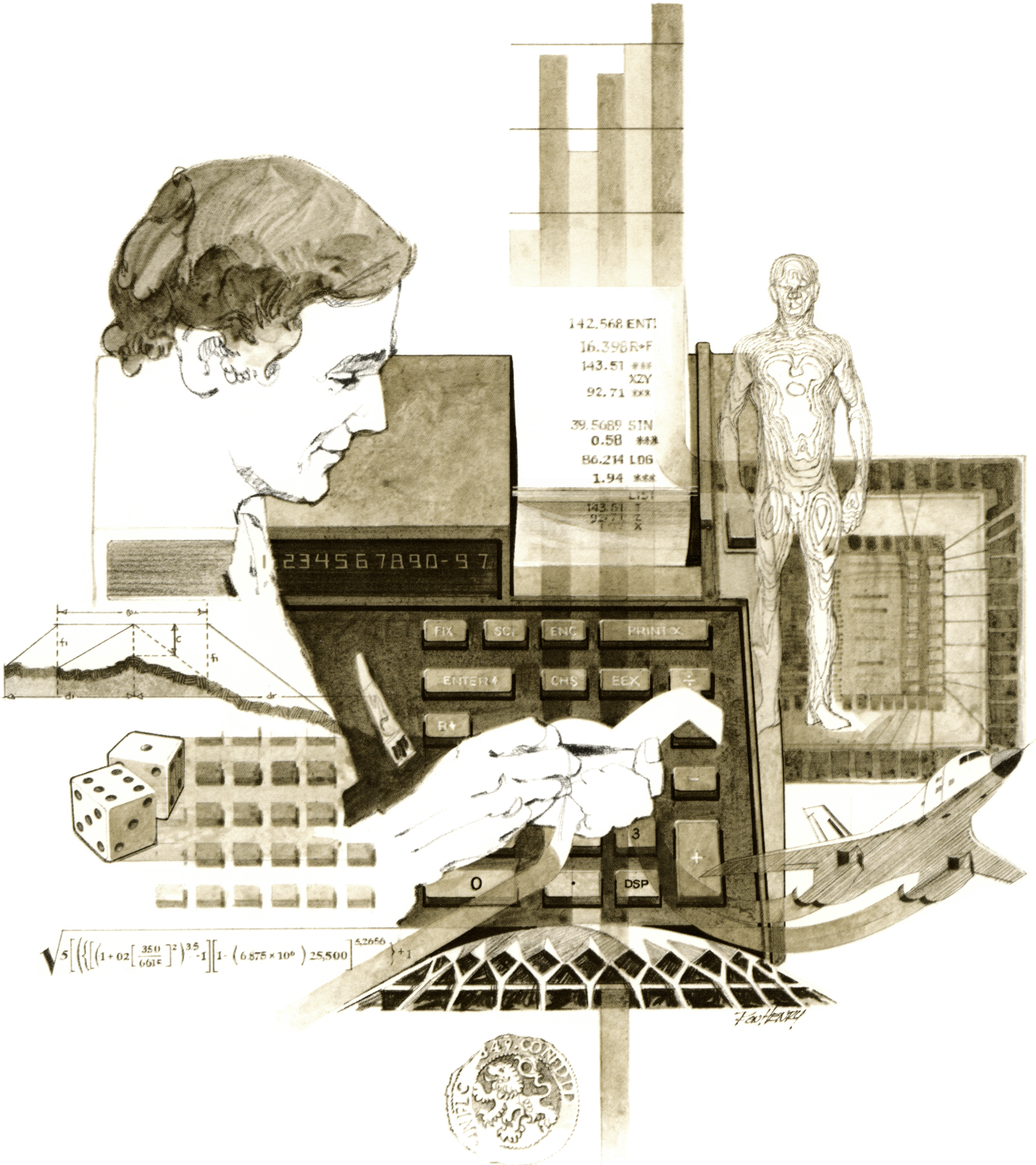
HEWLETT-PACKARD

HP-67/HP-97

Users' Library Solutions

Chemistry



INTRODUCTION

In an effort to provide continued value to it's customers, Hewlett-Packard is introducing a unique service for the HP fully programmable calculator user. This service is designed to save you time and programming effort. As users are aware, Programmable Calculators are capable of delivering tremendous problem solving potential in terms of power and flexibility, but the real genie in the bottle is program solutions. HP's introduction of the first handheld programmable calculator in 1974 immediately led to a request for program **solutions** — hence the beginning of the HP-65 Users' Library. In order to save HP calculator customers time, users wrote their own programs and sent them to the Library for the benefit of other program users. In a short period of time over 5,000 programs were accepted and made available. This overwhelming response indicated the value of the program library and a Users' Library was then established for the HP-67/97 users.

To extend the value of the Users' Library, Hewlett-Packard is introducing a unique service—a service designed to save you time and money. The Users' Library has collected the best programs in the most popular categories from the HP-67/97 and HP-65 Libraries. These programs have been packaged into a series of low-cost books, resulting in substantial savings for our valued HP-67/97 users.

We feel this new software service will extend the capabilities of our programmable calculators and provide a great benefit to our HP-67/97 users.

A WORD ABOUT PROGRAM USAGE

Each program contained herein is reproduced on the standard forms used by the Users' Library. Magnetic cards are not included. The Program Description I page gives a basic description of the program. The Program Description II page provides a sample problem and the keystrokes used to solve it. The User Instructions page contains a description of the keystrokes used to solve problems in general and the options which are available to the user. The Program Listing I and Program Listing II pages list the program steps necessary to operate the calculator. The comments, listed next to the steps, describe the reason for a step or group of steps. Other pertinent information about data register contents, uses of labels and flags and the initial calculator status mode is also found on these pages. Following the directions in your HP-67 or HP-97 **Owners' Handbook and Programming Guide,** "Loading a Program" (page 134, HP-67; page 119, HP-97), key in the program from the Program Listing I and Program Listing II pages. A number at the top of the Program Listing indicates on which calculator the program was written (HP-67 or HP-97). If the calculator indicated differs from the calculator you will be using, consult Appendix E of your **Owner's Handbook** for the corresponding keycodes and keystrokes converting HP-67 to HP-97 keycodes and vice versa. No program conversion is necessary. The HP-67 and HP-97 are totally compatible, but some differences do occur in the keycodes used to represent some of the functions.

A program loaded into the HP-67 or HP-97 is not permanent—once the calculator is turned off, the program will not be retained. You can, however, permanently save any program by recording it on a blank magnetic card, several of which were provided in the Standard Pac that was shipped with your calculator. Consult your **Owner's Handbook** for full instructions. A few points to remember:

> The Set Status section indicates the status of flags, angular mode, and display setting. After keying in your program, review the status section and set the conditions as indicated before using or permanently recording the program.
>
> REMEMBER! To save the program permanently, **clip** the corners of the magnetic card once you have recorded the program. This simple step will protect the magnetic card and keep the program from being inadvertently erased.

As a part of HP's continuing effort to provide value to our customers, we hope you will enjoy our newest concept.

TABLE OF CONTENTS

Program Description I

Program Title PH OF WEAK ACID/BASE SOLUTIONS BY NEWTON-RAPHSON ITERATION

Contributor's Name Alan J. Rubin
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City Columbus **State** Ohio **Zip Code** 43209

Program Description, Equations, Variables A flexible program for the calculation of the pH of a weak acid or a weak base solution by Newton-Raphson iteration of

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

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

$$x_o = (KC + K_w)^{\frac{1}{2}}$$

To calculate the pH of a weak acid solution, K_a (after conversion from pK_a, K_b or pK_b, if necessary) is entered with Key B, followed by C_a molar entered into Key D (mg/l may be converted to M). Hydrogen concentration is flashed for one second followed by pH. To recover (H^+), press A.

To calculate the pH of a weak base solution K_b and C_b are entered, as above, and (OH^-) is flashed for one second followed by pOH. To convert to pH, press R/S. pH or pOH may be recovered at any time from memory without going through the entire calculation by pressing f, D. The error in x, f(x)/f'(x), may be recalled by f,B.

Operating Limits and Warnings

R1 through R6 are used.

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

NEITHER HP NOR THE CONTRIBUTOR MAKES ANY EXPRESS OR IMPLIED WARRANTY OF ANY KIND WITH REGARD TO THIS PROGRAM MATERIAL, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE. NEITHER HP NOR THE CONTRIBUTOR SHALL BE LIABLE FOR INCIDENTAL OR CONSEQUENTIAL DAMAGES IN CONNECTION WITH OR ARISING OUT OF THE FURNISHING, USE OR PERFORMANCE OF THIS PROGRAM MATERIAL.

Program Description II

Sketch(es)

Sample Problem(s)

1.) Find the pH of 1.0X10^{-4} $\underline{M}$ acetic acid solution if K_a is 1.8X10^{-5}.

2.) Find the pH of 3.0X10^{-6} $\underline{M}$ NH_4Cl solution if the pK_b for ammonia is 4.75.

3.) Calculate the pH of 0.002 molar KCN solution (pK_a = 9.32).

4.) What is the molar concentration of a 150 mg/l solution of calcium if its molecular weight is 40.

5.) If the K_a of a weak acid is 1.68X10^{-3}, find the pK_b.

Solution(s) 1.) 1.8 EEX,CHS,5,B → 1.80000X10^{-5}; 4 A → 1.00X10^{-4};
D → 3.45X10^{-5}, 4.46 answer

2.) 4.75 A → 1.78X10^{-5}; R/S → 5.62X10^{-10}; B → 5.62X10^{-10};
3 EEX,CHS,6,D → 1.08X10^{-7}, 6.97 answer.

3.) 9.32 A → 4.79X10^{-10}; R/S → 2.09X10^{-5}; B → 2.09X10^{-5};
.002 D → 1.95X10^{-4},3.71; R/S → 10.29 answer.

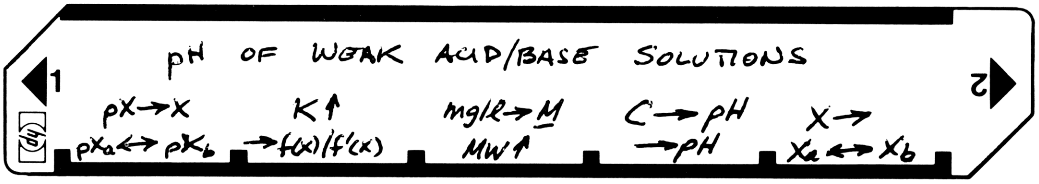
4.) 40 f,C → 40.00; 150 C → 3.75X10^{-3} answer.

5.) 1.68 EEX,CHS,3,E → 2.77; R/S → 11.23 answer
(alternate: 1.68 EEX,CHS,3,f,E → 5.95X10^{-12}; E → 11.23 answer)

Reference(s)

J.N. Butler, "Ionic Equilibrium. A Mathematical Approach," Addison-Wesley, Reading, Mass., 1964.

User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS		OUTPUT DATA/UNITS
1	Load side 1				0.00
2	(Optional) Enter molecular weight	MW	f	C	MW
3	CALC. OF pH OF WEAK ACID SOLUTION				
a	Enter K_a directly	K_a	B		
a	or after conversion of pK_a	pK_a	A	B	
a	or after conversion of K_b	K_b	f	E	
			B		
a	or after conversion of pK_b	pK_b	A	R/S	
			B		K_a
b	Enter molar conc. directly	C_a	D		
b	or after conversion from mg/l conc.	mg/l	C	D	pH *
3	CALC. OF pH OF WEAK BASE SOLUTION				
c	Enter K_b directly	K_b	B		
c	or after conversion of pK_b	pK_b	A	B	
c	or after conversion of K_a	K_a	f	E	
			B		
c	or after conversion of pK_a	pK_a	A	R/S	
			B		K_b
d	Enter molar conc. directly	C_b	D		
d	or after conversion of mg/l conc.	mg/l	C	D	pOH *
e	Convert pOH to pH		R/S		pH
4	Convert pH to $[H^+]$	pH	A		$[H^+]$
	or pH to $[OH^-]$	pH	A	R/S	$[OH^-]$
	or pH to pOH	pH	f	A	pOH
5	To determine error of calculation		f	B	$f(x)/f'(x)$
6	To recover pH or pOH		f	D	pX *
7	Convert pOH to pH or pK_b to pK_a		f	A	
	(or reverse)	pK_a	f	A	pK_b
	or $[H^+]$ to $[OH^-]$ or K_a to K_b				
	(or reverse)	$[OH^-]$	f	E	$[H^+]$
	* $[H^+]$ or $[OH^-]$ is displayed for one				
	second followed by pH or pOH				

67 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001	f LBL A	31 25 11	Convert
	CHS	42	
	10^x	32 53	pKa to Ka
	g SCI	32 23	pKb to Kb
	R/S	84	pH to [H+] etc.
	g LBL e	32 25 15	Interchange
	EEX	43	
	CHS	42	Ka and Kb
	1	01	or
010	4	04	[H+] and [OH-]
	h x≷y	35 52	
	÷	81	
	g SCI	32 23	
	h RTN	35 22	
	f LBL E	31 25 15	Convert
	LOG	31 53	[H+] to pH
	CHS	42	[OH-] to pOH
	f FIX	31 23	Ka to pKa
	R/S	84	etc.
020	g LBL a	32 25 11	Interchange
	1	01	
	4	04	
	h x≷y	35 52	pKa and pKb
	−	51	pH and pOH
	f FIX	31 23	
	h RTN	35 22	
	f LBL C	31 25 13	Calculate molarity
	EEX	43	from mg/l
	3	03	
030	÷	81	
	RCL 6	34 06	
	÷	81	
	g SCI	32 23	
	R/S	84	DISPLAY MW
	RCL 6	34 06	
	f FIX	31 23	
	h RTN	35 22	
	f LBL B	31 25 12	ENTER K
	STO 1	33 01	
040	h RTN	35 22	
	g LBL c	32 25 13	ENTER MW
	STO 6	33 06	
	h RTN	35 22	
	f LBL D	31 25 14	C → pH or pOH
	RCL 1	34 01	
	x	71	
	EEX	43	Calculates
	CHS	42	Constants
	1	01	
050	4	04	
	+	61	
	STO 3	33 03	
	h lst x	35 82	
	RCL 1	34 01	
	x	71	
	STO 4	33 04	

STEP	KEY ENTRY	KEY CODE	COMMENTS
	RCL 3	34 03	
	f √x	31 54	
	STO 2	33 02	
060	GTO 1	22 01	
	h RTN	35 22	
	g LBL b	32 25 12	→ f(x)/f′(x)
	RCL 5	34 05	
	g SCI	32 23	
	R/S	84	DISPLAY K
	RCL 1	34 01	
	h RTN	35 22	
	f LBL 1	31 25 01	
	RCL 2	34 02	Newton-Raphson
070	RCL 1	34 01	iteration
	+	61	
	RCL 2	34 02	
	x	71	
	RCL 3	34 03	
	−	51	
	RCL 2	34 02	
	x	71	
	RCL 4	34 04	
	−	51	
080	RCL 2	34 02	
	3	03	
	x	71	
	RCL 1	34 01	
	2	02	
	x	71	
	+	61	
	RCL 2	34 02	
	x	71	
	RCL 3	34 03	
090	−	51	
	÷	81	
	STO 5	33 05	
	h ABS	35 64	
	RCL 2	34 02	
	9	09	
	9	09	
	÷	81	
	h x≷y	35 52	
	g x≤y?	32 71	TEST
100	GTO f d	22 31 14	
	RCL 2	34 02	
	RCL 5	34 05	
	−	51	
	STO 2	33 02	
	GTO 1	22 01	ITERATE
	R/S	84	
	g LBL d	32 25 14	→ pH or pOH
	RCL 2	34 02	from memory
	g SCI	32 23	
110	h PAU	35 72	FLASH [X]
	GTO E	22 15	DISPLAY pX

REGISTERS

0	1 K	2 Hest	3 CK+Kw	4 KKw	5 f(x)/f′(x)	6 MW	7	8	9
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9

A	B	C	D	E	I

67 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
				170			
120							
				180			
130							
				190			
140							
				200			
150							
				210			
160							
				220			

LABELS					FLAGS
A $pX \to X$; $\frac{10^{-14}}{X}$	B $K\uparrow$	C $mg/l \to \underline{M}$	D $C \to pH$	E $X \to pX$; $14-pX$	0
a $pX_a \leftrightarrow pX_b$	b $f(x)/f'(x)$; K	c $MW\uparrow$	d $\to pH$	e $X_a \leftrightarrow X_b$	1
0	1 used	2	3	4	2
5	6	7	8	9	3

SET STATUS

FLAGS			TRIG		DISP	
	ON	OFF				
0	☐	☒	DEG	☐	FIX	☒
1	☐	☒	GRAD	☐	SCI	☐
2	☐	☒	RAD	☐	ENG	☐
3	☐	☒			n	2

Program Description I

Program Title Acid-base equilibrium (diprotic)

Contributor's Name Charles Kingston

Address John Jay College, 445 W 59 St

City New York **State** N.Y. **Zip Code** 10019

Program Description, Equations, Variables Program determines $[H_3O^+]$ or 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) $K_w = 1 \times 10^{-14}$

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

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

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

Mixture of (in H_2O) Equation

1. H_2A $$x^4 + K_1 x^3 + (K_1K_2 - K_w - K_1C_a)x^2 - (K_wK_1 + 2K_1K_2C_a)x - K_wK_1K_2 = 0$$
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. $NaHA$ $$x^4 + (C_{s,1} + K_1)x^3 + (K_1K_2 - K_w)x^2 - (K_wK_1 + K_1K_2C_{s,1})x - K_wK_1K_w = 0$$
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. $x \doteq (K_wK_2/C_{s,2})^{1/2}$

Operating Limits and Warnings

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

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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Program Description II

Sketch(es)

Sample Problem(s) What is the H_3O^+ concentration for a solution containing 0.05 m sodium hydrogen oxalate and 0.01 m oxalic acid? What pH is this?

