 50 FS? 02  |           |
| 02 0        |                | 51 RTN     |           |
| 03 SF 00    |                | 52 GTO IND |           |
| 04 GTO 00   |                | 10         |           |
| 05*LBL "RK" |                | 53*LBL 05  | -----     |
| 06 1        |                | 54 "P="    | Calculate |
| 07 CF 00    |                | 55 GTO 00  | unknown   |
| 08 "TC?"    |                | 56*LBL 06  |           |
| 09 PROMPT   |                | 57 "V="    |           |
| 10 STO 13   |                | 58*LBL 00  |           |
| 11 "PC?"    |                | 59 RCL 07  |           |
| 12 PROMPT   |                | 60 RCL 08  |           |
| 13 STO 14   |                | 61 *       |           |
| 14*LBL 00   |                | 62 RCL 09  |           |
| 15 SF 02    |                | 63 *       |           |
| 16 CF 01    |                | 64 RCL 05  |           |
| 17 FIX 2    |                | 65 RCL 06  |           |
| 18 "P?"     |                | 66 *       |           |
| 19 PROMPT   |                | 67 /       |           |
| 20 5        |                | 68 STO IND |           |
| 21 XEQ 00   |                | 10         |           |
| 22 "V?"     |                | 69 GTO 00  |           |
| 23 PROMPT   |                | 70*LBL 07  |           |
| 24 6        |                | 71 SF 01   |           |
| 25 XEQ 00   |                | 72 "N="    |           |
| 26 "N?"     |                | 73 GTO 01  |           |
| 27 PROMPT   |                | 74*LBL 08  |           |
| 28 7        |                | 75 SF 01   |           |
| 29 XEQ 00   |                | 76 "R="    |           |
| 30 "R?"     |                | 77 GTO 01  |           |
| 31 PROMPT   |                | 78*LBL 09  |           |
| 32 8        |                | 79 "T="    |           |
| 33 XEQ 00   |                | 80 SF 01   |           |
| 34 "T?"     |                | 81*LBL 01  |           |
| 35 PROMPT   |                | 82 RCL 05  |           |
| 36 CF 02    |                | 83 RCL 06  |           |
| 37 9        |                | 84 *       |           |
| 38*LBL 00   |                | 85 RCL 07  |           |
| 39 CF 01    |                | 86 /       |           |
| 40 STO 01   |                | 87 RCL 08  |           |
| 41 RDN      |                | 88 /       |           |
| 42 STO IND  |                | 89 RCL 09  |           |
| 01          |                | 90 /       |           |
| 43 X#0?     |                | 91 STO IND |           |
| 44 GTO 01   |                | 10         |           |
| 45 R↑       |                | 92*LBL 00  |           |
| 46 STO 10   |                | 93 FS? 00  |           |
| 47 1        |                | 94 GTO 10  |           |
| 48 STO IND  |                | 95 XEQ 01  |           |
| 01          |                | 96 GTO 00  |           |
| 49*LBL 01   |                | 97*LBL 02  |           |

# Program Listings

```

98 FS? 01
99 XEQ 01
100*LBL 00
101 RCL 00
102 RCL 09
103 *
104 RCL 06
105 RCL 12
106 -
107 STO 04
108 /
109 RCL 11
110 RCL 09
111 SQRT
112 /
113 STO 02
114 RCL 06
115 /
116 LASTX
117 RCL 12
118 +
119 STO 03
120 /
121 -
122 RCL 05
123 -
124 XEQ IND
10
125 /
126 ST- IND
10
127 RCL IND
10
128 /
129 ABS
130 1 E-4
131 X<=Y?
132 GTO 02
133 RCL IND
10
134 GTO 10
135*LBL 06
136 RCL 06
137 ENTER↑
138 +
139 RCL 12
140 +
141 RCL 02
142 *
143 RCL 03
144 RCL 06
145 *

```

|                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                          |
|----------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <p>-----</p> <p>If ideal,<br/>display</p> <p>-----</p>                           | <pre> 146 X↑2 147 / 148 RCL 00 149 RCL 09 150 * 151 RCL 04 152 X↑2 153 / 154 - 155 RTN </pre>                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                          |
| <p>-----</p> <p>Calculate using<br/>Redlich-Kwong<br/>equations</p> <p>-----</p> | <pre> 156*LBL 09 157 RCL 00 158 RCL 04 159 / 160 RCL 02 161 2 162 / 163 RCL 09 164 / 165 RCL 06 166 / 167 RCL 03 168 / 169 + 170 RTN 171*LBL 07 172*LBL 08 173 RCL 09 174 RCL 06 175 * 176 RCL 04 177 X↑2 178 / 179 RCL 06 180 ENTER↑ 181 + 182 RCL 12 183 + 184 RCL 00 185 / 186 RCL 06 187 / 188 RCL 03 189 X↑2 190 / 191 RCL 02 192 * 193 - 194 RCL 00 195 * 196 RCL IND </pre> | <p>-----</p> <p><math>\frac{\partial P}{\partial T}</math></p> <p>-----</p> <p><math>\frac{\partial P}{\partial n}</math> or <math>\frac{\partial P}{\partial R}</math></p> <p>-----</p> |
| <p>-----</p> <p><math>\frac{\partial P}{\partial V}</math></p> <p>-----</p>      |                                                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                          |

# Program Listings

|            |                         |    |  |
|------------|-------------------------|----|--|
| 10         |                         | 51 |  |
| 197 /      |                         |    |  |
| 198 RTN    |                         |    |  |
| 199*LBL 05 |                         |    |  |
| 200 LASTX  |                         |    |  |
| 201 +      |                         |    |  |
| 202 STO 05 |                         |    |  |
| 203 GTO 10 |                         |    |  |
| 204*LBL 01 |                         |    |  |
| 205 RCL 07 | -----<br>Calculate a, b | 60 |  |
| 206 RCL 08 |                         |    |  |
| 207 *      |                         |    |  |
| 208 STO 00 |                         |    |  |
| 209 .0867  |                         |    |  |
| 210 RCL 14 |                         |    |  |
| 211 /      |                         |    |  |
| 212 X<>Y   |                         |    |  |
| 213 RCL 13 |                         |    |  |
| 214 *      |                         |    |  |
| 215 *      |                         | 70 |  |
| 216 STO 12 |                         |    |  |
| 217 LASTX  |                         |    |  |
| 218 *      |                         |    |  |
| 219 RCL 13 |                         |    |  |
| 220 SQRT   |                         |    |  |
| 221 *      |                         |    |  |
| 222 4.934  |                         |    |  |
| 223 *      |                         |    |  |
| 224 STO 11 |                         |    |  |
| 225 RTN    |                         |    |  |
| 226*LBL 10 | -----<br>Display        | 80 |  |
| 227 ARCL X |                         |    |  |
| 228 AVIEW  |                         |    |  |
| 229 STOP   |                         |    |  |
| 230 .END.  |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
| 40         |                         | 90 |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
|            |                         |    |  |
| 50         |                         | 00 |  |

# REGISTERS, STATUS, FLAGS, ASSIGNMENTS

| DATA REGISTERS     |    |  | STATUS                                                                         |  |                |               |
|--------------------|----|--|--------------------------------------------------------------------------------|--|----------------|---------------|
| NR                 | 50 |  | SIZE <u>015</u> TOT. REG. <u>61</u> USER MODE                                  |  |                |               |
| temp storage index |    |  | ENG <u>      </u> FIX <u>2</u> SCI <u>      </u> ON <u>      </u> OFF <u>X</u> |  |                |               |
| $a/T^{1/2}$        |    |  | DEG <u>      </u> RAD <u>      </u> GRAD <u>      </u>                         |  |                |               |
| (V + b)            |    |  | <b>FLAGS</b><br># INIT S/C SET INDICATES CLEAR INDICATES                       |  |                |               |
| (V - b)            |    |  |                                                                                |  |                |               |
| P                  | 55 |  | 00                                                                             |  | Ideal          | Redlich-Kwong |
| V                  |    |  | 01                                                                             |  | Calc a, b      |               |
| n                  |    |  | 02                                                                             |  | Inputting data | Calculate     |
| f                  |    |  |                                                                                |  |                |               |
| T                  |    |  |                                                                                |  |                |               |
| control            | 60 |  |                                                                                |  |                |               |
| a                  |    |  |                                                                                |  |                |               |
| b                  |    |  |                                                                                |  |                |               |
| $T_c$              |    |  |                                                                                |  |                |               |
| $P_c$              |    |  |                                                                                |  |                |               |
|                    | 65 |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    | 70 |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    | 75 |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    | 80 |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    | 85 |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    |    |  | <b>ASSIGNMENTS</b>                                                             |  |                |               |
|                    |    |  | FUNCTION                                                                       |  | KEY            |               |
|                    | 90 |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    | 95 |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |
|                    |    |  |                                                                                |  |                |               |

EQUATIONS OF STATE

PROGRAM REGISTERS NEEDED: 47

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 1 (1 - 5)

ROW 2 (5 - 10)

ROW 3 (11 - 17)

ROW 4 (18 - 24)

ROW 5 (25 - 30)

ROW 6 (30 - 37)

ROW 7 (38 - 47)

ROW 8 (48 - 55)

ROW 9 (55 - 65)

ROW 10 (66 - 73)

ROW 11 (73 - 79)

ROW 12 (80 - 91)

ROW 13 (91 - 98)

ROW 14 (98 - 108)

ROW 15 (109 - 121)

ROW 16 (122 - 130)

ROW 17 (130 - 138)

ROW 18 (139 - 151)

## EQUATIONS OF STATE

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 19 (152 - 164)



ROW 20 (165 - 177)



ROW 21 (178 - 190)



ROW 22 (191 - 202)



ROW 23 (203 - 210)



ROW 24 (211 - 222)



ROW 25 (222 - 230)



ROW 26 (230 - 230)



## VAN DER WAALS GAS LAW

The Van der Waal gas equation is:

$$[P + (n^2 a/V^2)] [V - nb] = nRT$$

V must be calculated as the positive root of the cubic equation:

$$\bar{V}^3 - \bar{V}^2 [b + (RT/P)] + \bar{V} \cdot a/P - ab/P = 0, \text{ where } \bar{V} = V/n.$$

n must be calculated as the positive root of the cubic equation:

$$\bar{n}^3 - \bar{n}^2 \cdot 1/b + \bar{n} [(P/a) + (RT/ab)] - P/ab = 0$$

where  $\bar{n} = n/V$ .

The program solves these equations by non-iterative techniques, then converts to V or n.

The constant "R" is written into the program with the value of:

$$0.0820562.$$

The Critical Properties may be evaluated with the use of Key [E].

NOTE: Pressure must be in atmospheres.  
 Temperature must be in degrees Kelvin.  
 Volume must be in liters.  
 The number "n" must be in gram moles.

Example 1:

What is the temperature of 0.25 moles of Helium with a volume of 2.0 liters at a pressure of 2.5 atmospheres?

$$a = 0.03412, b = 0.0237$$

Keystrokes:

Display:

[XEQ] [ALPHA] SIZE [ALPHA] 014

[XEQ] [ALPHA] GAS [ALPHA]

a=?

.03412 [R/S]

b=?

