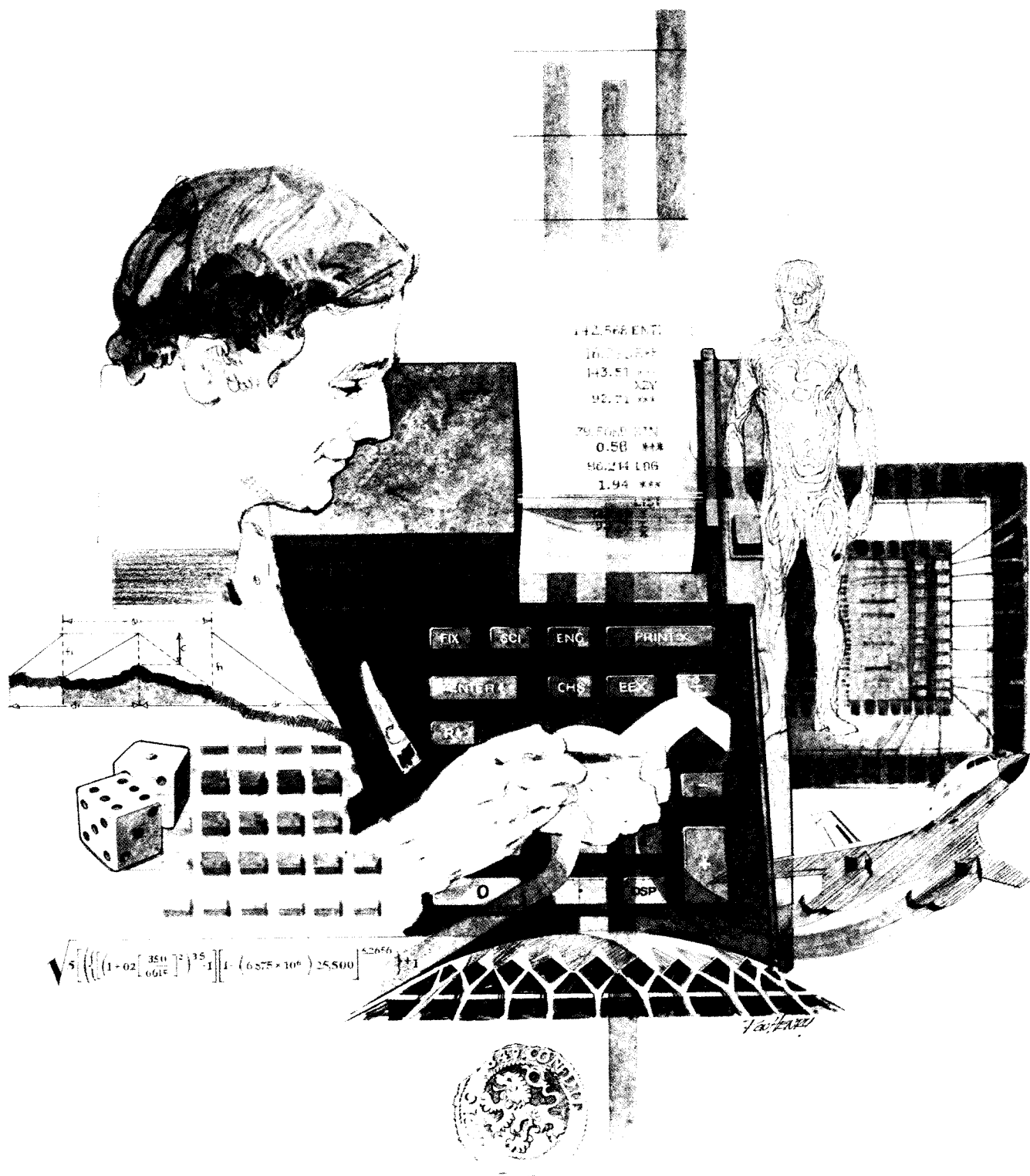


HEWLETT-PACKARD

HP-67/HP-97

Users' Library Solutions
Chemistry



INTRODUCTION

In an effort to provide continued value to its 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.

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Program Description I

1

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

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 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

$$x_0 = (KC + K_w)^{1/2}$$

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 1.0×10^{-4} M acetic acid solution if K_a is 1.8×10^{-5} .
- 2.) Find the pH of 3.0×10^{-6} M NH_4Cl solution if the $\text{p}K_b$ for ammonia is 4.75.
- 3.) Calculate the pH of 0.002 molar KCN solution ($\text{p}K_a = 9.32$).
- 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 1.68×10^{-3} , find the $\text{p}K_b$.