$K_1 = 5.90 \times 10^{-2}$

$C_a = 0.01$ m

$K_2 = 6.40 \times 10^{-5}$

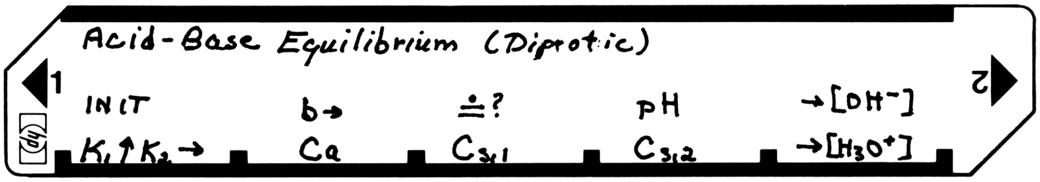
$C_{s,1} = 0.05$ m

Solution(s) Keystrokes

1.	[f] [A]		→ 0.00	00
2.	5.90 [EEX] [CHS] 2 [ENT↑] 6.40 [EEX] [CHS] 5 [A]		→ 5.90	-02
3.	.01 [B]		→ 1.00	-02
4.	.05 [C]		→ 5.00	-02
5.	[E]	Read [H_3O^+]	→ 5.54	-03
6.	[f] [D]	Read pH	→ 2.26	

Reference(s) J. G. Dick, *Analytical Chemistry*, McGraw Hill Book Co, 1973

User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS		OUTPUT DATA/UNITS
1	Load side 1 and 2				
2	Initialize		f	A	0.00 00
3	Optional: To stop at approx. $[H_3O^+]$ or to				
	cancel stop at approx $[H_3O^+]$		f	C	1.00/0.00 00
4	Enter K_1 value	K_1	ENT↑		K_1
5	Enter K_2 value	K_2	A		K_1
6	Enter Ca (omit if Ca = 0)	Ca M	B		Ca
7	Enter $C_{s,1}$ (omit if $C_{s,1} = 0$)	$C_{s,1}$ M	C		$C_{s,1}$
8	Enter $C_{s,2}$ (omit if $C_{s,2} = 0$)	$C_{s,2}$ M	D		$C_{s,2}$
9	To set mode for basic equilibrium		f	B	
10	Compute $[H_3O^+]$ **		E		$[H_3O^+]$ M
11	Optional: To convert display to pH *		f	D	pH
12	Optional: To convert display $[H_3O^+]$ to $[OH^-]$		f	E	$[OH^-]$ M
13	For new case go to step 2				
	If K_1 and K_2 are not to be changed,				
	steps 4 and 5 may be omitted. All values				
	for Ca, $C_{s,1}$ and $C_{s,2}$ must be entered for				
	each run (except 0).				
	*$[H_3O^+]$ may be recalled by :		RCL	4	$[H_3O^+]$ M
	** If ≐ mode is selected:				
10	Compute approx $[H_3O^+]$		E		$[H_3O^+]$ M
10a	(pH for approx. $[H_3O^+]$ will display w/pause)		R/S		pH
					$[H_3O^+]$ M

67 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBL 0	31 25 00	Solve quartic eq.
	STO 4	33 04	
	STO E	33 15	
	F? 1	35 71 01	
	R/S	84	
	F? 1	35 71 01	
	GSB d	32 22 14	
	FIX	31 23	
	DSP 8	23 08	
010	4	04	
	1	01	
	CHS	42	
	STO I	35 33	
	RCL 4	34 04	
	RCL 3	34 03	
	+	61	
	RCL 4	34 04	
	x	71	
	RCL 2	34 02	
020	+	61	
	RCL 4	34 04	
	x	71	
	RCL 1	34 01	
	+	61	
	RCL 4	34 04	
	x	71	
	RCL 0	34 00	
	+	61	
	RCL 4	34 04	
030	4	04	
	x	71	
	RCL 3	34 03	
	3	03	
	x	71	
	+	61	
	RCL 4	34 04	
	x	71	
	RCL 2	34 02	
	2	02	
040	x	71	
	+	61	
	RCL 4	34 04	
	x	71	
	RCL 1	34 01	
	+	61	
	÷	81	
	RCL 4	34 04	
	x⇌y	35 52	
	STO − 4	33 51 04	
050	CLX	44	
	RCL 4	34 04	
	−	51	
	RND	31 24	
	x≠0	31 61	
	GTO (i)	22 24	
	SCI	32 23	

STEP	KEY ENTRY	KEY CODE	COMMENTS
	RCL 4	34 04	
	DSP 2	23 02	
	F? 2	35 71 02	If basic mode set, convert $[OH^-]$ to $[H_3O^+]$
060	GTO e	22 31 15	
	RTN	35 22	
	*LBL e	32 25 15	Convert $[H_3O^+]$ to $[OH^-]$ or reverse
	RCL 8	34 08	
	÷	81	
	1/x	35 62	
	RTN	35 22	
	*LBL A	31 25 11	
	STO 9	33 09	
	↓	35 53	
070	STO A	33 11	
	RTN	35 22	
	*LBL B	31 25 12	
	STO B	33 12	
	1	01	1 sum to fn. indicator
	STO + 5	33 61 05	
	x⇌y	35 52	
	RTN	35 22	
	*LBL C	31 25 13	
	STO C	33 13	
080	2	02	2 sum to fn. indicator
	STO + 5	33 61 05	
	x⇌y	35 52	
	RTN	35 22	
	*LBL D	31 25 14	
	STO D	33 14	
	4	04	4 sum to fn. indicator
	STO + 5	33 61 05	
	x⇌y	35 52	
	RTN	35 22	
090	*LBL E	31 25 15	Set up proper coefficients used in all cases. Complete coefficients are calculated in subroutine pointed to by function indicator (Reg. 5)
	RCL A	34 11	
	STO 3	33 03	
	RCL 9	34 09	
	X	71	
	STO 2	33 02	
	STO 0	33 00	
	RCL 8	34 08	
	CHS	42	
	STO + 2	33 61 02	
100	STO x 0	33 71 00	
	RCL A	34 11	
	X	71	
	STO 1	33 01	
	RCL C	34 13	
	STO + 3	33 61 03	
	RCL D	34 14	
	STO + 3	33 61 03	
	STO + 3	33 61 03	
	RCL 5	34 05	Store fn. indicator in I and go to (i) for proper initial value.
110	STO I	35 33	
	GTO (i)	22 24	
	*LBL 1	31 25 01	

REGISTERS

0	1	2	3	4	5	6	7	8	9
a_0	a_1	a_2	a_3	x_n ; $[H_3O^+]$	Function indicator			K_w	K_2

S0	S1	S2	S3	S4	S5	S6	S7	S8	S9

A	B	C	D	E	I
K_1	C_a	$C_{s,1}$	$C_{s,2}$	approx $[H_3O^+]$	used

67 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS
	RCL A	34 11	
	RCL B	34 12	
	x	71	
	STO-2	33 51 02	
	STO 7	33 07	
	GSB 5	31 22 05	
	RCL 7	34 07	
120	√x	31 54	$(K_1C_a)^{1/2}$
	GTO 0	22 00	
	*LBL 2	31 25 02	
	GSB 7	31 22 07	
	RCL A	34 11	
	RCL 9	34 09	
	x	71	
	√x	31 54	$(K_1K_2)^{1/2}$
	GTO 0	22 00	
	*LBL 3	31 25 03	
130	GSB 5	31 22 05	
	GSB 7	31 22 07	
	RCL A	34 11	
	RCL B	34 12	
	x	71	
	STO-2	33 51 02	
	RCL C	34 13	
	÷	81	$K_1C_a/C_{s,1}$
	GTO 0	22 00	
	*LBL 4	31 25 04	
140	RCL A	34 11	
	RCL D	34 14	
	x	71	
	STO+2	33 61 02	
	RCL 8	34 08	
	RCL 9	34 09	
	x	71	
	RCL D	34 14	
	÷	81	
	√x	31 54	$(K_wK_2/C_{s,2})^{1/2}$
150	GTO 0	22 00	
	*LBL 6	31 25 06	
	GSB 7	31 22 07	
	RCL A	34 11	
	RCL D	34 14	
	x	71	
	STO+2	33 61 02	
	RCL 9	34 09	
	RCL C	34 13	
	x	71	
160	RCL D	34 14	
	÷	81	$K_2C_{s,1}/C_{s,2}$
	GTO 0	22 00	
	*LBL 5	31 25 05	
	RCL A	34 11	$-2K_1K_2C_a$ + Reg 1
	RCL 9	34 09	
	x	71	
	RCL B	34 12	
	x	71	

STEP	KEY ENTRY	KEY CODE	COMMENTS
	2	02	
170	x	71	
	STO-1	33 51 01	
	RTN	35 22	
	*LBL 7	31 25 07	
	RCL A	34 11	$-K_1K_2C_{s,1}$ + Reg 1
	RCL 9	34 09	
	x	71	
	RCL C	34 13	
	x	71	
	STO-1	33 51 01	
180	RTN	35 22	
	*LBL d	32 25 14	−log x
	log	31 53	
	CHS	42	
	FIX	31 23	
	Pause	35 72	
	RTN	35 22	
	*LBL b	32 25 12	
	SF2	35 51 02	
	RTN	35 22	
190	*LBL c	32 25 13	
	F? 1	35 71 01	
	GTO 9	22 09	
	1	01	
	SF 1	35 51 01	
	RTN	35 22	
	*LBL 9	31 25 09	
	0	00	
	CF 1	35 61 01	
	RTN	35 22	
200	*LBL a	32 25 11	
	EEX	43	
	CHS	42	
	1	01	
	4	04	
	STO 8	33 08	
	CLX	44	
	STO 5	33 05	
	CF2	35 61 02	
	SCI	32 23	
210	DSP 2	23 02	
	RTN	35 22	
220			

LABELS					FLAGS
A $K_1 \uparrow K_2 \rightarrow$	B C_a	C $C_{s,1}$	D $C_{s,2}$	E $[H_3O^+]$	0
a INIT	b b→	c ≐?	d pH	e $[OH^-]$	1 ≐?
0 Used	1 H_2A	2 NaHA	3 H_2A + NaHA	4 Na_2A	2 b →
5 Used	6 NaHA + Na_2A	7 Used	8	9 CF1	3

SET STATUS

FLAGS	ON	OFF	TRIG		DISP	
0	☐	☒	DEG	☒	FIX	☐
1	☐	☒	GRAD	☐	SCI	☒
2	☐	☒	RAD	☐	ENG	☐
3	☐	☒			n	2

Program Description I

Program Title Weak Acid/Base Titration Curve

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Program Description, Equations, Variables Consider a weak acid, H_4A. The electroneutrality of any solution containing this acid and its ions requires that

$$[H^+] + [Na^+] = [OH^-] + [H_3A^-] + 2[H_2A^{2-}] + 3[HA^{3-}] + 4[A^{4-}].$$

The $[Na^+]$ term must be included once neutralization is begun; NaOH is assumed to be the titrant. The acid ion concentrations must be expressed in terms of the dissociation constants and C, the "analytical concentration" of the acid:

$C = V_a\underline{M}_a/(V_a + V_b)$, where V_a = the volume of H_4A taken at the outset

$\underline{M}_a$ = the molarity of the H_4A solution taken

V_b = the volume of titrant added

See any beginning text on quantitative analysis for the derivation of the formulas for the fraction of each ionic species as a function of $[H^+]$. The results are used here. Let $Q = 1 + \frac{K_1}{[H^+]} + \frac{K_1K_2}{[H^+]^2} + \frac{K_1K_2K_3}{[H^+]^3} + \frac{K_1K_2K_3K_4}{[H^+]^4}$. For each acid ion concentration in the equation above, we now substitute its fraction times C:

$$[H^+] + [Na^+] = \frac{K_w}{[H^+]} + \frac{CK_1}{Q[H^+]} + \frac{2CK_1K_2}{Q[H^+]^2} + \frac{3CK_1K_2K_3}{Q[H^+]^3} + \frac{4CK_1K_2K_3K_4}{Q[H^+]^4}.$$

After substituting for Q, clearing fractions and collecting terms (a straightforward but very involved process, and one which is hard (for me at least) to do without errors) we arrive at the 6th degree equation given at the top of the next page.

Operating Limits and Warnings If you make a bad guess for pH_{est} and the calculator iterates until your patience is exhausted, you can press $\boxed{\text{R/S}}$ to halt the process, enter a guess which you hope will be better, and start again by re-entering your volume of titrant and pressing $\boxed{\text{A}}$. But make <u>sure</u> the primary and secondary storage registers are set "normally"; i.e. make sure that R_0 contains an integer equal to the number of K's entered plus 1. Press $\boxed{\text{f}}$ $\boxed{\text{P}\rightleftarrows\text{S}}$ if necessary. (You may have pressed $\boxed{\text{R/S}}$ while the primaries and secondaries were switched.)

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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$$[H^+]^6 + (K_1 + [Na^+])[H^+]^5 + (K_1K_2 + [Na^+]K_1 - CK_1 - K_w)[H^+]^4$$
$$+ (K_1K_2K_3 + [Na^+]K_1K_2 - 2CK_1K_2 - K_1K_w)[H^+]^3$$
$$+ (K_1K_2K_3K_4 + [Na^+]K_1K_2K_3 - 3CK_1K_2K_3 - K_1K_2K_w)[H^+]^2$$
$$+ ([Na^+]K_1K_2K_3K_4 - 4CK_1K_2K_3K_4 - K_1K_2K_3K_w)[H^+] - K_1K_2K_3K_4K_w = 0.$$

The equation is now re-written using the letters a, b, c, d, e, and f to represent the coefficients after the first one (i.e., 1):

$$[H^+]^6 + a[H^+]^5 + b[H^+]^4 + c[H^+]^3 + d[H^+]^2 + e[H^+] + f = 0$$

The Newton-Raphson method for finding roots of functions is discussed in most beginning calculus texts. If the polynomial in hydrogen ion on the left side of the above equation is called $g([H^+])$, the Newton-Raphson formula is

$$[H^+]_{n+1} = [H^+]_n - \frac{g([H^+]_n)}{g'([H^+]_n)}$$

where $[H^+]_n$ = a trial value of $[H^+]$;

$[H^+]_{n+1}$ = a new value of $[H^+]$, closer to the root of the equation than $[H^+]_n$ was;

$g([H^+]_n)$ = the function g evaluated at $[H^+] = [H^+]_n$ and

$g'([H^+]_n)$ = the first derivative of g evaluated at $[H^+] = [H^+]_n$.

Here, $g'([H^+]) = 6[H^+]^5 + 5a[H^+]^4 + 4b[H^+]^3 + 3c[H^+]^2 + 2d[H^+] + e$.

The iteration process continues, using each value of $[H^+]$ generated as the trial value for the next iteration, until a value for hydrogen ion is generated which differs by 1% or less from the previous value. The last value of hydrogen ion obtained is then converted to pH and presented as the answer. The 1% figure corresponds to ± 0.0043 in the pH, which means that these calculated pH's should agree about as well as can be expected with values obtained in the laboratory, since junction potentials, activity coefficients, etc., are not taken into account.

I have studied quite a few of the equations obtained in this computation, not only 6th degree ones but 5th, 4th and 3rd degree ones (see below). In every case I looked at, all 6 (or 5, 4, or 3) roots are real, but only one (the one of interest) is positive.

If a pH_{est} corresponding to too small a $[H^+]$ is taken, it is quite possible for the calculator to iterate its way to the largest of the negative roots. To prevent an "Error" message being produced when the calculator tries to take the log of a negative root, each value of hydrogen ion produced is checked at step 119 to see if it is negative. If it is, the program returns to LBLa (step 076), the pH_{est} is lowered (or raised, if the calculator is in "base mode") by 2 units, and the iteration process started anew. The calculator will thus always get the right answer, but the process can be quite lengthy if a really bad initial guess is made. See the "warning" on the previous page.

If a tribasic acid, H_3A is used, K_4 is zero, and the 6th degree equation given at the top of this page reduces to a 5th degree equation:

$$[H^+]^5 + (K_1 + [Na^+])[H^+]^4 + (K_1K_2 + [Na^+]K_1 - CK_1 - K_w)[H^+]^3$$
$$+ (K_1K_2K_3 + [Na^+]K_1K_2 - 2CK_1K_2 - K_1K_w)[H^+]^2$$
$$+ ([Na^+]K_1K_2K_3 - 3CK_1K_2K_3 - K_1K_2K_w)[H^+] - K_1K_2K_3K_w = 0$$

Here $g([H^+]) = [H^+]^5 + a[H^+]^4 + b[H^+]^3 + c[H^+]^2 + d[H^+] + e$ and

$$g'([H^+]) = 5[H^+]^4 + 4a[H^+]^3 + 3b[H^+]^2 + 2c[H^+] + d$$

If a dibasic acid, H_2A is used, K_3 and K_4 are both zero, and the 6th degree equation given at the top of the previous page reduces to a 4th degree equation:

$$[H^+]^4 + (K_1 + [Na^+])[H^+]^3 + (K_1K_2 + [Na^+]K_1 - CK_1 - K_w)[H^+]^2$$

$$+ ([Na^+]K_1K_2 - 2CK_1K_2 - K_1K_w)[H^+] - K_1K_2K_w = 0$$

Here $g([H^+]) = [H^+]^4 + a[H^+]^3 + b[H^+]^2 + c[H^+] + d$ and

$$g'([H^+]) = 4[H^+]^3 + 3a[H^+]^2 + 2b[H^+] + c$$

Finally, if a monobasic acid, HA is used, K_2, K_3 and K_4 are all zero, and the 6th degree equation reduces to

$$[H^+]^3 + (K + [Na^+])[H^+]^2 + ([Na^+]K - CK - K_w)[H^+] - KK_w = 0.$$

Here, $g([H^+]) = [H^+]^3 + a[H^+]^2 + b[H^+] + c$ and

$$g'([H^+]) = 3[H^+]^2 + 2a[H^+] + b$$

The 6th degree equation can not be used for fewer than 4 K's. It is true that f will turn out to be zero; unfortunately, the remaining polynomial is a multiple of $[H^+]$ and thus $[H^+] = 0$ will be a root and this is not the right answer. Thus a separate routine must be used for each different number of K's entered. The parts of the routines that are common to all are performed under LBL 8 and LBL 9.

If the weak electrolyte being titrated is a base rather than an acid, the mathematical treatment is identical. However, the equation that must be solved is an equation in $[OH^-]$ rather than in $[H^+]$, and the role of $[Na^+]$ is assumed by (say) $[Cl^-]$. Subroutine LBLd converts pH to pOH or vice versa, as needed, since even when titrating a base, the answer is pH and not pOH.

To get the computation of the coefficients a, b, c, d, e and f into few enough steps, I had to make the program calculate coefficients b through f by means of a loop. I hope that the chart on the next page will explain how the first part of LBLc does this. If 4 K's are entered, R_7 will be 5 initially, and the loop begins with the first column. If 3 K's are entered, R_7 will be 4 initially, and the loop begins with the second column, and so on. If n K's are entered, it is necessary that K_{n+1} and K_{n+2} be zero. Thus the initializing step $\boxed{f}\,\boxed{e}$ is necessary to initialize the registers properly.

If the volume of titrant added is zero, the program automatically takes $\sqrt{K_1C}$ as its first trial $[H^+]$. For titrant volumes greater than zero, usually the most practical trial pH to use is the one that was obtained for the previous volume (assuming that the previous volume was smaller than the present one!). It is not even necessary to key it in, as it is already in the display.

Program Description II

Sketch(es)

Sample Problem(s) 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 base added for 50.00 ml of 0.200 M H_2PO_4titrated with 0.500 N NaOH.