.0237 [R/S]

P V N T VPTc

.25 [C]

N=0.25

| Keystrokes: | Display: |
|-------------|----------|
| 2.00 [B]    | V=2.00   |
| 2.50 [A]    | P=2.50   |
| [D]         | T=243.07 |

#### Example 2:

What is the volume of 1.5 moles of CO<sub>2</sub> at 40 K & 10 atmospheres?

$$a = 3.592, b = 0.04267$$

| Keystrokes:               | Display:     |
|---------------------------|--------------|
| [XEQ] [ALPHA] GAS [ALPHA] | a=?          |
| 3.592 [R/S]               | b=?          |
| .04267 [R/S]              | P V N T VPTc |
| 1.50 [C]                  | N=1.50       |
| 40 [D]                    | T=40.00      |
| 10 [A]                    | P=10.00      |
| [B]                       | V=0.07       |
| [////] [FIX] 4            | 0.0667       |

#### Example 3:

How many moles H<sub>2</sub> in 3398 liters under 409 atmospheres at 294K?

$$a = 0.24444, b = 0.02661$$

What are the critical volume, pressure, and temperature of H<sub>2</sub>?

| Keystrokes:               | Display:     |
|---------------------------|--------------|
| [////] [FIX] 2            |              |
| [XEQ] [ALPHA] GAS [ALPHA] | a=?          |
| .24444 [R/S]              | b=?          |
| .02661 [R/S]              | P V N T VPTc |

Keystrokes:

3398 [B]

409 [A]

294 [D]

[C]

[E]

Display:

V=3,398.00

P=409.00

T=294.00

N=42,143.70

V<sub>C</sub>=0.06152

P<sub>C</sub>=12.78

T<sub>C</sub>=33.16

# User Instructions

|      |                                           |         |            | SIZE: 014     |
|------|-------------------------------------------|---------|------------|---------------|
| STEP | INSTRUCTIONS                              | INPUT   | FUNCTION   | DISPLAY       |
| 1    | Load program.                             |         |            |               |
| 2    | Begin execution and answer questions      |         | [XEQ] GAS  | a=?           |
|      | Van der Waals constant a                  | a       | [R/S]      | b=?           |
|      | Van der Waals constant b                  | b       | [R/S]      | P V N T PVTc  |
| 3    | Input any three of these values:          |         |            |               |
|      | Pressure in atmospheres                   | P, atm. | [A]        | P=(P)         |
|      | Volume in liters                          | V, l    | [B]        | V=(V)         |
|      | No. of gram moles                         | n       | [C]        | N=(n)         |
|      | Temperature in Kelvins                    | T, K    | [D]        | T=(T)         |
| 4    | Calculate the remaining value by pressing |         |            |               |
|      | the appropriate key:                      |         |            |               |
|      | Pressure in atmospheres                   |         | [A]        | P=(P)         |
|      | Volume in liters                          |         | [B]        | V=(V)         |
|      | No. of gram moles                         |         | [C]        | N=(n)         |
|      | Temperature in Kelvins                    |         | [D]        | T=(T)         |
| 5    | Calculate critical constants              |         | [E]        | Vc=(Vc)       |
|      |                                           |         | [R/S]      | Pc=(Pc)       |
|      |                                           |         | [R/S]      | Tc=(Tc)       |
| 6    | (Optional) After step 3, calculate molar  |         |            |               |
|      | volume                                    |         | [XEQ] 05   | ( $\bar{V}$ ) |
| 7    | (Optional) Calculate cube root of x       | x       | [////] [E] | $\sqrt[3]{x}$ |
|      |                                           |         |            |               |
|      | NOTE: Repeated calculations may be made   |         |            |               |
|      | for the same gas without reentry of a and |         |            |               |
|      | b by returning to step 3.                 |         |            |               |
|      |                                           |         |            |               |
|      |                                           |         |            |               |

# Program Listings

|             |                  |            |                  |
|-------------|------------------|------------|------------------|
| 01*LBL "GAS |                  | 51 3       |                  |
| 02 SF 27    |                  | 52 /       |                  |
| 03 "a=?"    |                  | 53 STO 00  |                  |
| 04 PROMPT   | Initialize       | 54 RCL 05  |                  |
| 05 STO 01   |                  | 55 3       |                  |
| 06 "b=?"    | Prompt for a and | 56 /       |                  |
| 07 PROMPT   | b                | 57 RCL 00  |                  |
| 08 STO 02   |                  | 58 X↑2     |                  |
| 09 .0820562 |                  | 59 -       |                  |
| 10 STO 03   |                  | 60 3       |                  |
| 11 GTO 06   |                  | 61 Y↑X     |                  |
| 12*LBL A    |                  | 62 STO 07  |                  |
| 13 FS?C 22  | Store or compute | 63 RCL 05  |                  |
| 14 GTO 01   | P                | 64 RCL 00  |                  |
| 15 XEQ 05   |                  | 65 *       |                  |
| 16 RCL 03   |                  | 66 RCL 04  |                  |
| 17 RCL 13   |                  | 67 -       |                  |
| 18 *        |                  | 68 2       |                  |
| 19 RCL 09   |                  | 69 /       |                  |
| 20 RCL 02   |                  | 70 RCL 00  |                  |
| 21 -        |                  | 71 3       |                  |
| 22 /        |                  | 72 Y↑X     |                  |
| 23 RCL 01   |                  | 73 -       |                  |
| 24 RCL 09   |                  | 74 STO 08  |                  |
| 25 X↑2      |                  | 75 X↑2     |                  |
| 26 /        |                  | 76 RCL 07  |                  |
| 27 -        |                  | 77 +       |                  |
| 28*LBL 01   |                  | 78 SQRT    |                  |
| 29 STO 10   |                  | 79 STO 07  |                  |
| 30 "P="     |                  | 80 RCL 08  |                  |
| 31 GTO 00   |                  | 81 +       |                  |
| 32*LBL B    |                  | 82 XEQ e   |                  |
| 33 FS?C 22  | Store or compute | 83 RCL 08  |                  |
| 34 GTO 02   | V                | 84 RCL 07  |                  |
| 35 RCL 02   |                  | 85 -       |                  |
| 36 RCL 01   |                  | 86 XEQ e   |                  |
| 37 RCL 10   |                  | 87 +       |                  |
| 38 /        |                  | 88 RCL 00  |                  |
| 39 STO 05   |                  | 89 -       |                  |
| 40 *        |                  | 90 RCL 12  |                  |
| 41 CHS      |                  | 91 *       |                  |
| 42 STO 04   |                  | 92 STO 11  |                  |
| 43 RCL 02   |                  | 93*LBL 02  |                  |
| 44 RCL 03   |                  | 94 STO 11  |                  |
| 45 RCL 13   |                  | 95 "V="    |                  |
| 46 *        |                  | 96 GTO 00  |                  |
| 47 RCL 10   |                  | 97*LBL C   |                  |
| 48 /        |                  | 98 FS?C 22 |                  |
| 49 +        |                  | 99 GTO 04  |                  |
| 50 CHS      |                  | 100 RCL 10 | Store or compute |
|             |                  | 101 RCL 02 | n                |

# Program Listings

|            |  |             |                        |
|------------|--|-------------|------------------------|
| 102 RCL 01 |  | 153 XEQ e   |                        |
| 103 *      |  | 154 RCL 08  |                        |
| 104 /      |  | 155 RCL 06  |                        |
| 105 CHS    |  | 156 -       |                        |
| 106 STO 04 |  | 157 XEQ e   |                        |
| 107 RCL 10 |  | 158 +       |                        |
| 108 RCL 01 |  | 159 RCL 00  |                        |
| 109 /      |  | 160 -       |                        |
| 110 RCL 03 |  | 161 RCL 11  |                        |
| 111 RCL 13 |  | 162 *       |                        |
| 112 *      |  | 163+LBL 04  |                        |
| 113 RCL 01 |  | 164 STO 12  |                        |
| 114 RCL 02 |  | 165 "N="    |                        |
| 115 *      |  | 166 GT0 00  |                        |
| 116 /      |  | 167+LBL D   |                        |
| 117 +      |  | 168 FS?C 22 |                        |
| 118 STO 05 |  | 169 GT0 03  |                        |
| 119 RCL 02 |  | 170 XEQ 05  | Store or compute<br>T  |
| 120 1/X    |  | 171 RCL 10  |                        |
| 121 CHS    |  | 172 RCL 01  |                        |
| 122 3      |  | 173 RCL 09  |                        |
| 123 /      |  | 174 X↑2     |                        |
| 124 STO 00 |  | 175 /       |                        |
| 125 RCL 05 |  | 176 +       |                        |
| 126 3      |  | 177 RCL 09  |                        |
| 127 /      |  | 178 RCL 02  |                        |
| 128 RCL 00 |  | 179 -       |                        |
| 129 X↑2    |  | 180 *       |                        |
| 130 -      |  | 181 RCL 03  |                        |
| 131 3      |  | 182 /       |                        |
| 132 Y↑X    |  | 183+LBL 03  |                        |
| 133 STO 07 |  | 184 STO 13  |                        |
| 134 RCL 05 |  | 185 "T="    |                        |
| 135 RCL 00 |  | 186 GT0 00  |                        |
| 136 *      |  | 187+LBL 05  |                        |
| 137 RCL 04 |  | 188 RCL 11  |                        |
| 138 -      |  | 189 RCL 12  | Calculate $\bar{V}$    |
| 139 2      |  | 190 /       |                        |
| 140 /      |  | 191 STO 09  |                        |
| 141 RCL 00 |  | 192 RTN     |                        |
| 142 3      |  | 193+LBL e   |                        |
| 143 Y↑X    |  | 194 X<0?    |                        |
| 144 -      |  | 195 SF 01   | Calculate cube<br>root |
| 145 STO 08 |  | 196 ABS     |                        |
| 146 X↑2    |  | 197 3       |                        |
| 147 RCL 07 |  | 198 1/X     |                        |
| 148 +      |  | 199 Y↑X     |                        |
| 149 SQRT   |  | 200 FS? 01  |                        |
| 150 STO 06 |  | 201 CHS     |                        |
| 151 RCL 08 |  | 202 CF 01   |                        |
| 152 +      |  | 203 RTN     |                        |

# Program Listings

```

204*LBL E
205 RCL 02
206 2.31207
207 *
208 FIX 5
209 "Vc="
210 ARCL X
211 AVIEW
212 8
213 RCL 01
214 *
215 9
216 /
217 RCL 03
218 /
219 RCL 01
220 9
221 /
222 RCL 02
223 /
224 RCL 02
225 3
226 *
227 FIX 2
228 /
229 "Pc="
230 ARCL X
231 AVIEW
232 X<>Y
233 LASTX
234 /
235 "Tc="
236*LBL 00
237 ARCL X
238 AVIEW
239 RTN
240*LBL 06
241 "P V N T
    VPTc"
242 AVIEW
243 .END.