Solution(s) 1.) 1.8 EEX,CHS,5,B $\rightarrow 1.80000 \times 10^{-5}$; 4 A $\rightarrow 1.00 \times 10^{-4}$;
 D $\rightarrow 3.45 \times 10^{-5}$, 4.46 answer

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

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

4.) 40 f,C $\rightarrow 40.00$; 150 C $\rightarrow 3.75 \times 10^{-3}$ answer.

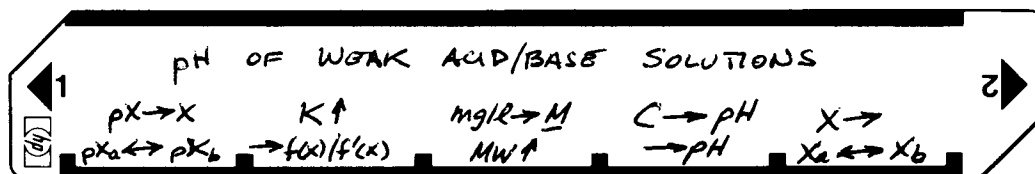
5.) 1.68 EEX,CHS,3,E $\rightarrow 2.77$; R/S $\rightarrow 11.23$ answer
 (alternate: 1.68 EEX,CHS,3,f,E $\rightarrow 5.95 \times 10^{-12}$; E $\rightarrow 11.23$ answer)

Reference(s)

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

User Instructions

3



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	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	f LBL A	31 25 11	Convert		RCL 3	34 03	
	CHS	42	pK_a to K_a		f V _X	31 54	
	10 ^x	32 53	pK_b to K_b		STD 2	33 02	
	g SCI	32 23	pH to $[H^+]$ etc.	060	GTD 1	22 01	
	RIS	84			h RTN	35 22	
	g LBL 2	32 25 15	Interchange		g LBL 6	32 25 12	$\rightarrow f(x)/f'(x)$
	EE _X	43	K_a and K_b		RCL 5	34 05	
	CHS	42			g SCI	32 23	
	1	01	or		RIS	84	DISPLAY K
010	+	04	$[H^+]$ and $[OH^-]$		RCL 1	34 01	
	h x _{xy}	35 52			h RTN	35 22	
	÷	81			f LBL 1	31 25 01	
	g SCI	32 23			RCL 2	34 02	
	h RTN	35 22		070	RCL 1	34 01	Newton-Raphson iteration
	f LBL E	31 25 15	Convert		+	61	
	LOG	31 53	$[H^+]$ to pH		RCL 2	34 02	
	CHS	42	$[OH^-]$ to pOH		X	71	
	f FIX	31 23	K_a to pK_a etc.		RCL 3	34 03	
	RIS	84			-	51	
020	g LBL a	32 25 11	Interchange		RCL 2	34 02	
	1	01	pK_a and pK_b		X	71	
	+	04	pH and pOH		RCL 4	34 04	
	h x _{xy}	35 52			-	51	
	-	51		080	RCL 2	34 02	
	f FIX	31 23			3	03	
	h RTN	35 22			X	71	
	f LBL C	31 25 13	Calculate molarity from mg/L		RCL 1	34 01	
	EE _X	43			2	02	
	3	03			X	71	
030	÷	81			+	61	
	RCL 6	34 06			RCL 2	34 02	
	÷	81			X	71	
	g SCI	32 23			RCL 3	34 03	
	RIS	84	DISPLAY MW	090	-	51	
	RCL 6	34 06			÷	81	
	f FIX	31 23			STD 5	33 05	
	h RTN	35 22			h ABS	35 64	
	f LBL B	31 25 12	ENTER K		RCL 2	34 02	
	STD 1	33 01			9	09	
040	h RTN	35 22			9	09	
	g LBL C	32 25 13	ENTER MW		÷	81	
	STD 6	33 06			h x _{xy}	35 52	
	h RTN	35 22			g x _{xy}	32 71	TEST
	f LBL D	31 25 14	$C \rightarrow pH$ or pOH	100	GTD f d	22 31 14	
	RCL 1	34 01			RCL 2	34 02	
	X	71			RCL 5	34 05	
	EE _X	43	Calculates Constants		-	51	
	CHS	42			STD 2	33 02	
	1	01			GTD 1	22 01	ITERATE
050	+	04			RIS	84	
	+	61			g LBL d	32 25 14	$\rightarrow pH$ or pOH
	STD 3	33 03			RCL 2	34 02	from memory
	h lst x	35 82			g SCI	32 23	
	RCL 1	34 01		110	h PAU	35 72	FLASH {X}
	X	71			GTD E	22 15	DISPLAY PX
	STD 4	33 04					