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:

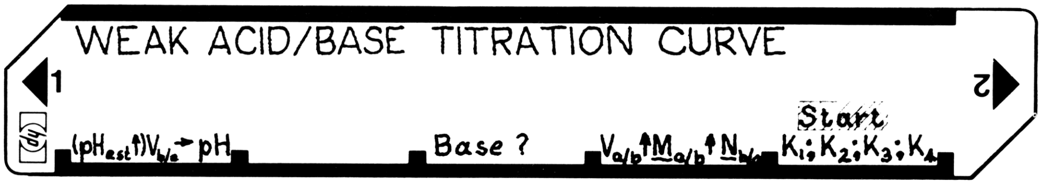
```
[f] [E] --------------   0.000
  [C]   --------------   1; Base mode
  [C]   --------------   0; Acid mode (correct)
7.5 [EEX] [CHS] 3[E] 6.2[EEX] [CHS] 8[E] [EEX] [CHS] 12[E]
50[ENTER ] .2[ENTER ] .5[D] ----------  3.000 (number of K's entered)
THEN:
```

```
0[A]  ---   0.000 Vol.        20.4[A]-- 20.400 Vol.        39.8[A]-- 39.800 Vol.
            1.454 pH                     5.527 pH                     9.142 pH
10[A] --- 10.000 Vol.         21[A] --- 21.000 Vol.        40.1[A]-- 40.100 Vol.
            2.192 pH                     5.930 pH                     9.832 pH
15[A] --- 15.000 Vol.         25[A] --- 25.000 Vol.        40.8[A]-- 40.800 Vol.
            2.637 pH                     6.730 pH                    10.584 pH
19.4[A]-- 19.400 Vol.         35[A] --- 35.000 Vol.        45[A] --- 45.000 Vol.
            3.654 pH                     7.685 pH                    11.457 pH
20[A] --- 20.000 Vol.         39[A] --- 39.000 Vol.        75[A] --- 75.000 Vol.
            4.677 pH                     8.483 pH                    12.845 pH
```

Reference(s) "A General Acid-Base Titration Curve Computer Program", G.L. Breneman, Journal of Chemical Education 51, 812-813 (197-)

Any beginning quantitative analysis text, such as Skoog & West, Fritz & Schenck, etc.

User Instructions



▨ = yellow

STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS		OUTPUT DATA/UNITS
1	Load both sides of card				0.000
2	Initialize		f	e	
3	(Optional) Set "base mode"		C		1
	" Reset "acid mode" *		C		0
4	Enter dissociation constants	K_1	E		K_1
	(If necessary)	K_2	E		K_2
	(If necessary)	K_3	E		K_3
	(If necessary)	K_4	E		K_4
5	Enter volume of weak acid or base to be titrated	V	ENT↑		
	Enter molarity of " " " " " " "	$\underline{M}$	ENT↑		
	Enter normality of strong base or acid titrant	$\underline{N}$	D		# of K's
6	(Semi-optional) Enter guess for pH **	pH_{est}	ENT↑		
	Enter volume of titrant added	V	A		pH
7	Repeat step 6 as often as needed to plot curve				
8	For a new problem go to 2.				
	*: When you press $\boxed{C}$, whether you get a "1" or				
	a "0" depends on the position of the program				
	pointer at the time the key is pressed. It may				
	be necessary to press $\boxed{C}$ twice to get the				
	response you want ("1" for base, "0" for acid).				
	**: A guess for pH need <u>not</u> be entered IF:				
	1) The volume of titrant is going to be zero				
	OR				
	2) The pH already in the display (usually from				
	the problem just done) is a suitable pH_{est};				
	it usually is suitable if the volume to be				
	entered is greater than the volume just				
	used.				

97 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBLC	21 13	
002	SF0	16 21 00	Reset F0 to acid mode
003	0	00	
004	RTN	24	
005	*LBLA	21 11	
006	X=0?	16-43	Vol.=0?
007	SF2	16 21 02	Y: set F2 N: leave it off
008	PRTX	-14	(HP-67 user should delete)
009	RCLB	36 12	
010	X⇄Y	-41	
011	×	-35	
012	LSTX	16-63	
013	RCLD	36 14	
014	+	-55	
015	÷	-24	
016	STOA	35 11	$[Na^+] \rightarrow R_A$
017	RCLE	36 15	
018	LSTX	16-63	
019	÷	-24	
020	STOC	35 13	$C \rightarrow R_C$
021	R↑	16-31	
022	STO8	35 08	$pH_{est} \rightarrow R_8$
023	RCL0	36 00	
024	STO7	35 07	Initialize coeff. counter
025	*LBLc	21 16 13	
026	RCL7	36 07	
027	STOI	35 46	
028	ISZI	16 26 46	
029	RCLi	36 45	
030	RCLA	36 11	
031	+	-55	
032	DSZI	16 25 46	
033	RCLI	36 46	Calculate coeff's. (See p. 4 for additional explanation)
034	RCLC	36 13	
035	×	-35	
036	-	-45	
037	RCLi	36 45	
038	×	-35	
039	EEX	-23	
040	CHS	-22	
041	1	01	
042	4	04	
043	-	-45	
044	*LBLb	21 16 12	
045	DSZI	16 25 46	
046	GTO0	22 00	
047	RCL7	36 07	
048	X⇄I	16-41	
049	X⇄Y	-41	
050	P⇄S	16-51	
051	STOi	35 45	
052	P⇄S	16-51	
053	7	07	
054	STOI	35 46	
055	DSZi	16 25 45	
056	GTOc	22 16 13	

STEP	KEY ENTRY	KEY CODE	COMMENTS
057	RCL0	36 00	#K's + 1 → R_I; R_I now ready for step 90
058	STOI	35 46	
059	RCL1	36 01	K_1
060	RCLA	36 11	$[Na^+]$
061	+	-55	
062	P⇄S	16-51	
063	STO0	35 00	Store a in R_{S0}
064	P⇄S	16-51	
065	RCL1	36 01	K_1
066	RCLC	36 13	C
067	×	-35	
068	√X	54	$\sqrt{K_1 C} = [H^+]_{trial}$ if Vol.=0
069	F2?	16 23 02	Was Vol.=0?
070	GTO1	22 01	Y: begin iterations
071	GTOB	22 12	N: use pH_{est} first
072	*LBL0	21 00	
073	RCLi	36 45	
074	×	-35	See p.4
075	GTOb	22 16 12	
076	*LBLa	21 16 11	
077	2	02	
078	F0?	16 23 00	Change pH_{est} by ±2
079	CHS	-22	
080	ST+8	35-55 08	
081	*LBLB	21 12	
082	RCL8	36 08	
083	GSBd	23 16 14	
084	CHS	-22	
085	10ˣ	16 33	$[H^+] = 10^{-pH}$
086	*LBL1	21 01	
087	P⇄S	16-51	
088	ENT↑	-21	
089	ENT↑	-21	Load stack with $[H^+]$
090	GTOi	22 45	Use correct N-R routine
091	*LBL5	21 05	Routine for 4 K's
092	6	06	
093	×	-35	
094	RCL0	36 00	
095	5	05	
096	GSB6	23 06	
097	RCL1	36 01	
098	4	04	
099	GSB6	23 06	Start forming $f'([H^+])$
100	RCL2	36 02	
101	3	03	
102	GSB6	23 06	
103	RCL3	36 03	
104	2	02	
105	GSB6	23 06	
106	RCL4	36 04	
107	GSB8	23 08	
108	RCL3	36 03	
109	GSB7	23 07	
110	RCL4	36 04	Continue forming $f([H^+])$
111	GSB7	23 07	
112	RCL5	36 05	

REGISTERS

0 #K's + 1	1 K_1	2 K_2	3 K_3	4 K_4	5 0	6 0	7 Counter	8 pH_{est}	9 $[H^+]_{trial}$
S0 a	S1 b	S2 c	S3 d	S4 e	S5 f	S6 $g'([H^+])$	S7	S8	S9

A $[Na^+]$	B $\underline{N}_b$	C C	D V_a	E $\underline{M}V_a$	I Control

97 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS
113	*LBL9	21 09	Finish forming $f([H^+])$
114	+	-55	
115	RCL6	36 06	RCL $f'([H^+])$
116	P⇄S	16-51	
117	÷	-24	
118	-	-45	Forms $[H^+]_{n+1}$
119	X<0?	16-45	Is $[H^+]$ negative?
120	GTOa	22 16 11	Y: start over w. new pH_{est}
121	STO9	35 09	N: continue
122	%CH	16 55	
123	ABS	16 31	
124	1	01	
125	X≤Y?	16-35	Is 1% ≤ |%CH| ?
126	SF2	16 21 02	Y: set F2 N: leave it off
127	RCL9	36 09	RCL $[H^+]$
128	F2?	16 23 02	Was 1% ≤ |%CH| ?
129	GTO1	22 01	Y: do another iteration
130	LOG	16 32	N: $[H^+]$ → pH
131	CHS	-22	
132	GSBd	23 16 14	
133	PRTX	-14	HP-67 user should delete
134	SPC	16-11	
135	RTN	24	
136	*LBLd	21 16 14	
137	F0?	16 23 00	Acid mode ?
138	RTN	24	Y: leave pH alone
139	1	01	N: 14 − pH = pOH or
140	4	04	14 − pOH = pH
141	X⇄Y	-41	
142	-	-45	
143	RTN	24	
144	*LBL6	21 06	
145	×	-35	
146	*LBL7	21 07	Steps repeatedly used in polynomial evaluation
147	+	-55	
148	×	-35	
149	RTN	24	
150	*LBL8	21 08	
151	+	-55	
152	STO6	35 06	
153	CLX	-51	Steps common to all 4 N-R routines; completes and stores $f'([H^+])$ in R_6; begins computation of $f([H^+])$
154	RCL0	36 00	
155	GSB7	23 07	
156	RCL1	36 01	
157	GSB7	23 07	
158	RCL2	36 02	
159	F2?	16 23 02	F2 set in LBL2 only
160	GTO9	22 09	
161	GTO7	22 07	
162	*LBL4	21 04	Routine for 3 K's
163	5	05	
164	×	-35	
165	RCL0	36 00	Start forming $f'([H^+])$
166	4	04	
167	GSB6	23 06	
168	RCL1	36 01	
169	3	03	
170	GSB6	23 06	
171	RCL2	36 02	
172	2	02	
173	GSB6	23 06	
174	RCL3	36 03	
175	GSB8	23 08	
176	RCL3	36 03	
177	GSB7	23 07	Continue forming $f([H^+])$
178	RCL4	36 04	
179	GTO9	22 09	
180	*LBL3	21 03	Routine for 2 K's
181	4	04	
182	×	-35	
183	RCL0	36 00	Start forming $f'([H^+])$
184	3	03	
185	GSB6	23 06	
186	RCL1	36 01	
187	2	02	
188	GSB6	23 06	
189	RCL2	36 02	
190	GSB8	23 08	
191	RCL3	36 03	Continue forming $f([H^+])$
192	GTO9	22 09	
193	*LBL2	21 02	Routine for 1 K
194	3	03	
195	×	-35	Start forming $f'([H^+])$
196	RCL0	36 00	
197	2	02	
198	GSB6	23 06	
199	RCL1	36 01	
200	SF2	16 21 02	Cause LBL 8 to exit to LBL9
201	GTO8	22 08	
202	*LBLe	21 16 15	
203	CLRG	16-53	
204	ISZi	16 26 45	Initialize R_0 to 1
205	RTN	24	
206	*LBLE	21 15	
207	ISZI	16 26 46	
208	STOi	35 45	$K_i \rightarrow R_i$
209	RTN	24	
210	*LBLD	21 14	
211	STOB	35 12	$N_b \rightarrow R_B$
212	R↓	-31	
213	X⇄Y	-41	
214	STOD	35 14	$V_a \rightarrow R_D$
215	×	-35	
216	STOE	35 15	$V_a \underline{M_a} \rightarrow R_E$
217	RCLI	36 46	# of K's
218	ST+0	35-55 00	# K's + 1 → R_0
219	RTN	24	
220	*LBLC	21 13	
221	CF0	16 22 00	Clear F0 to base mode
222	1	01	
223	RTN	24	

LABELS

A pH↑V→pH	B pH→N-R	C Base?	D V↑M↑N	E $K_1;K_2-K_4$
a [H+]<0 restart	b used	c used	d pH⇄pOH	e Start
0 used	1 N-R start	2 mono.	3 di.	4 tri.
5 quad.	6 × + ×	7 + ×	8 N-R mid.	9 N-R end

FLAGS

0	Acid mode
1	
2	Used
3	

SET STATUS

FLAGS	ON	OFF
0	☒	☐
1	☐	☒
2	☐	☒
3	☐	☒

TRIG	
DEG	☒
GRAD	☐
RAD	☐

DISP	
FIX	☒
SCI	☐
ENG	☐
n	3

Program Description I

Program Title EQUATIONS OF STATE

Contributor's Name

HEWLETT-PACKARD
1000 N. E. Circle Blvd.
Corvallis, Oregon 97330

Address

City **State**

Program Descriptio

This card 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^2	m^3/g mole	K
83.14	cm^3 - bar/g mole - K	bar	cm^3/g mole	K
82.05	cm^3 - atm/g mole - K	atm	cm^3/g mole	K
0.7302	atm - ft^3/lb mole - °R	atm	ft^3/lb mole	°R
10.73	psi - ft^3/lb mole - °R	psi	ft^3/lb mole	°R
1545	psf - ft^3/lb mole - °R	psf	ft^3/lb mole	°R

Critical Temperatures and Pressures

Substance	T_c, K	T_c, °R	P_c, 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-Hexane	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

Operating Limits ar

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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Program Description I

Program Title

Contributor's Nam

Address

City

Program Descripti

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 nor 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.

Operating Limits

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 an "error".

Registers R_0, R_1 and R_{S0}—R_{S9} are available for user storage.

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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Program Description II

Sketch(es)

Example 1:

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

Select ideal gas by pressing f A until 0.00 is displayed.

Keystrokes:	Outputs:	
f A f A	0.00	
25000 B .63 C 83.14 D		
1200 E A	2.51	(bars)

Example 2:

What is the specific volume (ft^3/lb) of a gas at atmospheric pressure and at a temperature of 513°R? The molecular weight is 29. Assume an ideal gas.

Sample Problem

Keystrokes:	Outputs:	
f A	0.00	
513 E 29 1/x C 0.7302		
D 1 A B	12.92	(ft^3/lb)

What is the density?

1/x	0.08	(lb/ft^3)

What is the density at 1.32 atmospheres and 555°R?

1.32 A 555 E B 1/x	0.09	(lb/ft^3)

Example 3:

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

P_c = 48.2 atm

T_c = 305.5 K

R = 82.05 cm^3 - atm/g mole-K

Keystrokes:	Outputs:	
f A	1.00	
305.5 f B 48.2 f C 82.05		
D 1 C 400 E 800 B A	36.27	(atm)

Solution(s)

Example 4:

6 gram moles of carbon dioxide gas are held at a pressure of 50 atmospheres, and at a temperature of 500 K. What is the volume in cubic centimeters? Use the Redlich-Kwong relation.

T_c = 304.2 K

P_c = 72.9 atm

R = 82.05 cm^3 - atm/g mole - K

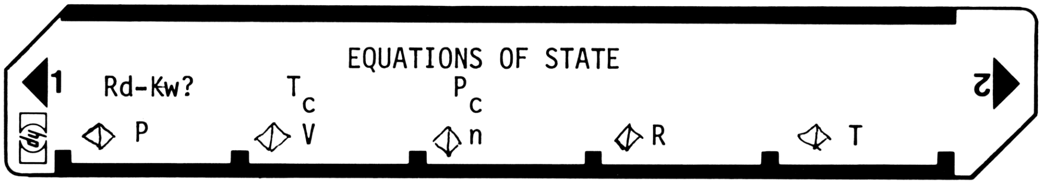
Keystrokes:	Outputs:	
f A	1.00	
72.9 f C 304.2 f B 82.05		
D 6 C 50 A 500 E B	4695.86	(cm^3)

Reference(s)

How many moles could be contained at this temperature and pressure in 5 liters?

5000 B C	6.39	(g moles)

User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS	OUTPUT DATA/UNITS
1	Load side 1 and side 2.			
2	Select Redlich-Kwong (1.00) or			
	ideal gas (0.00) using mode			
	toggle.		f A	1.00/0.00
3	If you selected ideal gas in			
	step 2, skip to step 5.			
4	Input critical temperature	T_c	f B	T_c
	and critical pressure.	P_c	f C	P_c
5	Input four of the following:			
	Absolute pressure	P	A	P
	Volume	V	B	V
	Number of moles	n	C	n
	Universal gas constant	R	D	R
	Absolute temperature	T	E	T
6	Calculate remaining value:			
	Absolute pressure		A	P
	Volume		B	V
	Number of moles		C	n
	Universal gas constant		D	R
	Absolute temperature		E	T
7	For a new case, go to steps 2,			
	4, or 5 and change values or			
	mode.			