```

Calculate  
Vc, Pc, Tc

Label top-row  
keys

51

60

70

80

90

00

# REGISTERS, STATUS, FLAGS, ASSIGNMENTS

| DATA REGISTERS |    |  | STATUS                                                                   |             |               |                 |  |
|----------------|----|--|--------------------------------------------------------------------------|-------------|---------------|-----------------|--|
| Used           | 50 |  | SIZE <u>014</u> TOT. REG. <u>62</u> USER MODE                            |             |               |                 |  |
| a              |    |  | ENG <u>    </u> FIX <u>2</u> SCI <u>    </u> ON <u>X</u> OFF <u>    </u> |             |               |                 |  |
| b              |    |  | DEG <u>    </u> RAD <u>    </u> GRAD <u>    </u>                         |             |               |                 |  |
| R              |    |  |                                                                          |             |               |                 |  |
| Used           |    |  | <b>FLAGS</b>                                                             |             |               |                 |  |
| Used           | 55 |  | #                                                                        | INIT<br>S/C | SET INDICATES | CLEAR INDICATES |  |
| Used           |    |  | 27                                                                       |             | USER ON       |                 |  |
| Used           |    |  |                                                                          |             |               |                 |  |
| V              |    |  |                                                                          |             |               |                 |  |
| P              | 60 |  |                                                                          |             |               |                 |  |
| V              |    |  |                                                                          |             |               |                 |  |
| n              |    |  |                                                                          |             |               |                 |  |
| T              |    |  |                                                                          |             |               |                 |  |
|                | 65 |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                | 70 |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                | 75 |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                | 80 |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                | 85 |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                |    |  | <b>ASSIGNMENTS</b>                                                       |             |               |                 |  |
|                |    |  | FUNCTION                                                                 |             | KEY           | FUNCTION        |  |
|                |    |  |                                                                          |             |               |                 |  |
|                | 90 |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                | 95 |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |
|                |    |  |                                                                          |             |               |                 |  |

## VAN DER WAALS GAS LAW

PROGRAM REGISTERS NEEDED: 49

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 1 (1 - 3)



ROW 2 (4 - 9)



ROW 3 (9 - 15)



ROW 4 (15 - 26)



ROW 5 (27 - 34)



ROW 6 (34 - 46)



ROW 7 (47 - 59)



ROW 8 (60 - 72)



ROW 9 (73 - 83)



ROW 10 (84 - 94)



ROW 11 (95 - 101)



ROW 12 (102 - 114)



ROW 13 (115 - 127)



ROW 14 (128 - 140)



ROW 15 (141 - 153)



ROW 16 (153 - 162)



ROW 17 (163 - 169)



ROW 18 (170 - 180)



## VAN DER WAALS GAS LAW

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 19 (181 - 190)



ROW 20 (191 - 200)



ROW 21 (201 - 206)



ROW 22 (206 - 213)



ROW 23 (214 - 226)



ROW 24 (227 - 234)



ROW 25 (235 - 241)



ROW 26 (241 - 243)



ROW 27 (243 - 243)



## BEER'S LAW AND ABSORPTIVITY CALCULATIONS

This is a flexible program for the calculation of the parameters of the Beer-Lambert law used in colorimetry,  $A = abC + i$ , where  $i$  is the intercept (an error term). Given the light path,  $b$ , and a set of concentration,  $C$ , and percent transmittance,  $\%T$ , or absorbance,  $A$ , data the program computes absorption coefficient,  $a$ , by the least squares method:

$$a = \frac{1}{b} \frac{n\sum AC - \sum A \sum C}{n\sum C^2 - (\sum C)^2}$$

Initialization (Key A) clears all registers and sets  $b$  equal to 1 cm. Either conc., absorbance (Key D) or conc.,  $\%T$  (Key C) data may be entered. In the latter case  $\%T$  is automatically converted to absorbance:

$$A = 2 - \log \%T$$

Corrections to  $C$ ,  $A$  or  $C$ ,  $\%T$  may be made by pressing [////] D or [////] C, respectively. If molecular weight has been entered ([////] B), mg/l data may be converted to molar concentration via Key B.

After completing data entry, pressing [R/S] repeatedly will display the absorption coefficient followed by the error intercept of  $i$ , and the correlation coefficient,  $r$ . Pressing [R/S] again repeats the sequence of  $a$ ,  $i$ ,  $r$ . Additional data may be added via Keys C or D, or corrected via Keys c or d. To enter a new data set requires only that Key A be pressed to clear the data registers (initialize).

NOTE: Unless  $b$  is 1 cm, then a new value must be entered ([////] A) each time the program is initialized. Initialization also removed molecular weight from memory. The least squares program requires at least two  $C$ ,  $A$  data pairs to calculate  $a$ . Enter 0, 0 into key D if only one pair is available.

Example: Calculate the molar absorption coefficient for phosphate as determined by the "ascorbic acid" method at 880 nm.

Concentrations expressed a phosphorus, therefore, the molecular weight is 30.98.

Light path was 1.2 cm.

## DATA

|    | <u>%T</u> | <u>mg/l as P</u> |
|----|-----------|------------------|
| a) | 97.9      | 0.0              |
| b) | 58.0      | 0.25             |
| c) | 37.2      | 0.50             |
| d) | 23.1      | 0.75             |
| e) | 14.5      | 1.00             |
| f) | 9.0       | 1.25             |

Keystrokes:

Display:

[XEQ] [ALPHA] SIZE [ALPHA] 010

[XEQ] [ALPHA] BEER [ALPHA] b=1.0?

1.2 [R/S] b=1.2

31 [///] [B] MW=31.0

0 [ENTER↑] 97.9 [C] N=1.

.25 [B] M=8.06E-6

58 [C] N=2.

.5 [B] M=1.61E-5

37.2 [C] N=3.

.75 [B] M=2.42E-5

23.1 [C] N=4.

1 [B] M=3.23E-5

14.1 [C] N=5.

1.25 [B] M=4.03E-5

9 [C] N=6.

[R/S] a=21,352.

I=0.0181

R=0.9998

# User Instructions

|      |                                             |              |                    | SIZE: 010 |
|------|---------------------------------------------|--------------|--------------------|-----------|
| STEP | INSTRUCTIONS                                | INPUT        | FUNCTION           | DISPLAY   |
| 1    | Load program                                |              |                    |           |
| 2    | Initialize (clears all reg., sets $b = 1$ ) |              | [XEQ] BEER or[A]   | $b=1.0?$  |
| 3    | (Optional) enter light path if $b \neq 1$   | $b$          | [R/S]              | $b=(b)$   |
| 4    | (Optional) enter molecular weight           | MW           | [///] [B]          | $MW=(MW)$ |
| 5    | Enter molar conc. and absorbance            |              |                    |           |
|      | or enter mg/l and absorbance                | $C_i, A_i$   | [ENTER↑] [D]       | $N=(n_i)$ |
|      | or enter mg/l concentration and             | $mg/l_i$     | [B]                | $M=(M_i)$ |
|      | enter absorbance                            | $A_i$        | [D]                | $N=(n_i)$ |
|      | or enter molar conc. and percent trans-     |              |                    |           |
|      | mittance                                    | $C_i, \%T_i$ | [ENTER↑] [C]       | $N=(n_i)$ |
|      | or enter mg/l and percent transmittance     | $C_i, \%T_i$ | [ENTER↑] [C]       | $N=(n_i)$ |
|      | or enter mg/l conc. and                     | $mg/l_i$     | [B]                | $M=(M_i)$ |
|      | enter percent transmittance                 | $\%T_i$      | [C]                | $N=(n_i)$ |
| 6    | Continue data entry                         |              |                    | $N=(n)$   |
|      | or correct an entry                         | $C_k, A_k$   | [ENTER↑] [///] [D] | $N=(n-1)$ |
|      | or correct an entry                         | $C_k, \%T_k$ | [ENTER↑] [///] [C] | $N=(n-1)$ |
| 7    | Display absorption coefficient, intercept   |              |                    |           |
|      | and correlation coefficient                 |              | [R/S]              | $a=(a)$   |
|      |                                             |              |                    | $I=(i)$   |
|      |                                             |              |                    | $R=(r)$   |
| 8    | To repeat a, i, r display                   |              | [R/S]              |           |
| 9    | To add further data, repeat step 5          |              |                    |           |
| 10   | To enter a new set of data, go to step 2    |              |                    |           |
|      | (initialize)                                |              |                    |           |
|      |                                             |              |                    |           |
|      | To calculate molar concentrations from      | MW           | [///] [B]          | $MW=(MW)$ |
|      | mg/l values                                 | $mg/l$       | [B]                | $M=(M)$   |



# Program Listings

|                   |                |            |                 |
|-------------------|----------------|------------|-----------------|
| 01*LBL "BEE<br>R" |                | 51 "N="    |                 |
| 02*LBL A          | Initialize     | 52 ARCL X  |                 |
| 03 SF 27          |                | 53 PROMPT  |                 |
| 04 CLRG           |                | 54 GTO 01  |                 |
| 05 ZREG 04        |                | 55*LBL c   | Correct Ci, %Ti |
| 06 1              |                | 56 XEQ 05  |                 |
| 07 STO 00         |                | 57 Z-      |                 |
| 08*LBL a          |                | 58 "N="    |                 |
| 09 FIX 1          |                | 59 ARCL X  |                 |
| 10 RCL 00         | Input b        | 60 PROMPT  |                 |
| 11 "b="           |                | 61 GTO 01  |                 |
| 12 ARCL X         |                | 62*LBL 05  |                 |
| 13 "F?"           |                | 63 SF 05   |                 |
| 14 PROMPT         |                | 64*LBL E   | Convert %T to A |
| 15 STO 00         |                | 65 LOG     |                 |
| 16 "b="           |                | 66 2       |                 |
| 17 ARCL X         |                | 67 -       |                 |
| 18 AVIEW          |                | 68 CHS     |                 |
| 19 RTN            |                | 69 FIX 4   |                 |
| 20*LBL B          |                | 70 FS?C 05 |                 |
| 21 RCL 01         | mg/l→M         | 71 RTN     |                 |
| 22 /              |                | 72 "A="    |                 |
| 23 1 E3           |                | 73 ARCL X  |                 |
| 24 /              |                | 74 AVIEW   |                 |
| 25 SCI 2          |                | 75 RTN     |                 |
| 26 "M="           |                | 76*LBL e   |                 |
| 27 ARCL X         |                | 77 2       |                 |
| 28 AVIEW          |                | 78 -       | Convert A to %T |
| 29 RTN            |                | 79 CHS     |                 |
| 30*LBL b          |                | 80 10↑X    |                 |
| 31 STO 01         |                | 81 FIX 1   |                 |
| 32 "MW="          |                | 82 "%T="   |                 |
| 33 ARCL X         | Input MW       | 83 ARCL X  |                 |
| 34 AVIEW          |                | 84 AVIEW   |                 |
| 35 RTN            |                | 85 RTN     |                 |
| 36*LBL D          |                | 86*LBL 01  |                 |
| 37 Z+             | Input Ci, Ai   | 87 RCL 09  |                 |
| 38 FIX 0          |                | 88 RCL 08  | Display a, i, r |
| 39 STOP           |                | 89 *       |                 |
| 40 GTO 01         |                | 90 RCL 04  |                 |
| 41*LBL d          |                | 91 RCL 06  |                 |
| 42 Z-             |                | 92 *       |                 |
| 43 "N="           | Correct Ci, Ai | 93 -       |                 |
| 44 ARCL X         |                | 94 STO 02  |                 |
| 45 PROMPT         |                | 95 RCL 09  |                 |
| 46 GTO 01         |                | 96 RCL 07  |                 |
| 47*LBL C          |                | 97 *       |                 |
| 48 XEQ 05         |                | 98 RCL 06  |                 |
| 49 Z+             | Input Ci, %Ti  | 99 X↑2     |                 |
| 50 FIX 0          |                | 100 -      |                 |
|                   |                | 101 STO 03 |                 |

# Program Listings

|            |  |    |  |
|------------|--|----|--|
| 102 /      |  | 51 |  |
| 103 RCL 00 |  |    |  |
| 104 /      |  |    |  |
| 105 FIX 0  |  |    |  |
| 106 "a="   |  |    |  |
| 107 ARCL X |  |    |  |
| 108 AVIEW  |  |    |  |
| 109 RCL 07 |  |    |  |
| 110 RCL 04 |  |    |  |
| 111 *      |  |    |  |
| 112 RCL 06 |  | 60 |  |
| 113 RCL 08 |  |    |  |
| 114 *      |  |    |  |
| 115 -      |  |    |  |
| 116 RCL 03 |  |    |  |
| 117 /      |  |    |  |
| 118 FIX 4  |  |    |  |
| 119 "I="   |  |    |  |
| 120 ARCL X |  |    |  |
| 121 AVIEW  |  |    |  |
| 122 RCL 02 |  | 70 |  |
| 123 RCL 03 |  |    |  |
| 124 SQRT   |  |    |  |
| 125 /      |  |    |  |
| 126 RCL 09 |  |    |  |
| 127 RCL 05 |  |    |  |
| 128 *      |  |    |  |
| 129 RCL 04 |  |    |  |
| 130 X↑2    |  |    |  |
| 131 -      |  |    |  |
| 132 SQRT   |  | 80 |  |
| 133 /      |  |    |  |
| 134 "R="   |  |    |  |
| 135 ARCL X |  |    |  |
| 136 PROMPT |  |    |  |
| 137 GTO 01 |  |    |  |
| 138 .END.  |  |    |  |
|            |  |    |  |
|            |  |    |  |
| 40         |  | 90 |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
|            |  |    |  |
| 50         |  | 00 |  |



BEER'S LAW AND ABSORPTIVITY  
CALCULATIONS  
PROGRAM REGISTERS NEEDED: 32

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 1 (1 - 4)



ROW 2 (5 - 12)



ROW 3 (12 - 19)



ROW 4 (20 - 26)



ROW 5 (27 - 33)



ROW 6 (34 - 42)



ROW 7 (43 - 48)



ROW 8 (49 - 55)



ROW 9 (56 - 62)



ROW 10 (63 - 71)



ROW 11 (72 - 80)



ROW 12 (81 - 88)



ROW 13 (89 - 101)



ROW 14 (102 - 110)



ROW 15 (111 - 120)



ROW 16 (120 - 132)



ROW 17 (133 - 138)



## ACTIVITY COEFFICIENTS FROM POTENTIOMETRIC DATA

This program calculates the Standard Electrode Potential (S.E.P.) and the activity coefficients of a system from values of the concentration and observed EMF.