REGISTERS

0	1 K	2 H _{est}	3 CK+K _w	4 K _{Kw}	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				

6 Program Listing II

5

[illegible]

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 *NY*

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 $x^4 + K_1 x^3 + (K_1 K_2 - K_w - K_1 C_a) x^2 - (K_w K_1 + 2 K_1 K_2 C_a) x - K_w K_1 K_2 = 0$
2. $H_2A + NaHA$ $x^4 + (C_{s,1} + K_1) x^3 + (K_1 K_2 - K_w - K_1 C_a) x^2 - (K_w K_1 + 2 K_1 K_2 C_a + K_1 K_2 C_{s,1}) x - K_w K_1 K_2 = 0$
3. $NaHA$ $x^4 + (C_{s,1} + K_1) x^3 + (K_1 K_2 - K_w) x^2 - (K_w K_1 + K_1 K_2 C_{s,1}) x - K_w K_1 K_w = 0$
4. $NaHA + Na_2A$ $x^4 + (C_{s,1} + 2 C_{s,2} + K_1) x^3 + (K_1 K_2 - K_w + K_1 C_{s,2}) x^2 - (K_w K_1 + K_1 K_2 C_{s,1}) x - K_w K_1 K_2 = 0$
5. Na_2A $x^4 + (2 C_{s,2} + K_1) x^3 + (K_1 K_2 - K_w + K_1 C_{s,2}) x^2 - K_w K_1 x - K_w K_1 K_2 = 0$

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

1. $x \doteq (K_1 C_a)^{1/2}$
2. $x \doteq K_1 C_a / C_{s,1}$
3. $x \doteq (K_1 K_2)^{1/2}$
4. $x \doteq K_2 C_{s,1} / C_{s,2}$
5. $x \doteq (K_w K_2 / C_{s,2})^{1/2}$

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

7

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?

$$K_1 = 5.40 \times 10^{-2}$$

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

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

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

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
6.	[F][D]	Read pH	→ 2.26

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

67 Program Listing I

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBL 0	31 25 00	Solve quartic eq.		RCL 4	34 04	If basic mode set, convert [OH ⁻] to [H ₃ O ⁺] Convert [H ₃ O ⁺] to [OH ⁻] or reverse
	STO 4	33 04			DSP 2	23 02	
	STO E	33 15			F? 2	35 71 02	
	F? 1	35 71 01		060	GTO C	22 31 15	
	R/S	84			RTN	35 22	
	F? 1	35 71 01			*LBL 0	32 25 15	
	GSD d	32 22 14			RCL 8	34 08	
	FLX	31 23			÷	81	
	DSP 8	23 08			1/x	35 62	
010	H	04			RTN	35 22	
	I	01			*LBL A	31 25 11	1 sum to fn. indicator
	CHS	42			STO 9	33 09	
	STO I	35 33			↓	35 53	
	RCL 4	34 04		070	STO A	33 11	
	RCL 3	34 03			RTN	35 22	
	+	61			*LBL B	31 25 12	
	RCL 4	34 04			STO B	33 12	
	X	71			I	01	
	RCL 2	34 02			STO+5	33 61 05	
020	+	61			X≠Y	35 52	
	RCL 4	34 04			RTN	35 22	2 sum to fn. indicator
	X	71			*LBL C	31 25 13	
	RCL 1	34 01			STO C	33 13	
	+	61		080	2	02	
	RCL 4	34 04			STO+5	33 61 05	
	X	71			X≠Y	35 52	
	RCL 0	34 00			RTN	35 22	
	+	61			*LBL D	31 25 14	
	RCL 4	34 04			STO D	33 14	
030	H	04			4	04	
	X	71			STO+5	33 61 05	4 sum to fn. indicator
	RCL 3	34 03			X≠Y	35 52	
	3	03			RTN	35 22	
	X	71		090	*LBL E	31 25 15	
	+	61			RCL A	34 11	
	RCL 4	34 04			STO 3	33 03	
	X	71			RCL 9	34 09	
	RCL 2	34 02			X	71	
	2	02			STO 2	33 02	
040	X	71			STO 0	33 00	
	+	61			RCL 8	34 08	Set up proper coefficients used in all cases. Complete coefficients are calculated in subroutine pointed to by function indicator (Reg. 5)
	RCL 4	34 04			CHS	42	
	X	71			STO+2	33 61 02	
	RCL 1	34 01		100	STO X 0	33 71 00	
	+	61			RCL A	34 11	
	÷	81			X	71	
	RCL 4	34 04			STO 1	33 01	
	X≠Y	35 52			RCL C	34 13	
	STO-4	33 51 04			STO+3	33 61 03	
050	CLX	44			RCL D	34 14	
	RCL 4	34 04			STO+3	33 61 03	
	—	51			STO+3	33 61 03	Store fn. indicator in I and go to (i) for proper initial value.
	RND	31 24			RCL 5	34 05	
	X≠0	31 61		110	STO I	35 33	
	GTO (i)	22 24			GTO (i)	22 24	
	SCI	32 23			*LBL 1	31 25 01	