97 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBLa	21 16 11	
002	F0?	16 23 00	Redlich-Kwong ideal gas toggle.
003	GTO0	22 00	
004	0	00	
005	SF0	16 21 00	
006	RTN	24	
007	*LBL0	21 00	
008	1	01	
009	CF0	16 22 00	
010	RTN	24	
011	*LBLb	21 16 12	Store T_c.
012	CF3	16 22 03	
013	STOC	35 13	
014	RTN	24	
015	*LBLc	21 16 13	Store P_c.
016	CF3	16 22 03	
017	STOD	35 14	
018	RTN	24	
019	*LBLA	21 11	P code.
020	5	05	
021	GTO0	22 00	
022	*LBLB	21 12	V code.
023	6	06	
024	GTO0	22 00	
025	*LBLC	21 13	n code.
026	7	07	
027	GTO0	22 00	
028	*LBLD	21 14	R code.
029	8	08	
030	GTO0	22 00	
031	*LBLE	21 15	T code.
032	9	09	
033	*LBL0	21 00	
034	CF1	16 22 01	Store input.
035	STOI	35 46	
036	R↓	-31	
037	STOi	35 45	
038	F3?	16 23 03	
039	RTN	24	
040	1	01	
041	STOi	35 45	Dummy 1.00 for unknown and GTO ideal gas.
042	GTOi	22 45	
043	*LBL5	21 05	
044	*LBL6	21 06	Ideal gas solution for P and V.
045	RCL7	36 07	
046	RCL8	36 08	
047	×	-35	
048	RCL9	36 09	
049	×	-35	
050	RCL5	36 05	
051	RCL6	36 06	
052	×	-35	
053	÷	-24	
054	STOi	35 45	
055	GTO0	22 00	
056	*LBL7	21 07	
057	*LBL8	21 08	Ideal gas solution for n, R and T.
058	SF1	16 21 01	
059	*LBL9	21 09	
060	RCL5	36 05	
061	RCL6	36 06	
062	×	-35	
063	RCL7	36 07	
064	÷	-24	
065	RCL8	36 08	
066	÷	-24	
067	RCL9	36 09	
068	÷	-24	
069	STOi	35 45	
070	*LBL0	21 00	Stop if ideal gas is desired.
071	F0?	16 23 00	
072	RTN	24	
073	GSB1	23 01	Calculate P by Redlich-Kwong
074	GTO0	22 00	
075	*LBL2	21 02	
076	F1?	16 23 01	
077	GSB1	23 01	
078	*LBL0	21 00	
079	RCLE	36 15	
080	RCL9	36 09	
081	×	-35	
082	RCL6	36 06	
083	RCLB	36 12	
084	-	-45	
085	STO4	35 04	
086	÷	-24	
087	RCLA	36 11	
088	RCL9	36 09	
089	√X	54	
090	÷	-24	
091	STO2	35 02	
092	RCL6	36 06	
093	÷	-24	
094	LSTX	16-63	
095	RCLB	36 12	
096	+	-55	
097	STO3	35 03	
098	÷	-24	
099	-	-45	
100	RCL5	36 05	
101	-	-45	Calculate f(P).
102	GSBi	23 45	
103	÷	-24	Calculate f'(P).
104	ST-i	35-45 45	
105	RCLi	36 45	Loop again?
106	÷	-24	
107	ABS	16 31	
108	EEX	-23	
109	CHS	-22	
110	4	04	
111	X≤Y?	16-35	
112	GTO2	22 02	

REGISTERS

0	1	2 $a/T^{1/2}$	3 (V+b)	4 (V-b)	5 P	6 V	7 n	8 R	9 T
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9

A a	B b	C T_c	D P_c	E nR	I Control

97 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS
113	RCLi	36 45	Display result of iteration
114	RTN	24	
115	*LBL6	21 06	$\frac{\partial P}{\partial V}$
116	RCL6	36 06	
117	ENT↑	-21	
118	+	-55	
119	RCLB	36 12	
120	+	-55	
121	RCL2	36 02	
122	×	-35	
123	RCL3	36 03	
124	RCL6	36 06	
125	×	-35	
126	X²	53	
127	÷	-24	
128	RCLE	36 15	
129	RCL9	36 09	
130	×	-35	
131	RCL4	36 04	
132	X²	53	
133	÷	-24	
134	-	-45	
135	RTN	24	
136	*LBL9	21 09	$\frac{\partial P}{\partial T}$
137	RCLE	36 15	
138	RCL4	36 04	
139	÷	-24	
140	RCL2	36 02	
141	2	02	
142	÷	-24	
143	RCL9	36 09	
144	÷	-24	
145	RCL6	36 06	
146	÷	-24	
147	RCL3	36 03	
148	÷	-24	
149	+	-55	
150	RTN	24	
151	*LBL7	21 07	
152	*LBL8	21 08	$\frac{\partial P}{\partial n}$ or $\frac{\partial P}{\partial R}$
153	RCL9	36 09	
154	RCL6	36 06	
155	×	-35	
156	RCL4	36 04	
157	X²	53	
158	÷	-24	
159	RCL6	36 06	
160	ENT↑	-21	
161	+	-55	
162	RCLB	36 12	
163	+	-55	
164	RCLE	36 15	
165	÷	-24	
166	RCL6	36 06	
167	÷	-24	
168	RCL3	36 03	

STEP	KEY ENTRY	KEY CODE	COMMENTS
169	X²	53	
170	÷	-24	
171	RCL2	36 02	
172	×	-35	
173	-	-45	
174	RCLE	36 15	
175	×	-35	
176	RCLi	36 45	
177	÷	-24	
178	RTN	24	
179	*LBL5	21 05	Display P.
180	LSTX	16-63	
181	+	-55	
182	STO5	35 05	
183	R/S	51	
184	*LBL1	21 01	
185	RCL7	36 07	Calculate a and b.
186	RCL8	36 08	
187	×	-35	
188	STOE	35 15	
189	.	-62	
190	0	00	
191	8	08	
192	6	06	
193	7	07	
194	RCLD	36 14	
195	÷	-24	
196	X⇄Y	-41	
197	RCLC	36 13	
198	×	-35	
199	×	-35	
200	STOB	35 12	
201	LSTX	16-63	
202	×	-35	
203	RCLC	36 13	
204	√X	54	
205	×	-35	
206	4	04	
207	.	-62	
208	9	09	
209	3	03	
210	4	04	
211	×	-35	
212	STOA	35 11	
213	RTN	24	
220			

LABELS					FLAGS
A ↔P	B ↔V	C ↔n	D ↔R	E ↔T	0 R-K
a R-K?	b T_c	c P_c	d	e	1 a,b
0 Used	1 a,b	2 Iter	3	4	2
5 P	6 V	7 n	8 R	9 T	3 Calc

SET STATUS

FLAGS	ON	OFF	TRIG		DISP	
0	☐	☑	DEG	☑	FIX	☑
1	☐	☑	GRAD	☐	SCI	☐
2	☐	☑	RAD	☐	ENG	☐
3	☐	☑			n	2

Program Description I

Program Title Van der Waals Gas Law

Contributor's Name Hewlett-Packard

Address 1000 N.E. Circle Blvd.

City Corvallis **State** Oregon **Zip Code** 97330

Program Description, Equations, Variables The Van der Waals gas equation is given by $(P + \frac{a}{\bar{V}^2})(\bar{V} - b) = RT$ where $\bar{V} = \frac{V}{n}$

Pressure and temperature may be solved for directly, but n and V must be calculated from the positive root of this cubic equation in $\bar{V}$:

$$\bar{V}^3 - \bar{V}^2 (b + \frac{RT}{P}) + \bar{V}\frac{a}{p} - \frac{ab}{p} = 0$$

The program solves this equation by fast, non-iterative techniques (see 2nd reference) and V and n can then be calculated. The critical temperature, pressure, and molar volume are given by $\bar{V}c = 3b$, $Pc = \frac{a}{27b^2}$ $Tc = \frac{8a}{27bR}$

NOTE: The constant R is preprogrammed and is initially in R_3. Also subroutine e may be of some use by itself as it calculates $\sqrt[3]{x}$ for positive or negative x.

Operating Limits and Warnings Temperatures must be in °K, pressures must be in atmospheres, volumes must be in liters.

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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Program Description II

Sketch(es)

Sample Problem(s)

1) What is the temperature of .250 moles of Helium with a volume of 2.00 ℓ. and a pressure of 2.5 atm. a = .03412, b = .02370

2) What is the volume of 1.5 moles of CO_2 at 40°K and 10 atm. pressure?
a = 3.592 b = .04267

3) What are the critical temperature, critical pressure and critical molar volume of H_2 where 0 = .2444 and 6 = .2661

Solution(s)

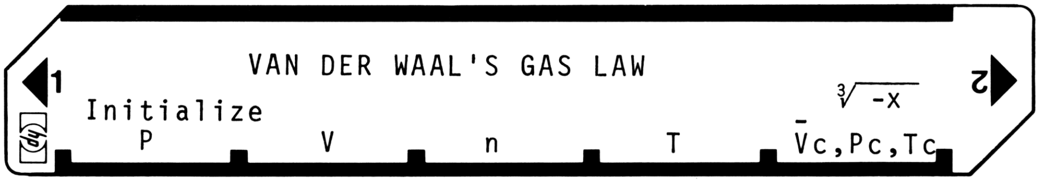
(1) .03412; ↑; .02370; [f] [A]; .25 [C] 2.00 [B] 2.5 [[]; [D] --->243.07°K
(2)3.592; ↑; .04267; [f] [A] 1.5 [C] 40 [D] 10; [A]; [B] ---------> .07 ℓ.
(3) .2444↑; .02661; [f] [A]; [E] ---------------------------->.07983 = $\bar{V}$c
12.78 atm = Pc
33.16°K = Tc

Reference(s) This program is a modification of the User's Library program #01743A submitted by Timothy McGrath.

Daniels, F., and R.A. Alberty, Physical Chemistry, 3rd edition, John Wiley and Sons, Inc., New York, 1966, pp 18-20.

Abramowitz, M. and I.A. Stegan, Handbook of Mathematical Functions, Nat'l Bureau of Standards, 1964, p 17.

User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS		OUTPUT DATA/UNITS
1.	Load side 1 and side 2				
2.	Input Van Der Waals constants a & b, &	a	ENT↑		
	initialize	b	f	A	.08
3.	Input data (any 3 of 4)				
	Pressure	P,atm.	A		P
	Volume	V, liters	B		V
	No. of Moles	n	C		n
	Temperature	T,°K	D		T
4.	Calculate Pressure		A		P,atm
5.	Calculate Volume		B		V, Liters
6.	Calculate No. of Moles		C		n, #
7.	Calculate Temperature		D		T, °K
8.	Calculate Molar Volume, $\bar{V}$c		E		$\bar{V}$c
	Critical Temperature, Tc				Tc
	Critical Pressure, Pc				Pc
9.	Optional: Calculate Molar Volume		GSB	5	$\bar{V}$
10.	Optional: To Calculate $\sqrt[3]{-x}$	x	CHS		
	i.e., cube root of a negative no.		f	E	
	NOTE: Calculations may be made in any order and repeated calculations may be made without re-entering a & b, or other values.				

97 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBLa	21 16 11	Initialize:
002	STO2	35 02	
003	R↓	-31	Store a,b & R
004	STO1	35 01	
005	.	-62	
006	0	00	
007	8	08	
008	2	02	
009	0	00	
010	5	05	
011	6	06	
012	2	02	
013	STO3	35 03	
014	RTN	24	Pressure
015	*LBLA	21 11	Data entry?
016	F3?	16 23 03	
017	GTO1	22 01	Calculate P
018	GSB5	23 05	
019	RCL3	36 03	.
020	RCLD	36 14	
021	×	-35	.
022	RCL9	36 09	.
023	RCL2	36 02	
024	-	-45	
025	÷	-24	
026	RCL1	36 01	
027	RCL9	36 09	
028	X^2	53	
029	÷	-24	
030	-	-45	
031	STOA	35 11	
032	PRTX	-14	
033	RTN	24	Store P
034	*LBL1	21 01	
035	STOA	35 11	
036	RTN	24	Volume
037	*LBLB	21 12	Date entry?
038	F3?	16 23 03	
039	GTO2	22 02	Calculate V
040	RCL2	36 02	
041	RCL1	36 01	
042	RCLA	36 11	
043	÷	-24	
044	STO5	35 05	
045	X⇄Y	-41	
046	×	-35	
047	CHS	-22	
048	STO4	35 04	
049	LSTX	16-63	
050	RCL3	36 03	
051	RCLD	36 14	
052	×	-35	
053	RCLA	36 11	
054	÷	-24	
055	+	-55	
056	CHS	-22	
057	3	03	
058	÷	-24	
059	STO0	35 00	
060	RCL5	36 05	
061	3	03	
062	÷	-24	
063	RCL0	36 00	
064	X^2	53	
065	-	-45	
066	ENT↑	-21	
067	ENT↑	-21	
068	×	-35	
069	×	-35	
070	STO7	35 07	
071	RCL5	36 05	
072	RCL0	36 00	
073	×	-35	
074	RCL4	36 04	
075	-	-45	
076	2	02	
077	÷	-24	
078	RCL0	36 00	
079	ENT↑	-21	
080	X^2	53	
081	×	-35	
082	-	-45	
083	STO8	35 08	
084	ENT↑	-21	
085	×	-35	
086	RCL7	36 07	
087	+	-55	
088	√X	54	
089	STO7	35 07	
090	RCL8	36 08	
091	+	-55	
092	GSBe	23 16 15	
093	RCL8	36 08	
094	RCL7	36 07	
095	-	-45	
096	GSBe	23 16 15	
097	+	-55	
098	RCL0	36 00	
099	-	-45	
100	RCLC	36 13	
101	X⇄Y	-41	
102	×	-35	
103	STOB	35 12	
104	PRTX	-14	
105	RTN	24	
106	*LBL2	21 02	Store V
107	STOB	35 12	
108	RTN	24	Moles
109	*LBLC	21 13	
110	F3?	16 23 03	Data entry?
111	GTO4	22 04	
112	RCLB	36 12	

REGISTERS

0	1	2	3	4	5	6	7	8	9
Used	a	b	R	Used	Used		Used	Used	$\bar{V}$
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9

A	B	C	D	E	I
P	V	n	T		

97 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS
113	RCL9	36 09	Calculate n
114	÷	-24	
115	STOC	35 13	
116	PRTX	-14	
117	RTN	24	
118	*LBL4	21 04	Store n
119	STOC	35 13	
120	RTN	24	
121	*LBLD	21 14	Temperature
122	F3?	16 23 03	Data entry?
123	GTO3	22 03	
124	GSB5	23 05	Calculate T
125	RCLA	36 11	
126	RCL1	36 01	
127	RCL9	36 09	
128	X^2	53	
129	÷	-24	
130	+	-55	
131	RCL9	36 09	
132	RCL2	36 02	
133	-	-45	
134	×	-35	
135	RCL3	36 03	
136	÷	-24	
137	STOD	35 14	
138	PRTX	-14	
139	RTN	24	
140	*LBL3	21 03	Store T
141	STOD	35 14	
142	RTN	24	
143	*LBL5	21 05	Calculate $\bar{V}$
144	RCLB	36 12	
145	RCLC	36 13	
146	÷	-24	
147	STO9	35 09	
148	RTN	24	
149	*LBLE	21 15	Calculate $\bar{V}$, Pc,
150	8	08	
151	RCL1	36 01	Tc
152	×	-35	
153	9	09	
154	÷	-24	
155	RCL3	36 03	
156	÷	-24	
157	RCL1	36 01	
158	9	09	
159	÷	-24	
160	RCL2	36 02	
161	÷	-24	
162	RCL2	36 02	
163	3	03	
164	×	-35	
165	DSP5	-63 05	
166	PRTX	-14	
167	DSP2	-63 02	
168	÷	-24	

STEP	KEY ENTRY	KEY CODE	COMMENTS
169	PRTX	-14	
170	X⇄Y	-41	
171	LSTX	16-63	
172	÷	-24	
173	PRTX	-14	
174	RTN	24	
175	*LBLe	21 16 15	
176	X<0?	16-45	Calculate
177	SF1	16 21 01	
178	ABS	16 31	$\sqrt[3]{-x}$
179	3	03	
180	1/X	52	
181	Y^x	31	
182	F1?	16 23 01	
183	CHS	-22	
184	CF1	16 22 01	
185	RTN	24	
190			
200			
210			
220			

LABELS

A P	B V	C n	D T	E $\bar{V}$c,Pc,Tc
a Initialize	b	c	d	e $\sqrt[3]{-x}$
0	1 Sto P	2 Sto V	3 Sto T	4 Sto n
5 $\bar{V}$	6	7	8	9

FLAGS

0	
1	$\sqrt[3]{-x}$
2	
3	Data Entry

SET STATUS

FLAGS	ON	OFF
0	☐	☑
1	☐	☑
2	☐	☑
3	☐	☑

TRIG	
DEG	☑
GRAD	☐
RAD	☐

DISP	
FIX	☑
SCI	☐
ENG	☐
n	2

Program Description I

Program Title Beer's Law/Absorbtivity Calculations

Contributor's Name Alan J. Rubin
Address 2577 Kenview
City Columbus **State** Ohio **Zip Code** 43209

Program Description, Equations, Variables 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 absorbtivity, a, by the least squares method:

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

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 f,D or f,C, respectively. If molecular weight has been entered (f,B), mg/l data may be converted to molar concentration via Key B.

After completing data entry, pressing R/S will display the absorbtivity for 5 seconds followed by the error intercept of A, 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 memories (initialize).

Operating Limits and Warnings Unless b is 1 cm, then a new value must be entered (f,A) each time the program is initialized. Initialization also removes 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. Primary registers 0 through 9 are unused. Only side 1 of the program card needs to be loaded (side 2 can be used to retain the reduced data).

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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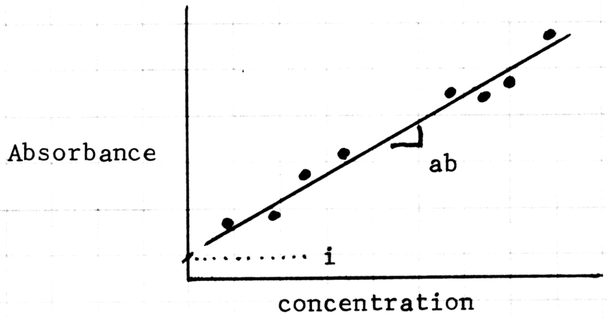
Program Description II

Sketch(es)



BEER'S LAW PLOT

A = abC

Sample Problem(s)

Calculate the molar absorbtivity for phosphate as determined by the "ascorbic acid" method at 880 nm.