Equations Used:

$$E + E_{\text{REF}} + A \log m + B \log F - 0.0602 \sqrt{m} = E^{\circ} - A \cdot C \cdot m$$

$$A = 0.059156 \text{ } v/n$$

$$B = 0.059156/n$$

$E$  = measured EMF's in volts (V)

$E_{\text{REF}}$  = EMF of reference electrode

$n$  = number of electrons involved in the reaction

$f = (v^{+}v^{-})$  e.g. for  $\text{CaCl}_2$ :  $v^{+}=1$ ;  $v^{-}=2$ ,  $f=[2^2 \cdot 1^1]=4$

$v$  = Total number of ions

$r$  = Activity coefficient

Program must be reinitialized for each case (e.g., push [XEQ] [ALPHA] ACT [ALPHA] since the summation registers are used.

Greater accuracy may be obtained if values used as constants in program could be obtained to more significant figures. Also remember that the valid number of significant figures in the answer is related to the number of significant figures in the data.

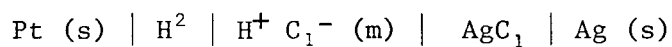
References: Beech, G., *Fortran IV In Chemistry*, pp 64-6, John Wiley and Sons. 1975.

Kemp, Marwin K., *Physical Chemistry for Engineering and the Physical Sciences: A Self-Paced Approach*, pp (10-144), University of Tulsa. 1974.

Example:

For the following data determine the Standard Electrode Potential and the activity coefficient at each point.

| Concentration (M) | Potential (V) | $f = 1$                  |
|-------------------|---------------|--------------------------|
| 0.003215          | 0.52053       | $\nu = 2$                |
| 0.004488          | 0.50384       | $E_{\text{REF}} = 0.000$ |
| 0.005619          | 0.49257       | $n = 1$                  |
| 0.007311          | 0.47948       |                          |
| 0.009138          | 0.46860       |                          |
| 0.011195          | 0.45861       |                          |



Keystrokes:

Display:

[XEQ] [ALPHA] SIZE [ALPHA] 015

[XEQ] [ALPHA] ACT [ALPHA]

F=?

1 [R/S]

NU=?

2 [R/S]

EREF=?

0 [R/S]

N=?

1 [R/S]

.003215 [ENTER↑] .52053 [A]

1.000

.004488 [ENTER↑] .50384 [A]

2.000

.005619 [ENTER↑] .49257 [A]

3.000

.007311 [ENTER↑] .47948 [A]

4.000

.009138 [ENTER↑] .46860 [A]

5.000

.011195 [ENTER↑] .45861 [A]

6.000

[D]

R↑2=0.9338

[R/S]

S.E.P.=0.2224

.007311 [ENTER↑] .47948 [E]

M=0.0073

[R/S]

GAMMA=0.9188

## DISPLAY

[illegible]

# Program Listings

|             |                   |              |                  |
|-------------|-------------------|--------------|------------------|
| 01*LBL "ACT |                   | 51 +         |                  |
| "           |                   | 52 /         |                  |
| 02 SF 27    | Initialize        | 53 "R↑2="    |                  |
| 03 EREG 04  |                   | 54 ARCL X    |                  |
| 04 GTO C    |                   | 55 PROMPT    |                  |
| 05*LBL A    |                   | 56 RCL 05    |                  |
| 06 XEQ 01   | Insert data pairs | 57 RCL 06    |                  |
| 07 E+       |                   | 58 *         |                  |
| 08 RTN      |                   | 59 RCL 04    |                  |
| 09*LBL B    |                   | 60 RCL 08    |                  |
| 10 XEQ 01   | Delete data pairs | 61 *         |                  |
| 11 E-       |                   | 62 -         |                  |
| 12 RTN      |                   | 63 RCL 09    |                  |
| 13*LBL C    |                   | 64 RCL 05    |                  |
| 14 CLRG     | Initialize and    | 65 *         |                  |
| 15 "F=?"    | store physical    | 66 RCL 04    |                  |
| 16 PROMPT   | parameters        | 67 X↑2       |                  |
| 17 STO 10   |                   | 68 -         |                  |
| 18 "NU=?"   |                   | 69 /         |                  |
| 19 PROMPT   |                   | 70 STO 14    |                  |
| 20 STO 11   |                   | 71 "S.E.P. = |                  |
| 21 "EREF=?" |                   | "            |                  |
| 22 PROMPT   |                   | 72 ARCL X    |                  |
| 23 STO 12   |                   | 73 AVIEW     |                  |
| 24 "N=?"    |                   | 74 RTN       |                  |
| 25 PROMPT   |                   | 75*LBL E     |                  |
| 26 STO 13   |                   | 76 STO 02    | Compute activity |
| 27 RTN      |                   | 77 RDN       | coefficient      |
| 28*LBL D    | Calculate         | 78 STO 01    |                  |
| 29 RCL 08   | coefficient of    | 79 RCL 14    |                  |
| 30 RCL 06   | determination and | 80 RCL 12    |                  |
| 31 RCL 04   | standard elec-    | 81 -         |                  |
| 32 *        | trode potential   | 82 RCL 02    |                  |
| 33 RCL 09   |                   | 83 -         |                  |
| 34 /        |                   | 84 XEQ 02    |                  |
| 35 -        |                   | 85 RCL 01    |                  |
| 36 X↑2      |                   | 86 LOG       |                  |
| 37 RCL 04   |                   | 87 *         |                  |
| 38 X↑2      |                   | 88 -         |                  |
| 39 RCL 09   |                   | 89 XEQ 02    |                  |
| 40 /        |                   | 90 RCL 11    |                  |
| 41 CHS      |                   | 91 /         |                  |
| 42 RCL 05   |                   | 92 RCL 10    |                  |
| 43 +        |                   | 93 LOG       |                  |
| 44 /        |                   | 94 *         |                  |
| 45 RCL 06   |                   | 95 -         |                  |
| 46 X↑2      |                   | 96 XEQ 02    |                  |
| 47 RCL 09   |                   | 97 /         |                  |
| 48 /        |                   | 98 10↑X      |                  |
| 49 CHS      |                   | 99 RCL 01    |                  |
| 50 RCL 07   |                   | 100 "M="     |                  |

# Program Listings

|              |                                                                                                                                                                                   |    |  |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|--|
| 101 ARCL X   |                                                                                                                                                                                   | 51 |  |
| 102 PROMPT   |                                                                                                                                                                                   |    |  |
| 103 X<>Y     |                                                                                                                                                                                   |    |  |
| 104 "GAMMA=" |                                                                                                                                                                                   |    |  |
| 105 ARCL X   |                                                                                                                                                                                   |    |  |
| 106 AVIEW    |                                                                                                                                                                                   |    |  |
| 107 RTN      |                                                                                                                                                                                   |    |  |
| 108+LBL 01   | Subroutine to<br>store molarity<br>and potential<br>values then<br>operate on the<br>potential value<br>converting it to<br>a form satisfac-<br>tory for a least-<br>squares fit. |    |  |
| 109 STO 02   |                                                                                                                                                                                   |    |  |
| 110 STO 03   |                                                                                                                                                                                   | 60 |  |
| 111 RDN      |                                                                                                                                                                                   |    |  |
| 112 STO 01   |                                                                                                                                                                                   |    |  |
| 113 RCL 12   |                                                                                                                                                                                   |    |  |
| 114 ST+ 03   |                                                                                                                                                                                   |    |  |
| 115 XEQ 02   |                                                                                                                                                                                   |    |  |
| 116 RCL 01   |                                                                                                                                                                                   |    |  |
| 117 LOG      |                                                                                                                                                                                   |    |  |
| 118 *        |                                                                                                                                                                                   |    |  |
| 119 ST+ 03   |                                                                                                                                                                                   |    |  |
| 120 XEQ 02   |                                                                                                                                                                                   | 70 |  |
| 121 RCL 11   |                                                                                                                                                                                   |    |  |
| 122 /        |                                                                                                                                                                                   |    |  |
| 123 RCL 10   |                                                                                                                                                                                   |    |  |
| 124 LOG      |                                                                                                                                                                                   |    |  |
| 125 *        |                                                                                                                                                                                   |    |  |
| 126 ST+ 03   |                                                                                                                                                                                   |    |  |
| 127 .0602    |                                                                                                                                                                                   |    |  |
| 128 RCL 01   |                                                                                                                                                                                   |    |  |
| 129 SQRT     |                                                                                                                                                                                   |    |  |
| 130 *        |                                                                                                                                                                                   | 80 |  |
| 131 ST- 03   |                                                                                                                                                                                   |    |  |
| 132 RCL 03   |                                                                                                                                                                                   |    |  |
| 133 RCL 01   |                                                                                                                                                                                   |    |  |
| 134 RTN      |                                                                                                                                                                                   |    |  |
| 135+LBL 02   |                                                                                                                                                                                   |    |  |
| 136 .059156  |                                                                                                                                                                                   |    |  |
| 137 RCL 11   |                                                                                                                                                                                   |    |  |
| 138 *        |                                                                                                                                                                                   |    |  |
| 139 RCL 13   |                                                                                                                                                                                   |    |  |
| 140 /        |                                                                                                                                                                                   | 90 |  |
| 141 RTN      |                                                                                                                                                                                   |    |  |
|              |                                                                                                                                                                                   |    |  |
|              |                                                                                                                                                                                   |    |  |
|              |                                                                                                                                                                                   |    |  |
|              |                                                                                                                                                                                   |    |  |
|              |                                                                                                                                                                                   |    |  |
|              |                                                                                                                                                                                   |    |  |
|              |                                                                                                                                                                                   |    |  |
|              |                                                                                                                                                                                   |    |  |
| 50           |                                                                                                                                                                                   | 00 |  |



ACTIVITY COEFFICIENTS FROM  
POTENTIOMETRIC DATA  
PROGRAM REGISTERS NEEDED: 33

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 1 (1 - 4)



ROW 2 (4 - 10)



ROW 3 (11 - 18)



ROW 4 (18 - 22)



ROW 5 (23 - 31)



ROW 6 (32 - 44)



ROW 7 (45 - 53)



ROW 8 (54 - 65)



ROW 9 (66 - 71)



ROW 10 (72 - 82)



ROW 11 (83 - 91)



ROW 12 (92 - 100)



ROW 13 (101 - 105)



ROW 14 (106 - 115)



ROW 15 (116 - 125)



ROW 16 (126 - 132)



ROW 17 (133 - 139)



ROW 18 (140 - 142)



## CRYSTALLOGRAPHIC TO CARTESIAN COORDINATE TRANSFORMATIONS

(This program requires one memory module)

Program transforms coordinates from any crystallographic (oblique) system into a cartesian system and calculates the distances and angles between three points in space.

## Equations Used:

$$x = a + b \cos \gamma + c \cos \beta$$

$$y = b \sin \gamma + c \cos (90-\beta) \cos \alpha'$$

$$z = c \cos (90-\beta) \sin \alpha'$$

$$\cos \alpha' = \frac{\cos \alpha - \cos \beta \cos \gamma}{\sin \beta \sin \gamma}$$

## Variables:

$a, b, c$  = length of oblique axes

$\alpha, \beta, \gamma$  = angle between oblique axes

$a_i, b_i, c_i$  = coordinates of point in oblique system

$x_i, y_i, z_i$  = coordinates of point in cartesian system

$D_{ij}$  = distance from point  $i$  to  $j$

$\theta_{1-2-3}$  = angle between points

$$\begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} = \begin{pmatrix} a & b \cos \gamma & c \cos \beta \\ 0 & b \sin \gamma & c \sin \beta \cos \alpha' \\ 0 & 0 & c \sin \beta \sin \alpha' \end{pmatrix} \begin{pmatrix} a_i \\ b_i \\ c_i \end{pmatrix}$$

$$D_{ij} = [(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2]^{\frac{1}{2}}$$

$$\theta_{1-2-3} = \cos^{-1} \left[ \frac{(x_1 - x_2)(x_3 - x_2) + (y_1 - y_2)(y_3 - y_2) + (z_1 - z_2)(z_3 - z_2)}{D_{12} \cdot D_{23}} \right]$$

One of the distances,  $D_{ij}$ , must be calculated before calculating the angle between three points. Input  $a, b, c$  before  $\alpha, \beta, \gamma$ .

Example:

Suppose one has a monoclinic crystal with unit cell dimensions:

$$\begin{array}{ll} a = 11.716\text{\AA} & \alpha = 90.00^\circ \\ b = 8.102\text{\AA} & \beta = 106.14^\circ \\ c = 11.166\text{\AA} & \gamma = 90.00^\circ \end{array}$$

The crystallographic fractional coordinates of a nitrogen atom and two carbons bonded to the nitrogen are:

|                |       |       |       |
|----------------|-------|-------|-------|
| N <sub>2</sub> | 0.508 | 0.259 | 0.170 |
| C <sub>1</sub> | 0.585 | 0.410 | 0.189 |
| C <sub>3</sub> | 0.430 | 0.249 | 0.034 |

What are the rectangular coordinates of the three atoms, the distances (bond lengths) between the atoms and the angle between the three atoms?

Keystrokes:

Display:

|                                |          |
|--------------------------------|----------|
| [XEQ] [ALPHA] SIZE [ALPHA] 026 |          |
| [XEQ] [ALPHA] XTAL [ALPHA]     | a=?      |
| 11.716 [R/S]                   | b=?      |
| 8.102 [R/S]                    | c=?      |
| 11.166 [R/S]                   | A=?      |
| 90 [R/S]                       | B=?      |
| 106.14 [R/S]                   | C=?      |
| 90 [R/S]                       | a1=?     |
| .585 [R/S]                     | b1=?     |
| .41 [R/S]                      | c1=?     |
| .189 [R/S]                     | X1=6.267 |
|                                | Y1=3.322 |
|                                | Z1=2.027 |
|                                | a2=?     |
| .508 [R/S]                     | b2=?     |
| .259 [R/S]                     | c2=?     |
| .17 [R/S]                      | X2=5.424 |
|                                | Y2=2.098 |
|                                | Z2=1.823 |
|                                | a3=?     |
| .43 [R/S]                      | b3=?     |

Keystrokes:

.249 [R/S]

.034 [R/S]

[ENTER↑] [////] [D]

Display:

c3=?

X3=4.932

Y3=2.017

Z3=0.365

D12=1.500

D13=2.499

D23=1.541

# User Instructions

SIZE: 026

| STEP | INSTRUCTIONS                          | INPUT          | FUNCTION   | DISPLAY              |
|------|---------------------------------------|----------------|------------|----------------------|
| 1    | Load program                          |                |            |                      |
| 2    | Begin program                         |                | [XEQ] XTAL | a=?                  |
| 3    | Input lengths of oblique axes         | a              | [R/S]      | b=?                  |
|      |                                       | b              | [R/S]      | c=?                  |
|      |                                       | c              | [R/S]      | A=?                  |
| 4    | Input angles between oblique axes     | $\alpha$       | [R/S]      | B=?                  |
|      |                                       | $\beta$        | [R/S]      | C=?                  |
|      |                                       | $\gamma$       | [R/S]      | a1=?                 |
| 5    | Input coordinates of point #1 and see | a <sub>1</sub> | [R/S]      | b1=?                 |
|      | rectangular coordinates               | b <sub>1</sub> | [R/S]      | c1=?                 |
|      |                                       | c <sub>1</sub> | [R/S]      | X1=(x <sub>1</sub> ) |
|      |                                       |                |            | Y1=(y <sub>1</sub> ) |
|      |                                       |                |            | Z1=(z <sub>1</sub> ) |
|      |                                       |                |            | a2=?                 |
| 6    | Input coordinates of point #2 and see | a <sub>2</sub> | [R/S]      | b2=?                 |
|      | rectangular coordinates               | b <sub>2</sub> | [R/S]      | c2=?                 |
|      |                                       | c <sub>2</sub> | [R/S]      | X2=(x <sub>2</sub> ) |
|      |                                       |                |            | Y2=(y <sub>2</sub> ) |
|      |                                       |                |            | Z2=(z <sub>2</sub> ) |
|      |                                       |                |            | a3=?                 |
| 7    | Input coordinates of point #3 and see | a <sub>3</sub> | [R/S]      | b3=?                 |
|      | rectangular coordinates               | b <sub>3</sub> | [R/S]      | c3=?                 |
|      |                                       | c <sub>3</sub> | [R/S]      | X3=(x <sub>3</sub> ) |
|      |                                       |                |            | Y3=(y <sub>3</sub> ) |
|      |                                       |                |            | Z3=(z <sub>3</sub> ) |
|      |                                       |                |            |                      |
|      |                                       |                |            |                      |

# User Instructions

[illegible]

# Program Listings

|                   |                                                         |            |                                                                             |
|-------------------|---------------------------------------------------------|------------|-----------------------------------------------------------------------------|
| 01*LBL "XTR<br>L" |                                                         | 51 /       |                                                                             |
| 02*LBL A          |                                                         | 52 ST* 08  |                                                                             |
| 03 CLRG           |                                                         | 53 ACOS    |                                                                             |
| 04 SF 27          |                                                         | 54 SIN     |                                                                             |
| 05 "a=?"          | Prompt for unit<br>cell dimensions                      | 55 ST* 09  | Atom 1                                                                      |
| 06 PROMPT         |                                                         | 56*LBL B   |                                                                             |
| 07 STO 01         |                                                         | 57 1       |                                                                             |
| 08 "b=?"          |                                                         | 58 STO 10  |                                                                             |
| 09 PROMPT         |                                                         | 59 XEQ 00  | Atom 2                                                                      |
| 10 STO 04         |                                                         | 60*LBL C   |                                                                             |
| 11 STO 05         |                                                         | 61 2       |                                                                             |
| 12 "c=?"          |                                                         | 62 STO 10  |                                                                             |
| 13 PROMPT         |                                                         | 63 XEQ 00  | Atom 3                                                                      |
| 14 STO 07         |                                                         | 64*LBL D   |                                                                             |
| 15 STO 08         |                                                         | 65 3       |                                                                             |
| 16 STO 09         |                                                         | 66 STO 10  |                                                                             |
| 17 "A=?"          | Prompt for angles<br>between crystal-<br>lographic axes | 67 XEQ 00  |                                                                             |
| 18 PROMPT         |                                                         | 68 RTN     |                                                                             |
| 19 COS            |                                                         | 69*LBL 00  |                                                                             |
| 20 STO 20         |                                                         | 70 FIX 0   |                                                                             |
| 21 "B=?"          |                                                         | 71 CF 29   |                                                                             |
| 22 PROMPT         |                                                         | 72 "a"     |                                                                             |
| 23 STO 21         |                                                         | 73 ARCL 10 |                                                                             |
| 24 "C=?"          |                                                         | 74 "f=?"   | Prompt for<br>crystallographic<br>fractional<br>coordinates of<br>ith atom. |
| 25 PROMPT         |                                                         | 75 PROMPT  |                                                                             |
| 26 STO 22         |                                                         | 76 STO 00  |                                                                             |
| 27 COS            |                                                         | 77 "b"     |                                                                             |
| 28 STO 23         |                                                         | 78 ARCL 10 |                                                                             |
| 29 ST* 04         |                                                         | 79 "f=?"   |                                                                             |
| 30 RCL 22         |                                                         | 80 PROMPT  |                                                                             |
| 31 SIN            |                                                         | 81 STO 20  |                                                                             |
| 32 STO 24         |                                                         | 82 "c"     |                                                                             |
| 33 ST* 05         |                                                         | 83 ARCL 10 |                                                                             |
| 34 RCL 21         |                                                         | 84 "f=?"   |                                                                             |
| 35 COS            |                                                         | 85 PROMPT  |                                                                             |
| 36 STO 00         |                                                         | 86 STO 21  |                                                                             |
| 37 ST* 07         |                                                         | 87 RCL 10  |                                                                             |
| 38 RCL 21         |                                                         | 88 3       |                                                                             |
| 39 SIN            |                                                         | 89 *       |                                                                             |
| 40 ST* 08         |                                                         | 90 8       |                                                                             |
| 41 ST* 09         |                                                         | 91 +       |                                                                             |
| 42 RCL 24         |                                                         | 92 STO 24  |                                                                             |
| 43 *              |                                                         | 93 1       |                                                                             |
| 44 RCL 23         |                                                         | 94 STO 25  |                                                                             |
| 45 RCL 00         |                                                         | 95 "X"     | Get x-coordinate                                                            |
| 46 *              |                                                         | 96 XEQ 01  |                                                                             |
| 47 RCL 20         |                                                         | 97 2       |                                                                             |
| 48 X<>Y           |                                                         | 98 STO 25  |                                                                             |
| 49 -              |                                                         | 99 "Y"     |                                                                             |
| 50 X<>Y           |                                                         | 100 XEQ 01 | Get y-coordinate                                                            |
|                   |                                                         | 101 3      |                                                                             |