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

Light path was 1.2 cm.

data

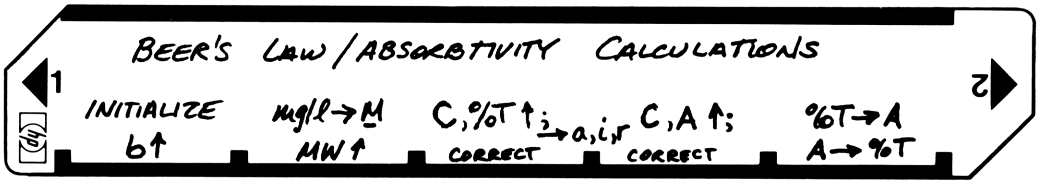
	%T	mg/l as P
a)	97.9	0
b)	58.0	0.25
c)	37.2	0.50
d)	23.1	0.75
e)	14.5	1.00
f)	9.0	1.25

Solution(s)

1. Read program and initialize: A ⟶	1.0
2. Enter light path: 1.2 f,A ⟶	1.2
3. Enter molecular weight: 31 f,B ⟶	31.0
4. Enter data:	
a) 0↑ , 97.9 C ⟶	1.
b) .25 B ⟶ 8.06×10^{-6} , 58 C ⟶	2.
continue as above	n_i
f) 1.25 B ⟶ 4.03×10^{-5}, 9 C ⟶	6.
5. Obtain a, i, r : R/S ⟶ 21245, 0.0187, 0.9998	answers

Reference(s)

User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS		OUTPUT DATA/UNITS
1	Load side 1				0.0000
2	Initialize (clears all reg., sets b = 1)		A		1.0
3	(optional) enter light bath if b ≠ 1	b	f	A	b
4	(optional) enter molecular weight	MW	f	B	MW
5	Enter molar conc. and absorbance	C_i, A_i	↑	D	n_i
	or				
5	Enter mg/l and absorbance	C_i, A_i	↑	D	n_i
	or				
5	Enter mg/l concentration	mg/l_i	B		$\underline{M}_i$
	Enter absorbance	A_i	D		n_i
	or				
5	Enter molar conc. and percent transmittance	C_i, $\%T_i$	↑	C	n_i
	or				
5	Enter mg/l and percent transmittance	C_i, $\%T_i$	↑	C	n_i
	or				
5	Enter mg/l conc.	mg/l_i	B		$\underline{M}_i$
	Enter percent transmittance	$\%T_i$	C		n_i
6	Continue data entry				n
	or correct an entry	C_k, A_k	↑	d	n-1
	or correct an entry	C_k, $\%T_k$	↑	c	n-1
7	Display absorbtivity, intercept and				
	correlation coefficient		R/S		a
					i
					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	MW	f	B	MW
	from mg/l values	mg/l	B		$\underline{M}$
	To calculate A from %T	%T	E		A
	To calculate %T from A	A	f	e	%T

67 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001	f LBL A	31 25 11	INITIALIZE Clear all reg. Set b=1
	f CL REG	31 43	
	f P⇄S	31 42	
	f CL REG	31 43	
	1	01	
	STO A	33 11	
	f FIX	31 23	
	DSP 1	23 01	
	h RTN	35 22	
010	g LBL a	32 25 11	ENTER b
	STO A	33 11	
	h RTN	35 22	
	f LBL B	31 25 12	mg/l → $\underline{M}$
	RCL B	34 12	
	÷	81	
	EEX	43	
	3	03	
	÷	81	
	DSP 2	23 02	
020	g SCI	32 23	
	h RTN	35 22	
	g LBL b	32 25 12	ENTER MW
	STO B	33 12	
	h RTN	35 22	
	f LBL D	31 25 14	ENTER C_i, A_i
	Σ+	21	
	f FIX	31 23	
	DSP 0	23 00	
	R/S	84	
030	GTO 1	22 01	→ a, i, r
	g LBL d	32 25 14	CORRECT C_i, A_i
	h Σ-	35 21	
	R/S	84	
	GTO 1	22 01	→ a, i, r
	f LBL C	31 25 13	ENTER C_i, $\%T_i$
	f GSB E	31 22 15	
	Σ+	21	
	f FIX	31 23	
	DSP 0	23 00	
040	R/S	84	
	GTO 1	22 01	→ a, i, r
	g LBL c	32 25 13	CORRECT C_i, $\%T_i$
	f GSB E	31 22 15	
	h Σ-	35 21	
	R/S	84	
	GTO 1	22 01	→ a, i, r
	f LBL E	31 25 15	ENTER %T
	f LOG	31 53	
	2	02	
050	−	51	
	CHS	42	
	f FIX	31 23	
	DSP 4	23 04	
	h RTN	35 22	→ A
	g LBL e	32 25 15	ENTER A
	2	02	
	−	51	
	CHS	42	
	g 10^x	32 53	
060	f FIX	31 23	
	DSP 1	23 01	
	h RTN	35 22	→ %T
	f LBL 1	31 25 01	CALCULATE absorbtivity intercept Correlation Coef.
	f P⇄S	31 42	
	RCL 9	34 09	
	RCL 8	34 08	
	×	71	
	RCL 4	34 04	
	RCL 6	34 06	
070	×	71	
	−	51	
	STO C	33 13	
	RCL 9	34 09	
	RCL 7	34 07	
	×	71	
	RCL 6	34 06	
	g x^2	32 54	
	−	51	
	STO D	33 14	
080	÷	81	
	RCL A	34 11	
	÷	81	
	f FIX	31 23	
	DSP 0	23 00	
	f -x-	31 84	DISPLAY a
	RCL 7	34 07	
	RCL 4	34 04	
	×	71	
	RCL 6	34 06	
090	RCL 8	34 08	
	×	71	
	−	51	
	RCL D	34 14	
	÷	81	
	DSP 4	23 04	
	f -x-	31 84	DISPLAY i
	RCL C	34 13	
	RCL D	34 14	
	f $\sqrt{x}$	31 54	
100	÷	81	
	RCL 9	34 09	
	RCL 5	34 05	
	×	71	
	RCL 4	34 04	
	g x^2	32 54	
	−	51	
	f $\sqrt{x}$	31 54	
	÷	81	DISPLAY r
	f P⇄S	31 42	
110	R/S	84	
	GTO 1	22 01	
	h RTN	35 22	DISPLAY a, i, r AGAIN

REGISTERS

0	1	2	3	4	5	6	7	8	9

S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
				ΣA	ΣA^2	ΣC	ΣC^2	ΣAC	n

A	B	C	D	E	I
b	MW	$n\Sigma AC - \Sigma A \Sigma C$	$n\Sigma C^2 - (\Sigma C)^2$		

67 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
				170			
120							
				180			
130							
				190			
140							
				200			
150							
				210			
160							
				220			

LABELS					FLAGS
A INITIALIZE	B mg/l → M	C C, %T ↑	D C, A ↑	E %T → A	0
a b ↑	b MW ↑	c −C, −%T	d −c, −%T	e A → %T	1
0	1 → a, i, r	2	3	4	2
5	6	7	8	9	3

SET STATUS

FLAGS			TRIG		DISP	
	ON	OFF				
0	☐	☑	DEG	☐	FIX	☑
1	☐	☑	GRAD	☐	SCI	☐
2	☐	☑	RAD	☐	ENG	☐
3	☐	☑			n	4

Program Description I

Program Title Activity Coefficients from Potentiometric Data

Contributor's Name John R. Joyce

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City Tulsa **State** Oklahoma **Zip Code** 74112

Program Description, Equations, Variables

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

$A = 0.059156\, \nu / n$

$B = 0.059156 / n$

E = measured EMF's in volts (V)

E_{REF} = E.M.F. of reference electrode

n = number of electrons invovled in the reaction

$f = (\nu_+^{\nu+} \nu_-^{\nu-})$ e.g. for $CaCl_2$: $\nu_+ = 1$; $\nu_- = 2$; $\nu=3$, $f=4$ $f=[2^2 \cdot 1^1]=4$

ν = Total number of ions

Operating Limits and Warnings Program must be reinitialized for each case (e.g., push START, [C]) 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.

This program has been verified only with respect to the numerical example given in *Program Description II*. User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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Program Description II

Sketch(es)

Sample Problem(s) For the following data determine the Standard Electrode Potential and the activity coefficient at each point.

Concentration (M)	Potential (V)
0.003215	0.52053
0.004488	0.50384
0.005619	0.49257
0.007311	0.47948
0.009138	0.46860
0.011195	0.45861

F = 1

ν = 2

E_{REF} = 0.000

n = 1

$$\mathrm{Pt\ (s)}\ \Big|\ \mathrm{H_2}\ \Big|\ \mathrm{H^+\ Cl^-\ (m)}\ \Big|\ \mathrm{AgCl}\ \Big|\ \mathrm{Ag\ (s)}$$

Solution(s)

```
         Keystrokes:  [C] 1[R/S] 2[R/S] 0[R/S] 1[R/S] --> 1
.003215[ENTER] .52053[A] .004488[ENTER] .50384[A]     --> 2
.005619[ENTER] .49257[A] .007311[ENTER] .47948[A]     --> 4
.0091384[ENTER] .46860[A] .011195[ENTER] .45861[A]    --> 6
[D]                                                   -->  .9334    (r^2)
                                                      -->  .2224    (S.E.P.)
.007311[ENTER] .47948[E]                              -->  .0073    (M)
                                                      -->  .9188    (γ)
```

Literature value (REF 2) for S.E.P. is 0.2225.

Reference(s) 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 (10-142)-(10-144), University of Tulsa, 1974.

User Instructions

STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS	OUTPUT DATA/UNITS
1.	Load sides 1 and 2.			
2.	Initialize program		c	
		f	R/S	f
		ν	R/S	ν
		E_{REF}	R/S	E_{REF}(V)
		n	R/S	n
3.	Input x value (molarity-M).	M_i	ENTER	M_i
4.	Input y value (electrode potential-V).	V_i	A	i+1
5.	Repeat steps 3 and 4 for all pairs.*			
6.	Compute coefficient of determination and the standard electrode potential.		D	V
7.	Input molarity	M	ENTER	M
8.	Input electrode potential	V	E	M, γ
9.	To insert additional data points repeat step 3-6			
10.	For a new case go to step 2.			
	* A set of data pairs may be deleted by entering them as in steps 3-4 and pressing [B].			

97 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBLA	21 11	Inserts data pairs
002	GSB1	23 01	
003	Σ+	56	
004	RTN	24	
005	*LBLB	21 12	Deletes data pairs
006	GSB1	23 01	
007	Σ-	16 56	
008	RTN	24	
009	*LBLC	21 13	Initializes program and stores physical parameters.
010	CLRG	16-53	
011	P⇄S	16-51	
012	CLRG	16-53	
013	R/S	51	
014	STOA	35 11	F
015	R/S	51	
016	STOB	35 12	ν
017	R/S	51	
018	STOC	35 13	E_{REF}
019	R/S	51	
020	STOD	35 14	#e⁻
021	RTN	24	
022	*LBLD	21 14	Calculates coefficient of determination and standard electrode potential.
023	P⇄S	16-51	
024	RCL8	36 08	
025	RCL6	36 06	
026	RCL4	36 04	
027	×	-35	
028	RCL9	36 09	
029	÷	-24	
030	-	-45	
031	X^2	53	
032	RCL4	36 04	
033	X^2	53	
034	RCL9	36 09	
035	÷	-24	
036	CHS	-22	
037	RCL5	36 05	
038	+	-55	
039	÷	-24	
040	RCL6	36 06	
041	X^2	53	
042	RCL9	36 09	
043	÷	-24	
044	CHS	-22	
045	RCL7	36 07	
046	+	-55	
047	÷	-24	
048	PRTX	-14	Coefficient of determination
049	RCL5	36 05	
050	RCL6	36 06	
051	×	-35	
052	RCL4	36 04	
053	RCL8	36 08	
054	×	-35	
055	-	-45	
056	RCL9	36 09	
057	RCL5	36 05	
058	×	-35	
059	RCL4	36 04	
060	X^2	53	
061	-	-45	
062	÷	-24	
063	STOE	35 15	S.E.P.
064	P⇄S	16-51	Standard Electrode potential. Computes activity coefficient.
065	RTN	24	
066	*LBLE	21 15	
067	STO2	35 02	
068	R↓	-31	
069	STO1	35 01	
070	RCLE	36 15	
071	RCLC	36 13	
072	-	-45	
073	RCL2	36 02	
074	-	-45	
075	GSB2	23 02	
076	RCL1	36 01	
077	LOG	16 32	
078	×	-35	
079	-	-45	
080	GSB2	23 02	
081	RCLB	36 12	
082	÷	-24	
083	RCLA	36 11	
084	LOG	16 32	
085	×	-35	
086	-	-45	
087	GSB2	23 02	
088	÷	-24	
089	10^x	16 33	
090	RCL1	36 01	
091	PRTX	-14	Molarity
092	X⇄Y	-41	
093	PRTX	-14	Activity coefficient
094	RTN	24	
095	*LBL1	21 01	
096	STO2	35 02	Stores molarity and potential values then operates on the potential value converting it to a form satisfactory for a least-squares fit.
097	STO3	35 03	
098	R↓	-31	
099	STO1	35 01	
100	RCLC	36 13	
101	ST+3	35-55 03	
102	GSB2	23 02	
103	RCL1	36 01	
104	LOG	16 32	
105	×	-35	
106	ST+3	35-55 03	
107	GSB2	23 02	
108	RCLB	36 12	
109	÷	-24	
110	RCLA	36 11	
111	LOG	16 32	
112	×	-35	

REGISTERS

0	1 M	2 V	3 γ	4	5	6	7	8	9
S0	S1	S2	S3	S4 Σ M	S5 Σ M^2	S6 Σ y	S7 Σ y^2	S8 Σ My	S9 n

A f	B ν	C Ref.Electrode(ν)	D #e⁻	E S.E.P.	I

97 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS
113	ST+3	35-55 03	
114	.	-62	
115	0	00	
116	6	06	
117	0	00	
118	2	02	
119	RCL1	36 01	
120	√X	54	
121	x	-35	
122	ST-3	35-45 03	
123	RCL3	36 03	
124	RCL1	36 01	
125	RTN	24	
126	*LBL2	21 02	
127	.	-62	
128	0	00	
129	5	05	
130	9	09	
131	1	01	
132	5	05	
133	6	06	
134	RCLB	36 12	
135	x	-35	
136	RCLD	36 14	
137	÷	-24	
138	RTN	24	
140			
150			
160			
170			
180			
190			
200			
210			
220			

LABELS

A M↑V(+)	B M↑V(-)	C START	D → S.E.P.	E M↑V→α
a	b	c	d	e
0	1 USED	2 A	3	4
5	6	7	8	9

FLAGS

0
1
2
3

SET STATUS

FLAGS	ON	OFF
0	☐	☑
1	☐	☑
2	☐	☑
3	☐	☑

TRIG	
DEG	☑
GRAD	☐
RAD	☐

DISP	
FIX	☑
SCI	☐
ENG	☐
n	4

Program Description I

Program Title Crystallographic to cartesian coordinate tranformations

Contributor's Name Craig G. Shaefer

Address 1335 Louisiana

City Lawrence **State** Kansas **Zip Code** 66044

Program Description, Equations, Variables 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:

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

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

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

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

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

$$D_{ij} = \left[(x_1 - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2\right]^{1/2}$$

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

variables:

a, b, c = length of oblique axes

α, β, γ = 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

θ_{1-2-3} = angle between points

Operating Limits and Warnings One of the distances, D_{ij}, must be calculated before calculating the angle between three points. Input a, b, c before α, β, γ.

This program has been verified only with respect to the numerical example given in *Program Description II*. User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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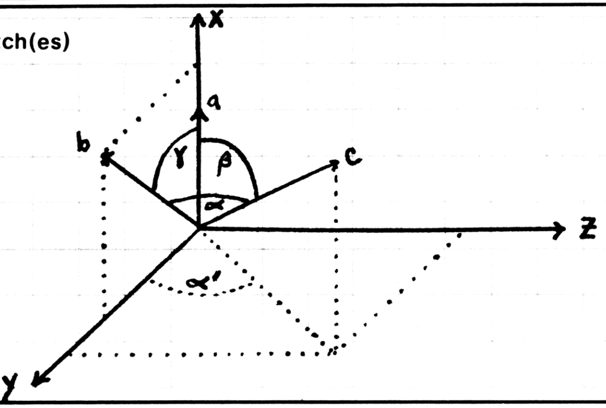
Program Description II

Sketch(es)



a, b, c = crystallographic (oblique) axes
x, y, z = cartesian axes
α, β, γ = angles between crystallographic axes

Sample Problem(s) Suppose one has a monoclinic crystal with unit cell dimensions:

a = 11.716 Å		α = 90.00°
b = 8.102 Å		β = 106.14°
c = 11.166 Å		γ = 90.00°

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

N_2	0.508	0.259	0.170
C_1	0.585	0.410	0.189
C_3	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?

Solution(s) 1.) 11.716 ↑ 8.102 ↑ 11.166 [A] → 0.000

2.) 90.00 ↑ 106.14 ↑ 90.00 [f] [A] → 0.000

3.) 0.585 ↑ 0.410 ↑ 0.189 [B] → 6.267 x_1, 3.322 y_1, 2.027 z_1, 1.000 atom #1

4.) 0.508 ↑ 0.259 ↑ 0.170 [C] → 5.424 x_2, 2.098 y_2, 1.823 z_2, 2.000 atom #2

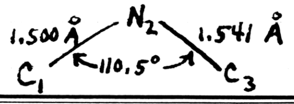
5.) 0.430 ↑ 0.249 ↑ 0.034 [D] → 4.932 x_3, 2.017 y_3, 0.365 z_3, 3.000 atom #3

~~Reference(s)~~ 6.) 12 [f] [D] → 1.500 Distance from atoms 1 to 2

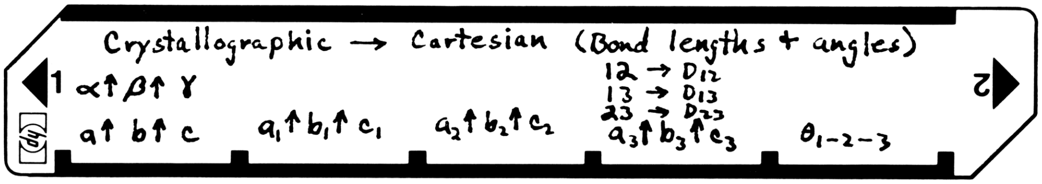
[RCL B] → 1.541 Distance from atoms 2 to 3

[RCL C] → 2.499 Distance from atoms 1 to 3

7.) [E] → 110.536 Angle from 1-2-3



User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS		OUTPUT DATA/UNITS
1	Load side 1 and side 2.				
2	Input lengths of oblique axes	a	↑		
		b	↑		
		c	A		0.000
3	Input angles between oblique axes	α	↑		
		β	↑		
		γ	f	A	0.000
4	Input coordinates of point #1	a_1	↑		
		b_1	↑		
		c_1	B		$X_1, Y_1, Z_1, 1.0$
5	Input coordinates of point #2	a_2	↑		
		b_2	↑		
		c_2	C		$X_2, Y_2, Z_2, 2.0$
6	Input coordinates of point #3	a_3	↑		
		b_3	↑		
		c_3	D		$X_3, Y_3, Z_3, 3.0$
7	Calculate distance between points i and j	ij	f	D	D_{ij}
	Note: The other two distances are also calculated and may be recalled from the appropriate register				
	RCL A → D_{12}				
	RCL B → D_{23}				
	RCL C → D_{13}				
8	Calculate angle from 1 to 2 to 3		E		θ_{1-2-3}
9	For new point to replace old one, go to step 4, 5, or 6 to replace the appropriate point.				
10	For new crystallographic system, go to step 2.				
	Note: Step 7 must be performed before step 8.				