# Program Listings

|             |                             |             |  |
|-------------|-----------------------------|-------------|--|
| 102 STO 25  | Get z-coordinates           | 151 XEQ 04  |  |
| 103 "Z"     |                             | 152 XEQ 04  |  |
| 104 XEQ 01  | Compute<br>coordinates      | 153 SQRT    |  |
| 105 RTN     |                             | 154 STO 22  |  |
| 106*LBL 01  |                             | 155 "D12="  |  |
| 107 0       |                             | 156 ARCL 20 |  |
| 108 RCL 00  |                             | 157 AVIEW   |  |
| 109 XEQ 02  |                             | 158 PSE     |  |
| 110 RCL 20  |                             | 159 "D13="  |  |
| 111 XEQ 02  |                             | 160 ARCL 22 |  |
| 112 RCL 21  |                             | 161 AVIEW   |  |
| 113 XEQ 02  |                             | 162 PSE     |  |
| 114 FIX 0   |                             | 163 "D23="  |  |
| 115 CF 29   |                             | 164 ARCL 21 |  |
| 116 ARCL 10 |                             | 165 AVIEW   |  |
| 117 "F="    |                             | 166 RTN     |  |
| 118 FIX 3   |                             | 167*LBL 03  |  |
| 119 ARCL X  |                             | 168 RCL IND |  |
| 120 AVIEW   | Matrix<br>multiplication    | 25          |  |
| 121 PSE     |                             | 169 XEQ 05  |  |
| 122 STO IND |                             | 170 RCL IND |  |
| 24          |                             | 25          |  |
| 123 ISG 24  |                             | 171 -       |  |
| 124 RTN     |                             | 172 X↑2     |  |
| 125 RTN     |                             | 173 +       |  |
| 126*LBL 02  |                             | 174 2       |  |
| 127 RCL IND |                             | 175 ST- 25  |  |
| 25          |                             | 176 RDN     |  |
| 128 *       |                             | 177 RTN     |  |
| 129 +       |                             | 178*LBL 04  |  |
| 130 3       |                             | 179 RCL IND |  |
| 131 ST+ 25  |                             | 25          |  |
| 132 RDN     |                             | 180 XEQ 07  |  |
| 133 RTN     |                             | 181 RCL IND |  |
| 134*LBL d   |                             | 25          |  |
| 135 11      |                             | 182 -       |  |
| 136 STO 25  | Distances between<br>points | 183 X↑2     |  |
| 137 0       |                             | 184 6       |  |
| 138 XEQ 03  |                             | 185 ST+ 25  |  |
| 139 XEQ 03  |                             | 186 RDN     |  |
| 140 XEQ 03  |                             | 187 +       |  |
| 141 SQRT    |                             | 188 1       |  |
| 142 STO 20  |                             | 189 ST+ 25  |  |
| 143 0       |                             | 190 RDN     |  |
| 144 XEQ 03  |                             | 191 RTN     |  |
| 145 XEQ 03  |                             | 192*LBL 05  |  |
| 146 XEQ 03  |                             | 193 ISG 25  |  |
| 147 SQRT    |                             | 194*LBL 00  |  |
| 148 STO 21  |                             | 195 ISG 25  |  |
| 149 0       |                             | 196*LBL 00  |  |
| 150 XEQ 04  |                             | 197 ISG 25  |  |
|             |                             |             |  |

# Program Listings

|             |                   |    |  |
|-------------|-------------------|----|--|
| 198*LBL 00  |                   | 51 |  |
| 199 RTN     |                   |    |  |
| 200*LBL 07  |                   |    |  |
| 201 RCL 25  |                   |    |  |
| 202 6       |                   |    |  |
| 203 -       |                   |    |  |
| 204 STO 25  |                   |    |  |
| 205 RDN     |                   |    |  |
| 206 RTN     |                   |    |  |
| 207*LBL 01  |                   | 60 |  |
| 208 RCL 20  |                   |    |  |
| 209 "D12="  |                   |    |  |
| 210 ARCL X  |                   |    |  |
| 211 AVIEW   |                   |    |  |
| 212 RTN     |                   |    |  |
| 213*LBL E   |                   |    |  |
| 214 RCL 11  | Calculate angle   |    |  |
| 215 RCL 14  | between atoms     |    |  |
| 216 -       | 1 and 3 at atom 2 |    |  |
| 217 RCL 17  |                   | 70 |  |
| 218 RCL 14  |                   |    |  |
| 219 -       |                   |    |  |
| 220 *       |                   |    |  |
| 221 RCL 12  |                   |    |  |
| 222 RCL 15  |                   |    |  |
| 223 -       |                   |    |  |
| 224 RCL 18  |                   |    |  |
| 225 RCL 15  |                   |    |  |
| 226 -       |                   |    |  |
| 227 *       |                   | 80 |  |
| 228 +       |                   |    |  |
| 229 RCL 13  |                   |    |  |
| 230 RCL 16  |                   |    |  |
| 231 -       |                   |    |  |
| 232 RCL 19  |                   |    |  |
| 233 RCL 16  |                   |    |  |
| 234 -       |                   |    |  |
| 235 *       |                   |    |  |
| 236 +       |                   |    |  |
| 237 RCL 20  |                   | 90 |  |
| 238 /       |                   |    |  |
| 239 RCL 21  |                   |    |  |
| 240 /       |                   |    |  |
| 241 ACOS    |                   |    |  |
| 242 "∠123=" |                   |    |  |
| 243 ARCL X  |                   |    |  |
| 244 AVIEW   |                   |    |  |
| 245 RTN     |                   |    |  |
| 246 .END.   |                   |    |  |
|             |                   | 00 |  |

[illegible]

CRYSTALLOGRAPHIC TO CARTESIAN  
COORDINATE TRANSFORMATIONS  
PROGRAM REGISTERS NEEDED: 62

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 1 (1 - 4)



ROW 2 (5 - 11)



ROW 3 (12 - 18)



ROW 4 (19 - 24)



ROW 5 (24 - 32)



ROW 6 (32 - 40)



ROW 7 (40 - 48)



ROW 8 (49 - 58)



ROW 9 (59 - 65)



ROW 10 (66 - 73)



ROW 11 (73 - 79)



ROW 12 (79 - 84)



ROW 13 (85 - 94)



ROW 14 (95 - 100)



ROW 15 (101 - 109)



ROW 16 (109 - 114)



ROW 17 (114 - 120)



ROW 18 (121 - 130)



CRYSTALLOGRAPHIC TO CARTESIAN  
COORDINATE TRANSFORMATIONSHEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 19 (131 - 138)



ROW 20 (138 - 144)



ROW 21 (144 - 150)



ROW 22 (150 - 155)



ROW 23 (155 - 160)



ROW 24 (161 - 168)



ROW 25 (168 - 176)



ROW 26 (177 - 185)



ROW 27 (185 - 195)



ROW 28 (195 - 204)



ROW 29 (205 - 211)



ROW 30 (212 - 222)



ROW 31 (223 - 232)



ROW 32 (233 - 242)



ROW 33 (242 - 246)



# KINETICS USING LINEWEAVER-BURK OR HOFSTEE PLOTS

(This program requires one memory module)

Using the methods of Lineweaver-Burk (1) or Hofstee (2) the program transforms reaction velocity (v) and substrate concentration (S) Data into the general form of a line ( $y = bx + a$ ). The values for the regression coefficients a and b

$$\frac{1}{v} = \frac{K_m}{V_{max}} \cdot \frac{1}{S} + \frac{1}{V_{max}} \quad (1) \quad v = -K_m \cdot \frac{v}{S} + V_{max} \quad (2)$$

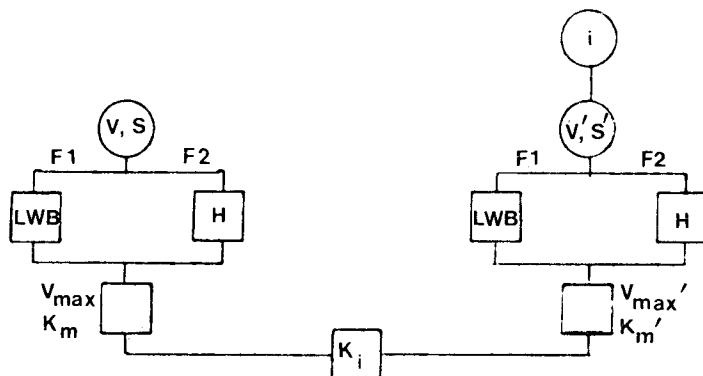
and the coefficient of determination are determined by use of the formulas in the curve fitting program. Since  $b = K_m/V_{max}$  and  $a = 1/V_{max}$  for the Lineweaver-Burk method and  $b = -K_m$  and  $a = V_{max}$  for the Hofstee method, the desired constants  $K_m$  and  $V_{max}$  may be calculated. Once constants for the line are found, projected values for velocity or substrate can be determined. If the same type of data in the presence of a competitive inhibitor is entered, then the  $V_{max}'$  and  $K_m'$  can be determined.  $K_i$  may be calculated from:

$$K_m' = K_m (1 - [i]/K_i)$$

Note: Because registers are cleared when selecting an operating mode, do not attempt to change from one type of curve fit to another during data entry. The methods of Lineweaver-Burk and Hofstee will give similar, but not necessarily identical results. For one discussion of the relative merits of each method see the last reference on the next page.

References: A. Lehninger, *Biochemistry*, Worth Publishers, Inc., New York, 1970, pp 147-168.  
 K. Plowman, *Enzyme Kinetics*, McGraw-Hill, New York, 1972, pp 7-38.  
 J. Dowd and D. Riggs, *Journal of Biological Chemistry*, vol. 240, p 863 (1965).

Example:



The following data on product formation at various substrate concentrations was determined in the presence and absence of a competitive inhibitor. Determine the  $K_m$  and  $V_{max}$  for product formation with and without the inhibitor. What is the  $K_i$ ?

|                                                        |     |     |     |      |      |
|--------------------------------------------------------|-----|-----|-----|------|------|
| Substrate concentration (mM)                           | 1.0 | 2.0 | 3.0 | 10.0 | 15.0 |
| Product formed ( $\mu\text{M/hr}$ )<br>(no inhibitor)  | 40  | 69  | 88  | 160  | 185  |
| Product formed ( $\mu\text{M/hr}$ )<br>(6mM inhibitor) | 24  | 44  | 60  | 126  | 158  |

Keystrokes:

Display:

[XEQ] [ALPHA] SIZE [ALPHA] 026

[XEQ] [ALPHA] KIN [ALPHA]

L-B OR H?

L [R/S]

LINEWEAVER-BURK

40 [A]

69 [A]

88 [A]

10 [ENTER↑]

160 [A]

Keystrokes:

15 [ENTER↑]  
185 [A] [C]  
[R/S]  
[R/S]  
[D]  
[R/S]  
6 [ ] [A]  
24 [A]  
44 [A]  
60 [A]  
10 [ENTER↑] 126 [A]  
15 [ENTER↑] 158 [A] [C]  
[R/S]  
[R/S]  
[D]  
[R/S]  
[E]

Display:

R↑2=0.9996  
a=0.0042  
b=0.0209  
VMAX=240.8340  
KM=5.0275  
  
R↑2=0.9999  
a=0.0040  
b=0.0377  
VMAX=249.7286  
KM=9.4028  
KI=6.8943

# User Instructions

|      |                                            |       |           | SIZE: 026             |
|------|--------------------------------------------|-------|-----------|-----------------------|
| STEP | INSTRUCTIONS                               | INPUT | FUNCTION  | DISPLAY               |
| 1    | Load program                               |       |           |                       |
| 2    | Begin program                              |       | [XEQ] KIN | L-B OR H?             |
| 3    | Select type of analysis                    |       |           |                       |
|      | Lineweaver-Burk                            | L     | [R/S]     | LINEWEAVER-           |
|      |                                            |       |           | BURK                  |
|      | or Hofstee                                 | H     | [R/S]     | HOFSTEE               |
| 4    | Input substrate concentration * **         | S     | [ENTER↑]  |                       |
| 5    | Input velocity                             | V     | [A]       | n+1                   |
| 6    | Repeat steps 4 and 5 for all data pairs    |       |           |                       |
| 7    | Compute and output coefficient of          |       |           |                       |
|      | determination ( $r^2$ ) and line parameter |       |           |                       |
|      | a and b                                    |       | [C]       | $R^2 = (r^2)$         |
|      |                                            |       | $[R/S]^+$ | $a = (a)$             |
|      |                                            |       | $[R/S]^+$ | $b = (b)$             |
| 8    | Optional: project substrate concentration  |       |           |                       |
|      | from a velocity                            | V     | [///] [D] | $S = (\hat{S})$       |
| 9    | Optional: project velocity from a          |       |           |                       |
|      | substrate concentration                    | S     | [///] [E] | $V = (\hat{V})$       |
| 10   | Compute and output Vmax and Km             |       | [D]       | $V_{MAX} = (V_{max})$ |
|      |                                            |       | $[R/S]^+$ | $K_M = (K_m)$         |
| 11   | Optional: if competitive inhibitor data    |       |           |                       |
|      | is available, the competitive mode may be  |       |           |                       |
|      | selected                                   |       |           |                       |
|      | a) input inhibitor concentration * **      | i     | [///] [A] | 1.0000                |
|      | b) input substrate concentration           | S     | [ENTER↑]  |                       |
|      | c) input velocity                          | V     | [A]       | n+1                   |
|      | d) repeat steps 11b) and 11c) for all      |       |           |                       |

# User Instructions

|      |                                                                                                                                                                          |       |           | SIZE:<br>(HP-41C)     |
|------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------|-----------|-----------------------|
| STEP | INSTRUCTIONS                                                                                                                                                             | INPUT | FUNCTION  | DISPLAY               |
| 12   | data pairs                                                                                                                                                               |       |           |                       |
|      | e) compute and output coefficient of determination ( $r^2$ ) and line parameters <u>a</u> and <u>b</u>                                                                   |       | [C]       | $R^2 = (r^2)$         |
|      |                                                                                                                                                                          |       | $[R/S]^+$ | $a = (a)$             |
|      |                                                                                                                                                                          |       | $[R/S]^+$ | $b = (b)$             |
|      | f) compute $V_{max}$ and $K_m$                                                                                                                                           |       | [D]       | $V_{MAX} = (V_{max})$ |
|      |                                                                                                                                                                          |       | $[R/S]^+$ | $KM = (K_m)$          |
|      | g) compute $K_i$                                                                                                                                                         |       | [E]       | $KI = (K_i)$          |
|      | a) To perform another lineweaver - Burk analysis                                                                                                                         |       | [b]       | LINEWEAVER-<br>BURK   |
|      | b) to perform another Hofstee analysis                                                                                                                                   |       | [c]       | HOFSTEE               |
|      | *This step may be skipped if the substrate equals the display counter.                                                                                                   |       |           |                       |
|      | **The last set of data pairs may be deleted by pressing $[R\downarrow]$ then [B]. A set of data may be deleted by entering the set as in steps 4 and 5 and pressing [B]. |       |           |                       |
|      | + No need if a printer is present                                                                                                                                        |       |           |                       |

# Program Listings

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <pre> 01♦LBL "KIN " 02 ΣREG 14 03 SF 27 04 SF 21 05 "L-B OR H?" 06 AON 07 PROMPT 08 AOFF 09 ASTO X 10 "H" 11 ASTO Y 12 X=Y? 13 GTO c 14♦LBL b 15 CF 00 16 XEQ 01 17 1 18 "LINEWEA VER-BURK" 19 AVIEW 20 RTN 21♦LBL c 22 SF 00 23 XEQ 01 24 1 25 "HOFSTEE " 26 AVIEW 27 RTN 28♦LBL 01 29 10.019 30 ENTER↑ 31 CLX 32♦LBL 15 33 STO IND Y 34 ISG Y 35 GTO 15 36 RTN 37♦LBL A 38 CF 03 39♦LBL 08 40 FC? 00 41 1/X 42 STO 23 43 X&lt;&gt;Y 44 FS? 00 45 GTO 09 46 1/X </pre> | <p>Initialization</p> <p>Prompt for type of plot</p> <p>Initialization for L-B plot</p> <p>Initialization for Hofstee plot</p> <p>Clear registers 10 thru 19</p> <p>Summation of data pairs</p> | <pre> 47 STO 22 48♦LBL 02 49 FS? 03 50 GTO 00 51 Σ+ 52♦LBL 07 53 ENTER↑ 54 1 55 + 56 RCL 22 57 X&lt;&gt;Y 58 RCL 23 59 X&lt;&gt;Y 60 RTN 61♦LBL B 62 SF 03 63 -1 64 RDN 65 GTO 08 66♦LBL 09 67 / 68 STO 22 69 RCL 23 70 X&lt;&gt;Y 71 GTO 02 72♦LBL 00 73 Σ- 74 GTO 07 75♦LBL d 76 STO 20 77 RCL 12 78 1/X 79 RCL 11 80 RCL 20 81 FC? 00 82 1/X 83 X&lt;&gt;Y 84 - 85 * 86 FC? 00 87 1/X 88 "S.=" 89 ARCL X 90 AVIEW 91 RTN 92♦LBL e 93 STO 20 94 RCL 11 95 RCL 12 96 RCL 20 97 FC? 00 </pre> | <p>Decrement data "counter". Prepare to delete data</p> <p>Compute v/s for Hofstee plot.</p> <p>Delete data pair.</p> <p>Project substrate concentration from velocity.</p> <p>Project velocity from substrate concentration</p> |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

# Program Listings

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                  |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <pre> 98 1/X 99 * 100 + 101 FC? 00 102 1/X 103 "V. =" 104 ARCL X 105 AVIEW 106 RTN 107♦LBL C 108 RCL 18 109 RCL 14 110 RCL 16 111 * 112 RCL 19 113 / 114 - 115 ENTER↑ 116 ENTER↑ 117 RCL 14 118 X↑2 119 RCL 19 120 / 121 RCL 15 122 X&lt;&gt;Y 123 - 124 / 125 STO 12 126 * 127 RCL 16 128 X↑2 129 RCL 19 130 / 131 CHS 132 RCL 17 133 + 134 / 135 "R↑2 =" 136 ARCL X 137 AVIEW 138 RCL 16 139 RCL 14 140 RCL 12 141 * 142 - 143 RCL 19 144 / 145 STO 11 146 "a =" 147 ARCL X 148 AVIEW </pre> | <p>Calculate and output coefficients</p> <p>Compute b</p> <p>Compute <math>r^2</math></p> <p>Compute a</p> | <pre> 149 RCL 12 150 "b =" 151 ARCL X 152 AVIEW 153 RTN 154♦LBL D 155 RCL 11 156 FC? 00 157 1/X 158 STO 10 159 "VMAX =" 160 ARCL X 161 AVIEW 162 RCL 12 163 FC? 00 164 GT0 04 165 CHS 166 STO 13 167 XEQ "PES" " 168♦LBL 04 169 RCL 11 170 / 171 STO 13 172 "KM =" 173 ARCL X 174 AVIEW 175 RTN 176♦LBL a 177 STO 25 178 .009 179 ENTER↑ 180 CLX 181 XEQ 15 182 XEQ "PES" " 183 1 184 RTN 185♦LBL E 186 XEQ "PES" " 187 RCL 25 188 RCL 03 189 RCL 13 190 / 191 1 192 - 193 / 194 STO 24 195 "KI =" 196 ARCL X </pre> | <p>Transform <math>\frac{a}{b}</math> to <math>V_{MAX}</math> &amp; <math>K_M</math></p> <p>Competitive inhibitor</p> <p>Compute and output <math>K_i</math></p> |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|

# Program Listings

|              |                                                      |    |  |
|--------------|------------------------------------------------------|----|--|
| 197 AVIEW    | Subroutine to<br>simulate HP-67/<br>97 P<>S function | 51 |  |
| 198 RTN      |                                                      |    |  |
| 199♦LBL "PES |                                                      |    |  |
| "            |                                                      |    |  |
| 200 10.01    |                                                      |    |  |
| 201 ENTER↑   |                                                      |    |  |
| 202 .009     |                                                      |    |  |
| 203 +        |                                                      |    |  |
| 204 LASTX    |                                                      |    |  |
| 205 ENTER↑   |                                                      | 60 |  |
| 206♦LBL 14   |                                                      |    |  |
| 207 X<> IND  |                                                      |    |  |
| Y            |                                                      |    |  |
| 208 X<> IND  |                                                      |    |  |
| Z            |                                                      |    |  |
| 209 X<> IND  |                                                      |    |  |
| Y            |                                                      |    |  |
| 210 ISG Y    |                                                      |    |  |
| 211 X<> X    |                                                      |    |  |
| 212 ISG Z    |                                                      | 70 |  |
| 213 GTO 14   |                                                      |    |  |
| 214 RTN      |                                                      |    |  |
| 215 .END.    |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
| 30           |                                                      | 80 |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
| 40           |                                                      | 90 |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
|              |                                                      |    |  |
| 50           |                                                      | 00 |  |

## REGISTERS, STATUS, FLAGS, ASSIGNMENTS

[illegible]

KINETICS USING LINEWEAVER-BURK  
OR HOFSTEE PLOTS  
PROGRAM REGISTERS NEEDED: 57

HEWLETT PACKARD  
SOLUTIONS BOOK:  
CHEMISTRY

ROW 1 (1 : 4)



ROW 2 (5 : 8)



ROW 3 (9 : 15)



ROW 4 (15 : 18)



ROW 5 (18 : 22)



ROW 6 (22 : 25)



ROW 7 (26 : 32)



ROW 8 (33 : 39)



ROW 9 (40 : 47)



ROW 10 (48 : 57)



ROW 11 (58 : 65)



ROW 12 (66 : 74)



ROW 13 (75 : 83)



ROW 14 (84 : 91)



ROW 15 (92 : 100)



ROW 16 (101 : 107)



ROW 17 (108 : 117)



ROW 18 (118 : 128)



KINETICS USING LINEWEAVER-BURK  
OR HOFSTEE PLOTS

HEWLETT PACKARD  
SOLUTIONS BOOK:  
CHEMISTRY

ROW 19 (129 : 135)



ROW 20 (136 : 145)



ROW 21 (146 : 152)



ROW 22 (153 : 159)



ROW 23 (159 : 167)



ROW 24 (167 : 173)



ROW 25 (174 : 181)



ROW 26 (181 : 186)



ROW 27 (186 : 194)



ROW 28 (195 : 199)



ROW 29 (199 : 203)



ROW 30 (204 : 211)



ROW 31 (212 : 215)



## MIXTURE VISCOSITIES

This program calculates the viscosity of a mixture of gases using Chapman Enskog theory. The Wilke formula is used.

$$\mu_{\text{mix}} = \sum_{i=1}^n \frac{X_i \mu_i}{\sum_{j=1}^n X_j \phi_{ij}}$$

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left( 1 + \frac{M_i}{M_j} \right)^{-1/2} \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \left( \frac{M_j}{M_i} \right)^{1/4} \right]^2$$

$X_i$  = Mole fraction of component  $i$

$\mu_i$  = Viscosity of component  $i$

$M_i$  = Molecular weight of component  $i$

Reference: R. Byron Bird, Warren E. Stewart, Edwin N. Lightfoot,  
*Transport Phenomena*, first edition, John Wiley & Sons, Inc.  
1960.

Example:

Predict the viscosity of this gas mixture at 1 atm and 293°K from given data of the independant gases at 1 atm and 293°K.

| Component           | $X_i$ | $M_i$  | $\mu_i \left( \frac{\text{g}}{\text{cm} \cdot \text{sec}} \right)$ |
|---------------------|-------|--------|--------------------------------------------------------------------|
| 1 : CO <sub>2</sub> | .133  | 44.010 | 1462 $\times 10^{-7}$                                              |
| 2 : O <sub>2</sub>  | .039  | 32.000 | 2031 $\times 10^{-7}$                                              |
| 3 : N <sub>2</sub>  | .828  | 28.016 | 1754 $\times 10^{-7}$                                              |

Keystrokes:

Display:

[XEQ] [ALPHA] SIZE [ALPHA] 029

[XEQ] [ALPHA] VISC [ALPHA]

N=?