67 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBL A	31 25 11	store a, b, c
	STO 7	33 07	
	STO 8	33 08	
	STO 9	33 09	
	R↓	35 53	
	STO 4	33 04	
	STO 5	33 05	
	R↓	35 53	
	STO 1	33 01	
010	CLX	44	
	RTN	35 22	
	*LBL a	32 25 11	store α, β, γ
	STO C	33 13	
	R↓	35 53	calculate
	STO B	33 12	transformation
	R↓	35 53	matrix
	COS	31 63	
	STO A	33 11	$\cos\alpha$
	RCL C	34 13	γ
020	COS	31 63	
	STO D	33 14	$\cos\gamma$
	STO×4	33 71 04	
	RCL C	34 13	
	SIN	31 62	
	STO E	33 15	$\sin\gamma$
	STO×5	33 71 05	
	RCL B	34 12	
	COS	31 63	
	STO 0	33 00	$\cos\beta$
030	STO×7	33 71 07	
	RCL B	34 12	
	SIN	31 62	$\sin\beta$
	STO×8	33 71 08	
	STO×9	33 71 09	
	RCL E	34 15	$\sin\gamma$
	×	71	$\sin\gamma\sin\beta$
	RCL D	34 14	$\cos\gamma$
	RCL 0	34 60	$\cos\beta$
	×	71	$\cos\gamma\cos\beta$
040	RCL A	34 11	
	X⇄Y	35 52	
	−	51	
	X⇄Y	35 52	$\dfrac{\cos\alpha - \cos\gamma\cos\beta}{\sin\gamma\sin\beta}$
	÷	81	
	STO×8	33 71 08	
	COS^{-1}	32 63	
	SIN	31 62	$\sin\alpha'$
	STO×9	33 71 09	
	CLX	44	
050	RTN	35 22	
	*LBL B	31 25 12	$a_i\ b_i\ c_i \rightarrow x_i\ y_i\ z_i$
	1	01	
	1	01	$i=1$
	STO E	33 15	
	R↓	35 53	
	GSB 0	31 22 00	

STEP	KEY ENTRY	KEY CODE	COMMENTS
	1	01	
	RTN	35 22	
	*LBL C	31 25 13	$i=2$
060	1	01	
	4	04	
	STO E	33 15	
	R↓	35 53	
	GSB 0	31 22 00	
	2	02	
	RTN	35 22	
	*LBL D	31 25 14	$i=3$
	1	01	
	7	07	
070	STO E	33 15	
	R↓	35 53	
	GSB 0	31 22 00	
	3	03	
	RTN	35 22	
	*LBL 0	31 25 00	store $a_i\ b_i\ c_i$
	STO B	33 12	
	R↓	35 53	
	STO A	33 11	
	R↓	35 53	
080	STO 0	33 00	
	1	01	
	STO I	35 33	
	GSB 1	31 22 01	
	2	02	
	STO I	35 33	
	GSB 1	31 22 01	
	3	03	
	STO I	35 33	
	GSB 1	31 22 01	
090	RTN	35 22	
	*LBL 1	31 25 01	multiply oblique
	0	00	coordinate by
	RCL 0	34 00	matrix element
	GSB 2	31 22 02	and add
	RCL A	34 11	
	GSB 2	31 22 02	
	RCL B	34 12	
	GSB 2	31 22 02	
	PSE	35 72	display rectangular
100	RCL E	34 15	coordinate
	X⇄I	35 24	
	R↓	35 53	store cartesian
	STO(i)	33 24	coordinates
	ISZ	31 34	
	R↑	35 54	
	X⇄I	35 24	
	STO E	33 15	
	RTN	35 22	
	*LBL 2	31 25 02	perform matrix
110	RCL(i)	34 24	multiplication
	×	71	
	+	61	

REGISTERS

0 USED	1 a	2 0	3 0	4 $b\cos\gamma$	5 $b\sin\gamma$	6 0	7 $c\cos\beta$	8 $c\sin\beta\cos\alpha'$	9 $c\sin\beta\sin\alpha'$
S0	S1 x_1	S2 y_1	S3 z_1	S4 x_2	S5 y_2	S6 z_2	S7 x_3	S8 y_3	S9 z_3

A D_{12}	B D_{23}	C D_{13}	D USED	E USED	I USED

67 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
	ISZ	31 34			ISZ	31 34	
	ISZ	31 34		170	RTN	35 22	
	ISZ	31 34			★ LBL 7	31 25 07	subtract 6 from I
	RTN	35 22			RCL I	35 34	
	★ LBL d	32 25 14	calculate distances between points		6	06	
	STO 0	33 00			−	51	
	1	01			STO I	35 33	
120	1	01			R↓	35 53	
	STO I	35 33			RTN	35 22	
	0	00			★ LBL 9	31 25 09	which distance should be displayed?
	GSB 3	31 22 03	$(x_i - x_j)^2$ +		1	01	
	GSB 3	31 22 03	$(y_i - y_j)^2$ +	180	2	02	
	GSB 3	31 22 03	$(z_i - z_j)^2$		RCL 0	34 00	
	$\sqrt{x}$	31 54			x=y?	32 51	
	STO A	33 11	D_{12}		GTO 1	22 01	
	0	00			1	01	
	GSB 3	31 22 03			3	03	
130	GSB 3	31 22 03			x=y?	32 51	
	GSB 3	31 22 03			GTO 3	22 03	
	$\sqrt{x}$	31 54			RCL B	34 12	D_{23}
	STO B	33 12	D_{23}		RTN	35 22	
	0	00		190	★ LBL 3	31 25 03	
	GSB 4	31 22 04			RCL C	34 13	D_{13}
	GSB 4	31 22 04			RTN	35 22	
	GSB 4	31 22 04			★ LBL 1	31 25 01	
	$\sqrt{x}$	31 54			RCL A	34 11	D_{12}
	STO C	33 13	D_{13}		RTN	35 22	
140	GTO 9	22 09			★ LBL E	31 25 15	calculate angle from 1−2−3
	★ LBL 3	31 25 03	$(x_i - x_j)^2$		P⇄S	31 42	
	RCL (i)	34 24			0	00	
	GSB 5	31 22 05	ISZ, ISZ, ISZ		STO I	35 33	
	RCL (i)	34 24		200	GSB e	32 22 15	$(x_1 - x_2)(x_3 - x_2)$ +
	−	51			GSB e	32 22 15	$(y_1 - y_2)(y_3 - y_2)$ +
	x^2	32 54			GSB e	32 22 15	$(z_1 - z_2)(z_3 - z_2)$
	+	61			RCL A	34 11	D_{12}
	DSZ	31 33			÷	81	
	DSZ	31 33			RCL B	34 12	D_{23}
150	RTN	35 22			÷	81	
	★ LBL 4	31 25 04	D_{13}		$\cos^{-1}$	32 63	θ_{1-2-3}
	RCL (i)	34 24			P⇄S	31 42	
	GSB 7	31 22 07	add −6 to I		RTN	35 22	
	RCL (i)	34 24		210	★ LBL e	32 25 15	
	−	51			ISZ	31 34	
	x^2	32 54			RCL (i)	34 24	
	ISZ	31 34			GSB 5	31 22 05	ISZ, ISZ, ISZ
	ISZ	31 34			RCL (i)	34 24	
	ISZ	31 34			STO E	33 15	
160	ISZ	31 34			−	51	
	ISZ	31 34			GSB 5	31 22 05	
	ISZ	31 34			RCL (i)	34 24	
	+	61			RCL E	34 15	
	ISZ	31 34		220	−	51	
	RTN	35 22			×	71	
	★ LBL 5	31 25 05	add 3 to I		+	61	
	ISZ	31 34			GSB 7	31 22 07	subtract 6 from I
	ISZ	31 34			RTN	35 22	

LABELS

A $a \uparrow b \uparrow c$	B $a_1 \uparrow b_1 \uparrow c_1$	C $a_2 \uparrow b_2 \uparrow c_2$	D $a_3 \uparrow b_3 \uparrow c_3$	E θ_{1-2-3}
a $\alpha \uparrow \beta \uparrow \gamma$	b	c	d D_{ij}	e dot product
0 store $a_i b_i c_i$	1 store cartesian coor.	2 matrix multiplication	3 $(x_i - x_j)^2$	4 D_{13}
5 I+3=I	6	7 I−6=I	8	9 which distance?

FLAGS

0
1
2
3

SET STATUS

FLAGS	ON	OFF	TRIG		DISP	
0	☐	☒	DEG	☒	FIX	☒
1	☐	☒	GRAD	☐	SCI	☐
2	☐	☒	RAD	☐	ENG	☐
3	☐	☒			n	3

Program Description I

Program Title Kinetics using Lineweaver-Burk or Hofstee plots

Contributor's Name R. Martin Bartholow
Address 1904 New Hampshire
City Lawrence **State** Ks **Zip Code** 66044

Program Description, Equations, Variables 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

$$\frac{1}{v} = \frac{Km}{Vmax} \cdot \frac{1}{S} + \frac{1}{Vmax} \quad (1) \qquad v = -Km \cdot \frac{v}{S} + Vmax \quad (2)$$

and the coefficient of determination are determined by use of the formulas in the curve fitting program. Since b = Km/Vmax and a = 1/Vmax for the Lineweaver-Burk method and b = -Km and a = Vmax for the Hofstee method, the desired constants Km and Vmax 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 Vmax' and Km' can be determined. Ki may be calculated from:

$$Km' = Km(1 - [i]/Ki)$$

Operating Limits and Warnings 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 page two.

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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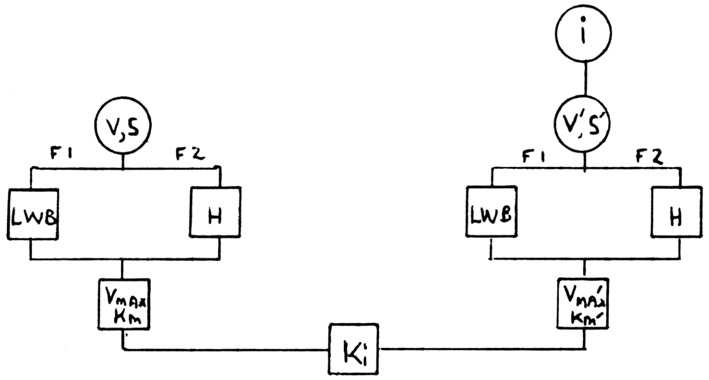
Program Description II

Sketch(es)



Sample Problem(s) The following data on product formation at various substrate concentrations was determined in the presence and absence of a competitive inhibitor. Determine the Km and Vmax for product formation with and without the inhibitor. What is the Ki?

Substrate concentration (mM)	1.0	2.0	3.0	10.0	15.0
Product formed (μM/hr) (no inhibitor)	40	69	88	160	185
Product formed (μM/hr) (6mM inhibitor)	24	44	60	126	158

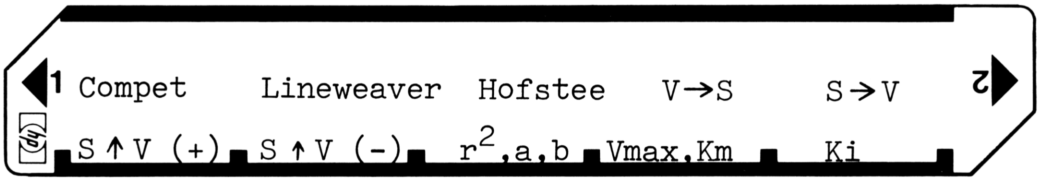
Solution(s)

$\boxed{\text{Dsp}}$ 4 $\boxed{\text{f}}\boxed{\text{B}}$	1.0000
40 $\boxed{\text{A}}$ 69 $\boxed{\text{A}}$ 88 $\boxed{\text{A}}$ 10 $\boxed{\uparrow}$ 160 $\boxed{\text{A}}$ 15 $\boxed{\uparrow}$ 185 $\boxed{\text{A}}$	6.0000
$\boxed{\text{C}}$	.9996 (r^2), .0042 (a), .0209 (b)
$\boxed{\text{D}}$	240.8340 (Vmax), 5.0275 (Km)
6.00 $\boxed{\text{f}}\boxed{\text{A}}$	1.0000
24 $\boxed{\text{A}}$ 44 $\boxed{\text{A}}$ 60 $\boxed{\text{A}}$ 10 $\boxed{\uparrow}$ 126 $\boxed{\text{A}}$ 15 $\boxed{\uparrow}$ 158 $\boxed{\text{A}}$	6.0000
$\boxed{\text{C}}$	.9999 (r^2), .0040 (a), .0377 (b)
$\boxed{\text{D}}$	249.7286 (Vmax'), 9.4028 (Km')
$\boxed{\text{E}}$	6.8943 (Ki)

Reference(s)

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, J. Biol. Chem., 240, 863 (1965).

User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS		OUTPUT DATA/UNITS
1	Load side 1 and side 2				0.00
2	Select type of analysis				
	a) Lineweaver-burk		f	B	1.00
	b) Hofstee		f	C	1.00
3	Input substrate concentration * **	S	Enter		S
4	Input velocity	V		A	n + 1
5	repeat steps 3 and 4 for all data pairs				
6	compute and output coefficient of				
	determination (r^2) and of the line:				
	a and b			C	r^2,a,b
7	optional: project substrate				
	concentration from a velocity	V	f	D	$\hat{S}$
8	optional: project velocity from a				
	substrate concentration	S	f	E	$\hat{V}$
9	compute and output Vmax and Km			D	Vmax,Km
10	Optional: if competitive inhibition				
	data is available, the competitive				
	mode may be selected				
	a) input inhibitor concentration * **	i	f	A	1.00
	b) input substrate concentration	S	Enter		S
	c) input velocity	V		A	n + 1
	d) repeat steps 10b and 10c for all				
	data pairs				
	e) compute and output coefficient of				
	determination (r^2) and of the line:				
	a and b			C	r^2,a,b
	f) compute Vmax' and Km'			D	Vmax',Km'
	g) compute Ki			E	Ki

* This step may be skipped if the substrate equals the display counter.

** The last set of data pairs may be deleted by pressing $\boxed{h}\boxed{R\downarrow}$ then $\boxed{B}$.
A set of data may be deleted by entering the set as in steps 3 and 4 and pressing $\boxed{B}$.

67 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*Lbl b	32 25 12	LINEWEAVER-BURK		*Lbl d	32 25 14	PROJECT V → S
	CF 0	35 61 00	Set flag 1 and		STO A	33 11	
	SF 1	35 51 01	clear secondary		P‹›S	31 42	
	P‹›S	31 42	register	060	Rcl 2	34 02	
	Cl Reg	31 43			1/X	35 62	
	P‹›S	31 42			Rcl 1	34 01	
	1	01			Rcl A	34 11	
	Rtn	35 22			F? 1	35 71 01	
	*Lbl c	32 25 13	HOFSTEE		1/X	35 62	
010	CF 1	35 61 01	Set flag 0 and		X‹›Y	35 52	
	SF 0	35 51 00	clear secondary		-	51	
	P‹›S	31 41	register		x	71	
	Cl Reg	31 43			F? 1	35 71 01	
	P‹›S	31 41		070	1/X	35 62	
	1	01			P‹›S	31 42	
	Rtn	35 22			Rtn	35 22	
	*Lbl A	35 25 11	SUMMATION		*Lbl e	32 25 15	PROJECT S → V
	CF 3	35 61 03	clear Σ- flag		STO A	33 11	
	*Lbl 8	31 25 08			P‹›S	31 42	
020	F? 1	35 71 01	if flag 1 then		Rcl 1	34 01	
	1/X	35 62	reciprocal		Rcl 2	34 02	
	STO D	33 14			Rcl A	34 11	
	X‹›Y	35 52			F? 1	35 71 01	
	F? 1	35 71 01	if flag 1 then	080	1/X	35 62	
	1/X	35 62	reciprocal		x	71	
	F? 0	35 71 00	if flag 0 then		+	61	
	GTO 9	22 09	go to label 9,		F? 1	35 71 01	
	STO C	33 13	returning by lbl2		1/X	35 62	
	*Lbl 2	31 25 02			P‹›S	31 42	
030	F? 3	35 71 03	if flag 3 then Σ-		Rtn	35 22	
	GTO 0	22 00			*Lbl C	31 25 13	COMPUTE b
	Σ+	21	compute sums		P‹›S	31 42	
	*Lbl 7	31 25 07			Rcl 8	34 08	
	Ent	41		090	Rcl 4	34 04	
	1	01	calculate n+1		Rcl 6	34 06	
	+	61			x	71	
	Rcl C	34 13			Rcl 9	34 09	
	X‹›Y	35 52			÷	81	
	Rcl D	34 14			-	51	
040	X‹›Y	35 52			Ent↑	41	
	Rtn	35 22			Ent↑	41	
	*Lbl B	31 25 12	DELETION		Rcl 4	34 04	
	SF 3	35 51 03	set flag 3		X^2	32 54	
	1	01		100	Rcl 9	34 09	
	CHS	42			÷	81	
	↓	35 53			Rcl 5	34 05	
	GTO 8	22 08			X‹›Y	35 52	
	*Lbl 9	31 25 09	COMPUTE V/S FOR		-	51	
	÷	81	HOFSTEE		÷	81	
050	STO C	33 13			STO 2	33 02	
	Rcl D	34 14			x	71	COMPUTE r^2
	X‹›Y	35 52			Rcl 6	34 06	
	GTO 2	22 02			x^2	32 54	
	*Lbl 0	31 25 00	Σ -	110	Rcl 9	34 09	
	Σ-	35 21			÷	81	
	GTO 7	22 07			CHS	42	

REGISTERS

0 Vmax	1 a'	2 b'	3 Km'	4 $\Sigma x'$	5 $\Sigma x^{2}{}'$	6 $\Sigma y'$	7 $\Sigma y^{2}{}'$	8 $\Sigma xy'$	9 n'
S0 Vmax	S1 a	S2 b	S3 Km	S4 Σx	S5 Σx^2	S6 Σy	S7 Σy^2	S8 Σxy	S9 n
A used	B	C used	D used	E Ki	I [i]				

67 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS
	Rcl 7	34 07	
	+	61	
	÷	81	
	Pause	35 72	
	Rcl 6	34 06	COMPUTE a
	Rcl 4	34 04	
	Rcl 2	34 02	
120	x	71	
	-	51	
	Rcl 9	34 09	
	÷	81	
	STO 1	33 01	
	Pause	35 72	
	Rcl 2	34 02	
	P<>S	31 42	
	Rtn	35 22	
	*Lbl D	31 25 14	TRANSFORM a AND
130	P<>S	31 42	b TO Vmax AND
	Rcl 1	34 01	Km
	F? 1	35 71 01	if flag 1 then
	1/X	35 62	reciprocal,
	STO 0	33 00	otherwise y-
	Pause	35 72	intercept is Vmax
	Rcl 2	34 02	
	F? 1	35 71 01	if flag 1 then
	GTO 4	22 04	label 4
	CHS	42	otherwise
140	STO 3	33 03	Km = -slope (b)
	Pause	35 72	
	Rtn	35 22	
	*Lbl 4	31 25 04	Km for lineweaver
	Rcl 1	34 01	burk method
	÷	81	
	STO 3	33 03	
	Pause	35 72	
	P<>S	31 42	
	Rtn	35 22	
150	*Lbl a	32 25 11	COMPETITIVE
	Cl Reg	31 43	INHIBITOR
	P<>S	31 42	positions
	ST i	35 33	primary register
	1	01	and stores [i]
	Rtn	35 22	
	*Lbl E	31 25 15	COMPUTE Ki
	P<>S	31 42	
	Rcl i	35 34	
	Rcl 3	34 03	
160	P<>S	31 42	Km recalled from
	Rcl 3	34 03	secondary reg
	P<>S	31 42	
	÷	81	
	1	01	
	-	51	
	÷	81	
	STO E	33 15	
	Rtn	35 72	

STEP	KEY ENTRY	KEY CODE	COMMENTS
170			
180			
190			
200			
210			
220			

LABELS

A S↑V(+)	B S↑V(-)	C r^2,a,b	D Vmax,Km	E Ki
a competit	b Linewea	c Hofstee	d V→S	e S→V
0 Σ-	1	2 V/S	3	4 Km (LWB)
5	6	7 Display	8 Σ-	9 V/S

FLAGS

0	Linewea
1	Hofstee
2	
3	Σ-

SET STATUS

FLAGS	ON	OFF	TRIG		DISP	
0	☐	☒	DEG	☒	FIX	☒
1	☐	☒	GRAD	☐	SCI	☐
2	☐	☒	RAD	☐	ENG	☐
3	☐	☒			n	2

Program Description I

Program Title Mixture Viscosities

Contributor's Name Richard D. Hyman
Address 23822 80th West
City Edmonds **State** Wash **Zip Code** 98020

Program Description, Equations, Variables

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

$$\mu_{mix} = \sum_{i=1}^{n} \frac{x_i \mu_i}{\sum_{j=1}^{n} x_j \Phi_{ij}}$$

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

X_i = Mole fraction of component i
μ_i = Viscosity " " i
M_i = Molecular wieght of " i

Operating Limits and Warnings This Program is made for four gases if using only 3 or 2 gases a 0 must be entered into the extra Registers for mole fractions. And a non-zero number must be entered for the Molecular wieght and viscosity even though there are less than 4 gases being used.

This program has been verified only with respect to the numerical example given in *Program Description II*. User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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Program Description II

Sketch(es)

Sample Problem(s) Predict the viscosity of this gas mixture at 1 atm + 293°K from given data of the independent gases at 1atm + 293°K.

Component	X_i	M_i	μ_i $\left(\frac{g}{cm\ sec}\right)$
1: CO_2	.133	44.01	1462×10^{-7}
2: O_2	.039	32.000	2031×10^{-7}
3: N_2	.828	28.016	1754×10^{-7}

Solution(s)

44.01 [↑] 32.0 [↑] 28.016 [↑] 1 [A] → 44.01

1462 [↑] 2031 [↑] 1754 [↑] 1 [B] → 1462

.133 [↑] .039 [↑] .828 [↑] 0 [C] → .133

[D] → 1714.29912

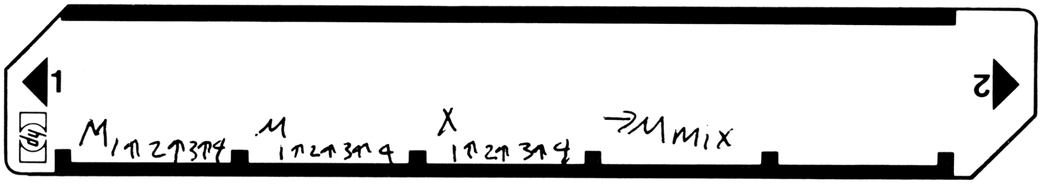
The answer is 1714×10^{-7} $\frac{g}{cm\,sec}$ This agrees with the observed value of 1793 to within 4%.

Reference(s) R. Byron Bird, Warren E. Stewart, Edwin N. Lightfoot.

Transport Phenomena I edition

John Wiley + Sons Inc. 1960

User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS	OUTPUT DATA/UNITS
1	Load side 1+2 of card			
2	In put Molecular wieght of Component 1 (M_1) must Be a non zero #	M_1		
3	Enter		↑	
4	Input M_2 (must be ≠ 0)	M_2		
5	Enter		↑	
6	Input M_3 "	M_3		
7	Enter		↑	
8	Input M_4 "	M_4	A	
9	Input Viscosity of 1 μ_1	μ_1		
10	Enter		↑	
11	Input μ_2 (non zero)	μ_2		
12	Enter		↑	
13	Input μ_3 "	μ_3		
14	Enter		↑	
15	Input μ_4 "	μ_4	B	
16	Input Mole fraction of 1 x_1	X_1		
17	Enter		↑	
18	Input X_2	X_2		
19	Enter		↑	
20	Input X_3 (Must Be = 0 if only 2 gas mixture)	X_3		
21	Enter		↑	
22	Input X_4 ($x_4 = 0$ if only 2 or 3 gas mixture)	X_4	C	
23	Solve for μ_{mix}		D	μ_{mix}
24	For a new case go To step 16 if only the mole fractions change.			
25	If new gases are involved go to step 2			

97 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS

```
 001  *LBLA      21 11
 002   CLRG      16-53
 003    P⇄S      16-51
 004   CLRG      16-53
 005    P⇄S      16-51
 006   STO4      35 04
 007     R↓        -31
 008   STO3      35 03
 009     R↓        -31
 010   STO2      35 02
 011     R↓        -31
 012   STO1      35 01
 013    RTN         24
 014  *LBLB      21 12
 015   STO8      35 08
 016     R↓        -31
 017   STO7      35 07
 018     R↓        -31
 019   STO6      35 06
 020     R↓        -31
 021   STO5      35 05
 022    RTN         24
 023  *LBLC      21 13
 024   STOD      35 14
 025     R↓        -31
 026   STOC      35 13
 027     R↓        -31
 028   STOB      35 12
 029     R↓        -31
 030   STOA      35 11
 031    RTN         24
 032  *LBLD      21 14
 033   RCL5      36 05
 034   RCL8      36 08
 035   RCL1      36 01
 036   RCL4      36 04
 037   GSBE      23 15
 038   RCLD      36 14
 039      x        -35
 040   STO0      35 00
 041   RCL5      36 05
 042   RCL7      36 07
 043   RCL1      36 01
 044   RCL3      36 03
 045   GSBE      23 15
 046   RCLC      36 13
 047      x        -35
 048   ST+0   35-55 00
 049   RCL5      36 05
 050   RCL6      36 06
 051   RCL1      36 01
 052   RCL2      36 02
 053   GSBE      23 15
 054   RCLB      36 12
 055      x        -35
 056   ST+0   35-55 00
```

STEP	KEY ENTRY	KEY CODE	COMMENTS

```
 057   RCLA      36 11
 058   ST+0   35-55 00
 059   RCL5      36 05
 060   RCLA      36 11
 061      x        -35
 062   RCL0      36 00
 063      ÷        -24
 064   STO9      35 09
 065   RCL6      36 06
 066   RCL8      36 08
 067   RCL2      36 02
 068   RCL4      36 04
 069   GSBE      23 15
 070   RCLD      36 14
 071      x        -35
 072   STO0      35 00
 073   RCL6      36 06
 074   RCL7      36 07
 075   RCL2      36 02
 076   RCL3      36 03
 077   GSBE      23 15
 078   RCLC      36 13
 079      x        -35
 080   ST+0   35-55 00
 081   RCLB      36 12
 082   ST+0   35-55 00
 083   RCL6      36 06
 084   RCL5      36 05
 085   RCL2      36 02
 086   RCL1      36 01
 087   GSBE      23 15
 088   RCLA      36 11
 089      x        -35
 090   ST+0   35-55 00
 091   RCL6      36 06
 092   RCLB      36 12
 093      x        -35
 094   RCL0      36 00
 095      ÷        -24
 096   ST+9   35-55 09
 097   RCL7      36 07
 098   RCL8      36 08
 099   RCL3      36 03
 100   RCL4      36 04
 101   GSBE      23 15
 102   RCLD      36 14
 103      x        -35
 104   STO0      35 00
 105   RCLC      36 13
 106   ST+0   35-55 00
 107   RCL7      36 07
 108   RCL6      36 06
 109   RCL3      36 03
 110   RCL2      36 02
 111   GSBE      23 15
 112   RCLB      36 12
```

REGISTERS

0	1	2	3	4	5	6	7	8	9
	M_1	M_2	M_3	M_4	μ_1	μ_2	μ_3	μ_4	

S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
	μ_i	μ_j	M_i	M_j					

A	B	C	D	E	I
X_1	X_2	X_3	X_4		

97 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS
113	x	-35	
114	ST+0	35-55 00	
115	RCL7	36 07	
116	RCL5	36 05	
117	RCL3	36 03	
118	RCL1	36 01	
119	GSBE	23 15	
120	RCLA	36 11	
121	x	-35	
122	ST+0	35-55 00	
123	RCL7	36 07	
124	RCLC	36 13	
125	x	-35	
126	RCL0	36 00	
127	÷	-24	
128	ST+9	35-55 09	
129	RCLD	36 14	
130	ST00	35 00	
131	RCL8	36 08	
132	RCL7	36 07	
133	RCL4	36 04	
134	RCL3	36 03	
135	GSBE	23 15	
136	RCLC	36 13	
137	x	-35	
138	ST+0	35-55 00	
139	RCL8	36 08	
140	RCL6	36 06	
141	RCL4	36 04	
142	RCL2	36 02	
143	GSBE	23 15	
144	RCLB	36 12	
145	x	-35	
146	ST+0	35-55 00	
147	RCL8	36 08	
148	RCL5	36 05	
149	RCL4	36 04	
150	RCL1	36 01	
151	GSBE	23 15	
152	RCLA	36 11	
153	x	-35	
154	ST+0	35-55 00	
155	RCL8	36 08	
156	RCLD	36 14	
157	x	-35	
158	RCL0	36 00	
159	÷	-24	
160	ST+9	35-55 09	
161	RCL9	36 09	
162	RTN	24	
163	*LBLE	21 15	
164	P⇄S	16-51	
165	ST04	35 04	
166	R↓	-31	
167	ST03	35 03	
168	R↓	-31	

STEP	KEY ENTRY	KEY CODE	COMMENTS
169	ST02	35 02	
170	R↓	-31	
171	ST01	35 01	
172	RCL4	36 04	
173	RCL3	36 03	
174	÷	-24	
175	4	04	
176	1/X	52	
177	Y^X	31	
178	RCL1	36 01	
179	RCL2	36 02	
180	÷	-24	
181	√X	54	
182	x	-35	
183	1	01	
184	+	-55	
185	X^2	53	
186	RCL3	36 03	
187	RCL4	36 04	
188	÷	-24	
189	1	01	
190	+	-55	
191	√X	54	
192	÷	-24	
193	8	08	
194	√X	54	
195	÷	-24	
196	P⇄S	16-51	
197	RTN	24	
200			
210			
220			

LABELS					FLAGS
A	B $\mu_{1\uparrow 2\uparrow 3\uparrow 4}$	C $X_{1\uparrow 2\uparrow 3\uparrow 4}$	D μ_{mix}	E Φ_{ij}	0
a $\mu_{1\uparrow 2\uparrow 3\uparrow 4}$	b	c	d	e	1
0	1	2	3	4	2
5	6	7	8	9	3

SET STATUS

FLAGS			TRIG		DISP	
	ON	OFF				
0	☐	☒	DEG	☒	FIX	☒
1	☐	☒	GRAD	☐	SCI	☐
2	☐	☒	RAD	☐	ENG	☐
3	☐	☒			n 5	

Program Description I

Program Title 67 VAPOR PRESSURE, BUBBLE AND DEW POINT CALCULATION

Contributor's Name ROGER N. LABAS

Address 1231-B ARCHDALE DR.

City CHARLOTTE **State** NC **Zip Code** 28210

Program Description, Equations, Variables THIS PROGRAM UTILIZES TWO VAPOR-PRESS VS TEMP POINTS (FOR EACH COMPONENT, UP TO FIVE) TO FIND THE TWO COEFFICIENTS OF THE ANTOINE EQUATION BELOW (TWO CONSTANT MODEL)

$\text{LOG } P_v = A/T + B$ WHERE P_v = VAPOR PRESSURE, T = ABS TEMP. HAVING FOUND THESE COEFFICIENTS, THE PROGRAM CALCULATES INDIVIDUAL EQUILIBRIUM CONSTANTS (K VALUE) AND, VAPOR MOLE FRACTIONS (BUBBLE POINT) OR LIQUID MOLE FRACTIONS (DEW POINT) ACCORDING TO: FOR IDEAL-LIQUID, GAS PHASES ⇒

$K_i = P_{vi}/P_T$, $x_i = y_i/K_i$, $y_i = K_i x_i$ WHERE

K_i = EQUILIBRIUM CONST. COMPONENT i, P_{vi} = VAPOR PRESS. COMPONENT i, P_T = SYSTEM TOTAL PRESS., x_i = LIQUID MOLE FRACT. COMPONENT i, y_i = VAPOR MOLE FRACT. COMPONENT i. FOR BUBBLE POINTS, THE PROGRAM USES A SEED GUESS (USUALLY LOWEST BOILING POINT OF COMPONENTS) AND INCREMENTS TEMPERATURE CHECKING Σy_i FOR THE FIRST BUBBLE. SIMILARLY FOR DEW POINTS, THE PROGRAM DECREMENTS FROM SEED (USU. HIGHEST CONDENSING POINT) CHECKING Σx_i FOR THE FIRST DROP. THE DECREMENTS OR INCREMENTS ARE CHOSEN BY USER, AS IS THE ACCURACY WITH WHICH THE PROGRAM COMPARES ITS Σx_i, Σy_i TO THE IDEAL 1.0. THE PRESENT TEMP AND Σx_i OR Σy_i ARE ALWAYS AVAILABLE TO VIEW.

Operating Limits and Warnings OBVIOUSLY THIS IS ONLY APPLICABLE TO SYSTEMS THAT CAN BE APPROXIMATED BY A STRAIGHT LINE PLOT OF P_v VS $1/T$ OVER THE RANGE IN QUESTION. MANY SYSTEMS FOLLOW THIS QUITE WELL HOWEVER, AND MANY MORE CAN BE SHOWN TO FIT FOR INTERVALS IN QUESTION. WHEN INPUTTING P_v VS T DATA IT IS WISE TO USE POINTS CLOSE TO THE EXPECTED RANGE OF BUBBLE OR DEW POINTS. THIS INSURES A REPRESENTIVE RANGE FOR RELIABLE INTERPOLATION OF THE VAPOR PRESSURE AND SUBSEQUENT CALCULATIONS.

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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Program Description II

Sketch(es)

Sample Problem(s) TO COMPLETE A BOILING POINT DIAGRAM THE BUBBLE POINT AND DEW POINTS OF AN ETHYLENE GLYCOL AND WATER SYSTEM ARE NEEDED. THE TOTAL PRESSURE IS 760 mm Hg AND CONCENTRATIONS (MOLE FRAC.) ARE EG = 0.196 H_2O = 0.804 ALSO THE VAPOR PRESSURE OF EG AT 3 5 °F (855 °R) IS NEEDED. THE FOLLOWING IS GIVEN

AT 338 °F P_v EG = 310 mm Hg P_v H_2O = 5942 mm Hg
AT 320 °F P_v EG = 220 mm Hg P_v H_2O = 4636 mm Hg

BOILING POINTS PURE COMPONENTS (CONDENSING POINTS SAME)
AT 760 mm Hg
EG = 338 °F H_2O = 212 °F

FIND BUBBLE AND DEW POINTS TO CORRESPOND WITH 0.1 % OF VAPOR AND LIQUID MOLE FRACTION SUMS (ie Σx_i or $y_i \leq 1.001$)

Solution(s) FOLLOW INSTRUCTIONS

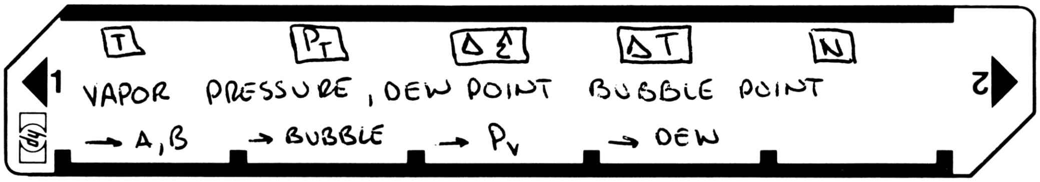
KEYSTROKES

2 [h] [ST I] 310 [E↑] 338 [E↑] 220 [E↑] 320 [A] → −5150.31
5942 [E↑] 338 [E↑] 4636 [E↑] 320 [R/S] [R/S] → −3727.35
760 [STO] [B] .001 [STO] [C] 2 [STO] [D] [STO] [E] [f] [P⇄S] .196 [STO] [2] .804 [STO] [1] [f] [P⇄S] → 0.80
212 [E↑] 460 [+] [STO] [A] [B] → RUNS ≈ 100 SEC. 221.12 BUBBLE POINT °F
2 [STO] [D] 338 [E↑] 460 [+] [STO] [A] [D] → RUNS ≈ 130 SEC 308.8 DEW POINT °F
2 [h] [ST I] 395 [E↑] 460 [+] [STO] [A] [C] → 834.89 mm Hg LITERATURE GIVES US 848 mm Hg AT 395 °F SO ERROR IS 1.55 % FOR P_v CALCULATION

Reference(s)

"INTRODUCTION TO CHEMICAL ENGINEERING THERODYNAMICS" SMITH & VAN NESS
2nd ED. COPYWRIGHT 1959 McGRAW-HILL Pg 375, 210, 352
EQs 12-40, 12-32, 7-25

User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS		OUTPUT DATA/UNITS
1	LOAD SIDES 1 AND 2				
2	LOAD R_I WITH NUMBER COMPONENTS N	(N)	(N)	STO I	
3	LOAD STACK WITH P_v VS T DATA	N^{TH} COMP.	P_N	E↑	mm Hg
	N^{TH} COMPONENT FIRST, ABS. PRESS mm		T_N	E↑	°F
	Hg AND °F PRESS A		P_N'	E↑	mm Hg
4	LOAD STACK WITH P_v VS T DATA FOR		T_N'	A	°F
	$N-1^{TH}$ COMPONENT NEXT, PRESS R/S TWICE	$N-1^{TH}$ COMP	P_{N-1}	E↑	
			T_{N-1}	E↑	
	FOLLOW STEP 4 UNTIL ALL COMPONENT		P_{N-1}'	E↑	
	DATA HAS BEEN ENTERED.		T_{N-1}'	R/S	
			R/S		
5	STORE R_A WITH SEED GUESS TEMP.	T OR	(T)	STO A	
6	STORE R_B WITH TOTAL PRESSURE	P_T mmHg	(P_T)	STO B	
7	STORE R_C WITH ΔΣ, ie IF YOU WANT				
	Σx_i OR $\Sigma y_i \le 1.001$ STORE 0.001		.001	STO C	
8	STORE R_D WITH ΔT OR INTERVAL	OR	(ΔT)	STO D	
9	STORE R_E WITH N	N	(N)	STO E	
10*	FOR BUBBLE POINT STORE x_N IN	MOLE FRACT	P⇄S	STO N	
	R_{10+N}		P⇄S		
11*	FOR DEW POINT STORE y_N IN	MOLE FRACT	P⇄S	STO N	
	R_{10+N}		P⇄S		
12*	FOR DEW POINT PRESS D		D		°F
13*	FOR BUBBLE POINT PRESS B		B		°F
14**	FOR VAPOR PRESSURE STORE N IN R_I		(N)	STO I	
15**	STORE T IN R_A	OR	(T)	STO A	
16**	PRESS C		C		mm Hg
*	ONLY ONE POINT BUBBLE OR DEW CAN				
	BE CALCULATED AT ONCE, BUT SUBSEQUENT				
	CASES FOR SAME SYSTEM CAN START AT STEP 5				
**	THESE STEPS OPTIONAL FOR VAPOR				
	PRESSURE CALCULATION, AND CAN BE				
	EXECUTED AFTER STEP 4.				
	NOTE: SPEED OF PROGRAM IS RELATIVELY				
	INSENSITIVE TO N.				