3 [R/S]

M1=?

44.01 [R/S]

M2=?

32 [R/S]

M3=?

28.016 [R/S]

MU1=?

1462 [R/S]

MU2=?

2031 [R/S]

MU3=?

1754 [R/S]

X1=?

.133 [R/S]

X2=?

.039 [R/S]

X3=?

.828 [R/S]

MUMIX-1714.30

[illegible]

# Program Listings

|                   |                                  |            |                              |
|-------------------|----------------------------------|------------|------------------------------|
| 01*LBL "VIS<br>C" |                                  | 50 STO 26  |                              |
| 02 SF 27          |                                  | 51 RCL 27  |                              |
| 03 "N=?"          | Prompt for N                     | 52 FRC     |                              |
| 04 PROMPT         |                                  | 53 1       | Reset i                      |
| 05 1 E3           |                                  | 54 +       |                              |
| 06 /              |                                  | 55 STO 27  | Begin loop 8                 |
| 07 1              |                                  | 56*LBL 08  |                              |
| 08 +              |                                  | 57 0       | D=0                          |
| 09 STO 27         |                                  | 58 STO 00  |                              |
| 10 STO 28         |                                  | 59 RCL 28  |                              |
| 11*LBL A          |                                  | 60 FRC     | Reset j                      |
| 12 "M"            |                                  | 61 1       |                              |
| 13 0              |                                  | 62 +       | Begin loop 0                 |
| 14 XEQ 07         | Prompt for Mi;<br>i=1 to N       | 63 STO 28  |                              |
| 15*LBL B          |                                  | 64*LBL 09  | Compute                      |
| 16 "MU"           |                                  | 65 RCL 27  | $\sum_{j=1}^N X_j \phi_{ij}$ |
| 17 7              | Prompt for $\mu_i$ ;<br>i=1 to N | 66 7       |                              |
| 18 XEQ 07         |                                  | 67 +       |                              |
| 19*LBL C          |                                  | 68 RCL IND |                              |
| 20 "X"            | Prompt for $X_i$ ;<br>i=1 to N   | 69 RCL 28  |                              |
| 21 14             |                                  | 70 7       |                              |
| 22 XEQ 07         |                                  | 71 +       |                              |
| 23 GTO D          |                                  | 72 RDN     |                              |
| 24*LBL 07         |                                  | 73 RCL IND |                              |
| 25 ASTO 00        |                                  | T          |                              |
| 26 STO 26         |                                  | 74 RCL IND |                              |
| 27 RCL 27         |                                  | 27         |                              |
| 28 FRC            |                                  | 75 RCL IND |                              |
| 29 1              | Reset pointer                    | 28         |                              |
| 30 +              |                                  | 76 XEQ E   | $\phi_{ij}$                  |
| 31 STO 27         |                                  | 77 RCL 28  |                              |
| 32*LBL 06         |                                  | 78 14      |                              |
| 33 CLA            |                                  | 79 +       |                              |
| 34 ARCL 00        |                                  | 80 RDN     |                              |
| 35 FIX 0          |                                  | 81 RCL IND |                              |
| 36 CF 29          |                                  | T          |                              |
| 37 ARCL 27        |                                  | 82 *       |                              |
| 38 "F=?"          |                                  | 83 ST+ 00  |                              |
| 39 PROMPT         |                                  | 84 ISG 28  | End loop 9                   |
| 40 RCL 27         |                                  | 85 GTO 09  |                              |
| 41 RCL 26         |                                  | 86 RCL 27  |                              |
| 42 +              |                                  | 87 7       |                              |
| 43 X<>Y           |                                  | 88 +       |                              |
| 44 STO IND        | Store input value                | 89 RCL IND |                              |
| Y                 |                                  | X          |                              |
| 45 ISG 27         |                                  | 90 X<>Y    |                              |
| 46 GTO 06         |                                  | 91 7       |                              |
| 47 RTN            |                                  | 92 +       |                              |
| 48*LBL D          | Compute $\mu_{mix} \Sigma=0$     | 93 RDN     |                              |
| 49 0              |                                  | 94 RCL IND |                              |
|                   |                                  | T          |                              |

[illegible]

| DATA REGISTERS |                |    |  | STATUS             |             |               |                 |
|----------------|----------------|----|--|--------------------|-------------|---------------|-----------------|
| 00             | Denominator    | 50 |  | SIZE               | 029         | TOT. REG.     | 62              |
|                | M <sub>1</sub> |    |  | ENG                |             | FIX           | 2               |
|                | M <sub>2</sub> |    |  | DEG                |             | SCI           |                 |
|                | M <sub>3</sub> |    |  | RAD                |             | GRAD          |                 |
|                | M <sub>4</sub> |    |  |                    |             |               |                 |
| 05             | M <sub>5</sub> | 55 |  | <b>FLAGS</b>       |             |               |                 |
|                | M <sub>6</sub> |    |  | #                  | INIT<br>S/C | SET INDICATES | CLEAR INDICATES |
|                | M <sub>7</sub> |    |  |                    |             |               |                 |
|                | μ <sub>1</sub> |    |  |                    |             |               |                 |
|                | μ <sub>2</sub> |    |  |                    |             |               |                 |
| 10             | μ <sub>3</sub> | 60 |  |                    |             |               |                 |
|                | μ <sub>4</sub> |    |  |                    |             |               |                 |
|                | μ <sub>5</sub> |    |  |                    |             |               |                 |
|                | μ <sub>6</sub> |    |  |                    |             |               |                 |
|                | μ <sub>7</sub> |    |  |                    |             |               |                 |
| 15             | X <sub>1</sub> | 65 |  |                    |             |               |                 |
|                | X <sub>2</sub> |    |  |                    |             |               |                 |
|                | X <sub>3</sub> |    |  |                    |             |               |                 |
|                | X <sub>4</sub> |    |  |                    |             |               |                 |
|                | X <sub>5</sub> |    |  |                    |             |               |                 |
| 20             | X <sub>6</sub> | 70 |  |                    |             |               |                 |
|                | X <sub>7</sub> |    |  |                    |             |               |                 |
|                | not used       |    |  |                    |             |               |                 |
|                | μ <sub>i</sub> |    |  |                    |             |               |                 |
|                | μ <sub>j</sub> |    |  |                    |             |               |                 |
| 25             | M <sub>i</sub> | 75 |  |                    |             |               |                 |
|                | M <sub>j</sub> |    |  |                    |             |               |                 |
|                | i              |    |  |                    |             |               |                 |
|                | j              |    |  |                    |             |               |                 |
| 30             |                | 80 |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
| 35             |                | 85 |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
| 40             |                | 90 |  | <b>ASSIGNMENTS</b> |             |               |                 |
|                |                |    |  | FUNCTION           | KEY         | FUNCTION      | KEY             |
|                |                |    |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
| 45             |                | 95 |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |
|                |                |    |  |                    |             |               |                 |

## MIXTURE VISCOSITIES

PROGRAM REGISTERS NEEDED: 34

HEWLETT PACKARD  
SOLUTION BOOK:  
CHEMISTRY

ROW 1 (1 - 3)



ROW 2 (3 - 11)



ROW 3 (11 - 17)



ROW 4 (18 - 23)



ROW 5 (23 - 31)



ROW 6 (31 - 38)



ROW 7 (38 - 45)



ROW 8 (46 - 54)



ROW 9 (55 - 64)



ROW 10 (65 - 73)



ROW 11 (74 - 80)



ROW 12 (81 - 88)



ROW 13 (89 - 98)



ROW 14 (99 - 102)



ROW 15 (103 - 111)



ROW 16 (111 - 120)



ROW 17 (120 - 129)



ROW 18 (130 - 139)



## **Hewlett-Packard Software**

In terms of power and flexibility, the problem-solving potential of the HP-41 programmable calculator is nearly limitless. And in order to see the practical side of this potential, HP has different types of software to help save you time and programming effort. Every one of our software solutions has been carefully selected to effectively increase your problem-solving potential. Chances are, we already have the solutions you're looking for.

## **Application Pacs**

To increase the versatility of your HP-41, HP has an extensive library of "Application Pacs". These programs transform your HP-41 into a specialized calculator in seconds. Included in these pacs are detailed manuals with examples, miniature plug-in Application Modules, and keyboard overlays. Every Application Pac has been designed to extend the capabilities of the HP-41.

You can choose from:

**Aviation (Pre-Flight Only) 00041-15018**  
**Clinical Lab 00041-15024**  
**Circuit Analysis 00041-15024**  
**Financial Decisions 00041-15004**  
**Mathematics 00041-15003**  
**Structural Analysis 00041-15021**  
**Surveying 00041-15005**  
**Securities 00041-15026**

**Statistics 00041-15002**  
**Stress Analysis 00041-15027**  
**Games 00041-15022**  
**Home Management 00041-15023**  
**Machine Design 00041-15020**  
**Navigation 00041-15017**  
**Real Estate 00041-15016**  
**Thermal and Transport Science 00041-15019**  
**Petroleum Fluids 00041-15039**

## **Users' Library**

The Users' Library provides the best programs from contributors and makes them available to you. By subscribing to the HP-41 Users' Library you'll have at your fingertips literally hundreds of different programs from many different application areas.

## **\*Users' Library Solutions Books**

Hewlett-Packard offers a wide selection of Solutions Books complete with user instructions, examples, and listings. These solution books will complement our other software offerings and provide you with a valuable tool for program solutions.

You can choose from:

**Business Stat/Marketing/Sales 00041-90094**  
**Home Construction Estimating 00041-90096**  
**Lending, Saving and Leasing 00041-90086**  
**Real Estate 00041-90136**  
**Small Business 00041-90137**  
**Geometry 00041-90084**  
**High-Level Math 00041-90083**  
**Test Statistics 00041-90082**  
**Antennas 00041-90093**  
**Chemical Engineering 00041-90100**  
**Control Systems 00041-90092**  
**Electrical Engineering 00041-90088**  
**Fluid Dynamics and Hydraulics 00041-90139**  
**Games II 00041-90443**

**Civil Engineering 00041-90089**  
**Heating, Ventilating & Air Conditioning 00041-90140**  
**Mechanical Engineering 00041-90090**  
**Solar Engineering 00041-90138**  
**Calendars 00041-90145**  
**Cardiac/Pulmonary 00041-90097**  
**Chemistry 00041-90102**  
**Games 00041-90099**  
**Optometry I (General) 00041-90143**  
**Optometry II (Contact Lens) 00041-90144**  
**Physics 00041-90142**  
**Surveying 00041-90141**  
**Time Module Solutions 00041-90395**

\*Some books require additional memory modules to accommodate all programs.

## **CHEMISTRY**

pH OF WEAK ACID/BASE SOLUTIONS  
ACID-BASE EQUILIBRIUM (DIPROTIC)  
WEAK ACID/BASE TITRATION CURVE  
EQUATIONS OF STATE  
VAN DER WAALS GAS LAW  
BEER'S LAW AND ABSORBPTIVITY CALCULATIONS  
ACTIVITY COEFFICIENTS FROM POTENTIOMETRIC DATA  
CRYSTALLOGRAPHIC TO CARTESIAN COORDINATE  
TRANSFORMATIONS  
KINETICS USING LINEWEAVER-BURK OR HOFSTEE PLOTS  
MIXTURE VISCOSITIES



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