67 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001 *	LBL A	31 25 11	LOADING FOR
	STO A	33 11	COEFFICIENT
	R↓	35 53	SOLUTIONS
	STO B	33 12	
	R↓	35 53	
	STO C	33 13	
	R↓	35 53	
	STO D	33 14	
	LOG	31 53	
010	RCL C	34 13	
	4	04	CONVERTING °F → °R
	6	06	
	0	00	
	+	61	
	STO C	33 13	
	x	71	
	RCL B	34 12	
	LOG	31 53	
	RCL A	34 11	
020	4	04	
	6	06	
	0	00	
	+	61	
	STO A	33 11	
	x	71	
	−	51	
	RCL C	34 13	
	RCL A	34 11	
	−	51	
030	÷	81	SOLVED FOR COEFF. B
	STO (i)	33 24	STORE IN R_N
	RCL D	34 14	
	LOG	31 53	
	RCL C	34 13	
	x	71	
	RCL (i)	34 24	
	RCL C	34 13	
	x	71	
	−	51	SOLVED FOR COEFF. A
040	x↔I	35 24	
	5	05	
	+	61	
	x↔I	35 24	
	STO (i)	33 24	STORE IN R_{N+5}
	x↔I	35 24	
	5	05	
	−	51	
	x↔I	35 24	
	DSZ	31 33	NEXT COMPONENT
050	R/S	84	
	R/S	84	STOP AT N COMPONENTS
	GTO A	22 11	
*	LBL B	31 25 12	BUBBLE POINT
	RCL E	34 15	STORE N IN R_I
	STO I	35 33	
	CL X	44	CLEAR R_0
	STO 0	33 00	
*	LBL 0	31 25 00	BEGIN LOOP DO N
	GSB 1	31 22 01	CALCULATE K_i, X_i
060	x	71	CALCULATE y_i
	GSB 2	31 22 02	Σy_i
	DSZ	31 33	
	GTO 0	22 00	LOOP UNTIL N
	RCL 0	34 00	COMPARE Σ WITH
	1	01	1.
	−	51	
	x>0	31 81	CHECK FOR CORRECT
	GTO 3	22 03	APPROACH, IF NOT
	ABS	35 64	CHANGE ΔT
070	RCL C	34 13	COMPARE ACCURACY
	x↔y	35 52	
	x≤y	32 71	
	GTO 4	22 04	DISPLAY BUBBLE
	GSB 5	31 22 05	TRY NEW T
	GTO B	22 12	START AGAIN
*	LBL C	31 25 13	CALC. P_v
	RCL A	34 11	
	x↔I	35 24	
	5	05	
080	+	61	
	x↔I	35 24	
	RCL (i)	34 24	
	x↔y	35 52	
	÷	81	
	x↔I	35 24	
	5	05	
	−	51	
	x↔I	35 24	
	RCL (i)	34 24	
090	+	61	
	10^x	32 53	
	RTN	35 22	
*	LBL D	31 25 14	DEW POINT
	RCL E	34 15	STORE N IN R_I
	STO I	35 33	
	CL x	44	CLEAR R_0
	STO 0	33 00	
*	LBL 6	31 25 06	BEGIN DO LOOP
	GSB 1	31 22 01	CALCULATE K_i, y_i
100	x↔y	35 52	CALCULATE x_i
	÷	81	
	GSB 2	31 22 02	Σx_i
	DSZ	31 33	
	GTO 6	22 06	LOOP UNTIL N
	RCL 0	34 00	COMPARE Σ WITH
	1	01	1.
	−	51	
	x>0	31 81	CHECK FOR CORRECT
	GTO 7	22 07	APPROACH, IF NOT
110	ABS	35 64	CHANGE ΔT
	RCL C	34 13	COMPARE ACCURACY
	x↔y	35 52	

REGISTERS

0	1	2	3	4	5	6	7	8	9
Σ xi or yi	A_N	A_{N-1}	A_{N-2}	A_{N-3}	A_{N-4}	B_N	B_{N-1}	B_{N-2}	B_{N-3}
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
B_{N-4}	x, y N	x, y N−1	x, y N−2	x, y N−3	x, y N−4				

A	B	C	D	E	I
SEED T	TOTAL PRESS	ΔΣ	ΔT	N	

67 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
	X≤Y	32 71					
	GTO 4	22 04	DISPLAY DEW	170			
	GSB b	32 22 12	TRY NEW T				
	GTO D	22 14	START AGAIN				
*	LBL 1	31 25 01	CALCULATE Ki:				
	GSB C	31 22 13					
	RCL B	34 12					
120	÷	81					
	X↔I	35 24					
	1	01					
	0	00					
	+	61		180			
	X↔I	35 24					
	RCL(i)	34 24	RCL Xi OR Yi:				
	RTN	35 22					
*	LBL 2	31 25 02	Σ Xi OR Yi:				
	X↔I	35 24					
130	1	01					
	0	00					
	-	51					
	X↔I	35 24					
	STO +0	33 61 00		190			
	RTN	35 22					
*	LBL 3	31 25 03	CHANGE ΔT FOR				
	GSB b	32 22 12	DEW				
	GSB a	32 22 11					
	GTO B	22 12					
140 *	LBL 4	31 25 04	CONVERT °R TO °F				
	RCL A	34 11	DISPLAY T				
	4	04					
	6	06					
	0	00		200			
	-	51					
	RTN	35 22					
*	LBL 5	31 25 05	NEW T				
	RCL A	34 11					
	RCL D	34 14					
150	+	61					
	STO A	33 11					
	RTN	35 22					
*	LBL 7	31 25 07	CHANGE ΔT FOR				
	GSB 5	31 22 05	BUBBLE	210			
	GSB a	32 22 11					
	GTO D	22 14					
*	LBL a	32 25 11					
	RCL D	34 14					
	5	05					
160	÷	81					
	STO D	33 14					
	RTN	35 22					
*	LBL b	32 25 12					
	RCL A	34 11		220			
	RCL D	34 14					
	+	51					
	STO A	33 11					
	RTN	35 22					

LABELS

A CALC A,B	B CALC BUB.	C CALC Pv	D CALC DEW	E
a CHANGE ΔT	b CHANGE ΔT	c	d	e
0 DO LOOP	1 CALC Ki	2 Σ Xi OR Yi	3 CHANGE ΔT	4 DISP T
5 CHANGE ΔT	6 DO LOOP	7 CHANGE ΔT	8	9

FLAGS

0
1
2
3

SET STATUS

FLAGS	ON	OFF	TRIG		DISP	
0	☐	☒	DEG	☒	FIX	☒
1	☐	☒	GRAD	☐	SCI	☐
2	☐	☒	RAD	☐	ENG	☐
3	☐	☒			n 2	

Program Description I

Program Title SINGLE STAGE EQUILIBRIUM FLASH CALCULATION

Contributor's Name Kerry R. Kelly
Address 4208 Salem Drive
City Baton Rouge **State** Louisiana **Zip Code** 70814

Program Description, Equations, Variables Given the number of components (n), the mole fraction (z_i), the equilibrium ratio between phases (K_i) for each component in the feed and a first guess for the mole ratio (V/F), the program will use a second order Newton convergence scheme to converge the Rachford-Rice equation to nearly zero (10^{-6}).

$$f(V/F) = \sum_{i=1}^{n} z_i(K_i-1) \Big/ \left[(K_i-1)(V/F)+1\right] = 0, \text{ Rachford-Rice Eq'n}$$

$$\left.\begin{aligned} (V/F)_{i+1} &= (V/F)_i - f\left[(V/F)_i\right] / f'\left[(V/F)_i\right] \\ f'\left[(V/F)_i\right] &= -\sum_{i=1}^{n} z_i(K_i-1)^2 \Big/ \left[(K_i-1)(V/F)+1\right]^2 \end{aligned}\right\} \text{Newton Convergence Method}$$

Next the program can solve for (V/L) and the final compositions of the liquid and the vapor by: $(V/L) = (V/F)/\left[1-(V/F)\right]$

$$x_i = z_i\left[1+(V/L)\right] / \left[1+K_i(V/L)\right]$$

$$y_i = z_i\left[1+(L/V)\right] / \left[1+(1/K_i)(L/V)\right]$$

Operating Limits and Warnings

Maximum number of components = 10

This program has been verified only with respect to the numerical example given in *Program Description II.* User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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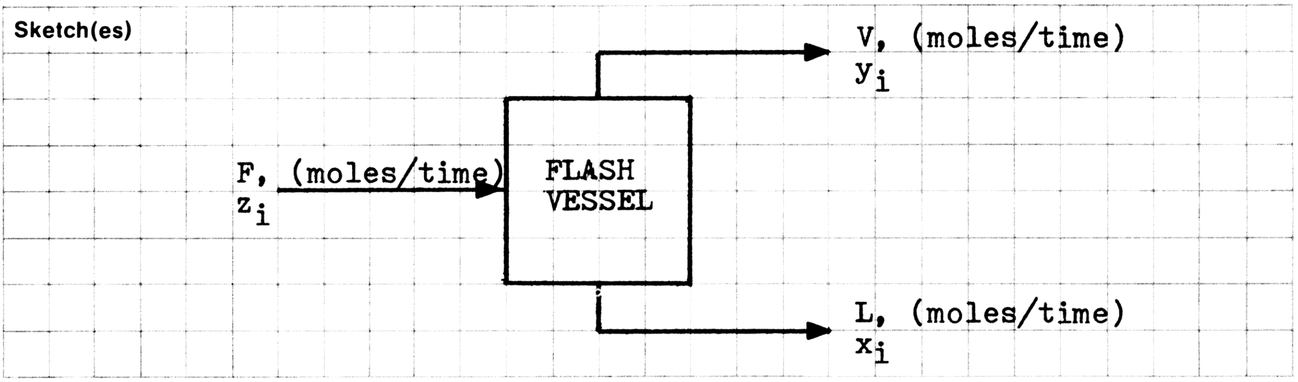
Program Description II

Sketch(es)



Sample Problem(s) A five component mixture of hydrocarbons is fed to a steady-state flash vaporization giving product equilibrium at 270°F and 50 psia. The details are given below:

Component	z_i	K_i @ 270°F & 50 psia
C_3	0.15	12.75
C_4	0.25	5.61
C_6	0.05	1.40
C_7	0.30	0.705
C_8	0.25	0.375

Calculate (V/F) and the composition of both the vapor and the liquid product streams.

Solution(s) 5(A) → 5.00000; .15 ↑ 12.75(B) .25 ↑ 5.61(B) .05 ↑ 1.4(B)

.3 ↑ .705(B) .25 ↑ .375(B) → 0.00000

.5(C)(calculation time ≈ 72 sec) → 0.80243

(D) →

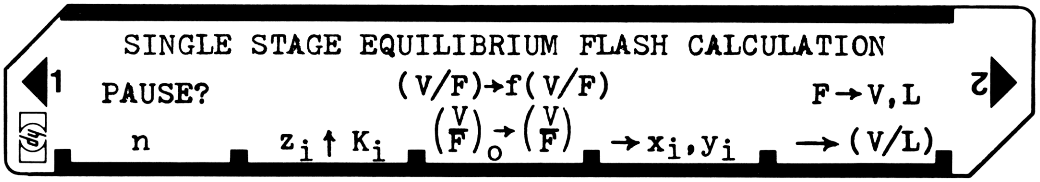
x_i	y_i
0.01438***	0.18339***
0.05320***	0.29845***
0.03785***	0.05299***
0.39304***	0.27709***
0.50153***	0.18807***

Reference(s)

(1) King, C. Judson; SEPARATION PROCESSES; First Ed.; Page 513; McGraw-Hill; 1971

(2) Kern, Donald Q.; PROCESS HEAT TRANSFER; First Ed.; Page 332; McGraw-Hill; 1950

User Instructions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS		OUTPUT DATA/UNITS
1	Load side 1 and side 2				
2	Input number of components.	n	A		n
3	Input mole fraction of component i				
	in the feed.	z_i	ENTER↑		z_i
4	Input equilibrium ratio between				
	phases for component i.	K_i	B		n - i
5	Repeat steps 3 and 4 for i = 1 to n				
6	Input a first guess for the mole ratio				
	(V/F) and compute and output the				
	actual ratio.*	$(V/F)_o$	C		(V/F)
7	Optional: Compute and output the				
	mole fraction of each component in				
	both the liquid (x_i) and the vapor(y_i)				
	for i = 1 to n **		D		x_1, y_1
					x_2, y_2
					⋮
					⋮
					x_n, y_n
8	Optional: Compute and output the				
	mole ratio (V/L)**		E		(V/L)
9	Optional: Input the mole feed rate				
	and compute and output the vapor mole				
	and then the liquid mole rate.**	F	f	E	V, L
10	Optional: Toggle pause mode. Used				
	to watch f(V/F) converge to less than				
	10^{-6}.		f	A	1.00/0.00
	* This calculation is trial and error				
	and may take several minutes if a				
	large number of components is				
	involved and/or the first guess is				
	poor.				
	** This step can be performed only				
	after step 6.				

67 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS
001	f LBL A	31 25 11	Set up the I register for data input by storing the no. of components minus one. (n-1)
	1	01	
	-	51	
	h ST I	35 33	
	STO D	33 14	
	1	01	
	+	61	
	h RTN	35 22	
	f LBL B	31 25 12	Store K_i and z_i in the proper register and then display the number of components for which data has not yet been entered. (n-i)
010	STO (i)	33 24	
	h x≷y	35 52	
	f P≷S	31 42	
	STO (i)	33 24	
	f P≷S	31 42	
	f DSZ	31 33	
	GTO 0	22 00	
	f LBL 0	31 25 00	
	h RC I	35 34	
	1	01	
020	+	61	
	h RTN	35 22	
	g LBL c	32 25 13	Prepare for calculation of f(V/F) or f'(V/F).
	STO A	33 11	
	RCL D	34 14	
	h ST I	35 33	
	0	00	
	STO E	33 15	
	f LBL 6	31 25 06	Calculate f(V/F) $= \sum_{i=1}^{n} \frac{z_i(K_i-1)}{(K_i-1)(V/F)+1}$ or If flag 0 is set Calc. f'(V/F) $= -\sum_{i=1}^{n} \frac{z_i(K_i-1)^2}{[(K_i-1)(V/F)+1]}$
	f GSB 1	31 22 01	
030	f DSZ	31 33	
	GTO 6	22 06	
	f GSB 1	31 22 01	
	RCL E	34 15	
	h RTN	35 22	
	f LBL 1	31 25 01	
	RCL A	34 11	
	RCL (i)	34 24	
	1	01	
	-	51	
040	X	71	
	1	01	
	+	61	
	h F0?	35 71 00	
	g x^2	32 54	
	RCL (i)	34 24	
	f P≷S	31 42	
	RCL (i)	34 24	
	h x≷y	35 52	
	1	01	
050	-	51	
	h F0?	35 71 00	
	g x^2	32 54	
	X	71	
	h x≷y	35 52	
	↑	81	
	f P≷S	31 42	

STEP	KEY ENTRY	KEY CODE	COMMENTS
	RCL E	34 15	
	+	61	
	STO E	33 15	
060	h RTN	35 22	
	f LBL 2	31 25 02	Set flag 0 so that subroutine c will calc. f'(V/F).
	RCL A	34 11	
	h SF 0	35 51 00	
	g GSB c	32 22 13	
	CHS	42	
	h CF 0	35 61 00	
	h RTN	35 22	
	f LBL C	31 25 13	Must constrain trials to $0 \leq (V/F) \leq 1$
	STO A	33 11	
070	h ABS	35 64	
	g FRAC	32 83	
	g GSB c	32 22 13	Calc. f(V/F)
	STO C	33 13	
	h F1?	35 71 00	Pause?
	h PAUSE	35 72	
	h ABS	35 64	Is $\lvert f(V/F)\rvert < 10^{-6}$?
	EEX	43	
	6	06	
	CHS	42	
080	g x>y	32 81	
	GTO 4	22 04	
	f GSB 2	31 22 02	Adjust (V/F) by Newton's method and check the new value by returning to C.
	RCL C	34 13	
	h x≷y	35 52	
	↑	81	
	RCL A	34 11	
	h x≷y	35 52	
	-	51	
	GTO C	22 13	
090	f LBL 4	31 25 04	Return with the latest value of (V/F) in dsply.
	RCL A	34 11	
	h RTN	35 22	
	f LBL D	31 25 14	Compute the value of x_i then y_i for i = 1 to n.
	f GSB E	31 22 15	
	RCL D	34 14	
	h ST I	35 33	
	f LBL 7	31 25 07	
	f GSB 5	31 22 05	
	f DSZ	31 33	
100	GTO 7	22 07	
	f GSB 5	31 22 05	
	h RTN	35 22	
	f LBL 5	31 25 05	
	RCL (i)	34 24	
	RCL E	34 15	
	X	71	
	1	01	
	+	61	
	RCL E	34 15	
110	1	01	
	+	61	
	h x≷y	35 52	

REGISTERS

0 K_n	1 K_{n-1}	2 K_{n-2}	3 . . .	4 . . .	5	6	7	8	9 K_{n-9}
S0 z_n	S1 z_{n-1}	S2 z_{n-2}	S3 . . .	S4 . . .	S5	S6	S7	S8	S9 z_{n-9}
A Trial (V/F)	B Used	C f(V/F)	D n-1	E Used	I Used				

67 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS
	↑	81	
	f P⇄S	31 42	
	RCL (i)	34 24	
	X	71	
	f -x-	31 84	
	RCL (i)	34 24	
	1	01	
120	RCL E	34 15	
	h 1/x	35 62	
	+	61	
	X	71	
	RCL E	34 15	
	h 1/x	35 62	
	f P⇄S	31 42	
	RCL (i)	34 24	
	↑	81	
	1	01	
130	+	61	
	↑	81	
	f -x-	31 84	
	h RTN	35 22	
	f LBL E	31 25 15	Convert (V/F) to (V/L).
	RCL A	34 11	
	1	01	
	RCL A	34 11	
	-	51	
	↑	81	
140	STO E	33 15	
	h RTN	35 22	
	g LBL e	32 25 15	Compute and display both the vapor rate (V) and the liquid rate (L) given the feed rate (F).
	ENTER↑	41	
	ENTER↑	41	
	RCL A	34 11	
	X	71	
	f -x-	31 84	
	-	51	
	f -x-	31 84	
150	h RTN	35 22	
	g LBL a	32 25 11	Pause toggle to watch convergence.
	h F1?	35 71 01	
	GTO 8	22 08	
	h SF 1	35 51 01	
	1	01	
	h RTN	35 22	
	f LBL 8	31 25 08	
	0	00	
	h CF 1	35 61 01	
160	h RTN	35 22	

STEP	KEY ENTRY	KEY CODE	COMMENTS
170			
180			
190			
200			
210			
220			

LABELS					FLAGS
A n	B z_i ↑ K_i	C $(\frac{V}{F})_0 \rightarrow (\frac{V}{F})$	D → x_i, y_i	E → (V/L)	0 Used
a PAUSE?	b	c $(\frac{V}{F}) \rightarrow f(\frac{V}{F})$	d	e F → V, L	1 Used
0 (n-i)	1 Used	2 f'(V/F)	3	4 Used	2
5 → x_i, y_i	6 Used	7 Used	8 Used	9	3

SET STATUS

FLAGS	ON	OFF	TRIG		DISP	
0	☐	☒	DEG	☒	FIX	☒
1	☐	☒	GRAD	☐	SCI	☐
2	☐	☒	RAD	☐	ENG	☐
3	☐	☒			n	5

NOTES

NOTES

NOTES

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