REGISTERS

0	a ₀	1	a ₁	2	a ₂	3	a ₃	4	x _n ; [H ₃ O ⁺]	5	Function indicator	6		7		8	K _w	9	K ₂
S0		S1		S2		S3		S4		S5		S6		S7		S8		S9	
A	K ₁		B	C _a		C	C _{s,1}		D	C _{s,2}		E	approx [H ₃ O ⁺]		I	used			

67 Program Listing II

STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS	
	RCL A	34 11			2	02		
	RCL B	34 12		170	X	71		
	X	71			STO-1	33 51 01		
	STO-2	33 51 02			RTN	35 22		
	STO 7	33 07			*LBL 7	31 25 07	$-K_1 K_2 C_{s,1} + \text{Reg 1}$	
	GSB 5	31 22 05			RCL A	34 11		
	RCL 7	34 07			RCL 9	34 09		
120	$\sqrt{x}$	31 54	$(K_1 C_a)^{1/2}$		X	71		
	GTO 0	22 00			RCL C	34 13		
	*LBL 2	31 25 02			X	71		
	GSB 7	31 22 07		180	STO-1	33 51 01		
	RCL A	34 11			RTN	35 22		
	RCL 9	34 09			*LBL d	32 25 14	$-\log x$	
	X	71			log	31 53		
	$\sqrt{x}$	31 54	$(K_1 K_2)^{1/2}$		CHS	42		
	GTO 0	22 00			FIX	31 23		
	*LBL 3	31 25 03			Parse	35 72		
130	GSB 5	31 22 05			RTN	35 22		
	GSB 7	31 22 07			*LBL b	32 25 12		
	RCL A	34 11			SF 2	35 51 02		
	RCL B	34 12			RTN	35 22		
	X	71		190	*LBL c	32 25 13		
	STO-2	33 51 02			F?1	35 71 01		
	RCL C	34 13			GTO 9	22 09		
	$\div$	81	$K_1 C_a / C_{s,1}$		1	01		
	GTO 0	22 00			SF 1	35 51 01		
	*LBL 4	31 25 04			RTN	35 22		
140	RCL A	34 11			*LBL 9	31 25 09		
	RCL D	34 14			0	00		
	X	71			CF 1	35 61 01		
	STO+2	33 61 02			RTN	35 22		
	RCL 8	34 08		200	*LBL a	32 25 11		
	RCL 9	34 09			EEX	43		
	X	71			CHS	42		
	RCL D	34 14			1	01		
	$\div$	81			4	04		
	$\sqrt{x}$	31 54	$(K_w K_2 / C_{s,2})^{1/2}$		STO 8	33 08		
150	GTO 0	22 00			CLX	44		
	*LBL 6	31 25 06			STO 5	33 05		
	GSB 7	31 22 07			CF 2	35 61 02		
	RCL A	34 11			SCI	32 23		
	RCL D	34 14		210	DSP 2	23 02		
	X	71			RTN	35 22		
	STO+2	33 61 02						
	RCL 9	34 09						
	RCL C	34 13						
	X	71						
160	RCL D	34 14						
	$\div$	81	$K_2 C_{s,1} / C_{s,2}$					
	GTO 0	22 00						
	*LBL 5	31 25 05						
	RCL A	34 11	$-2K_1 K_2 C_a + \text{Reg 1}$	220				
	RCL 9	34 09						
	X	71						
	RCL B	34 12						
	X	71						
LABELS				FLAGS	SET STATUS			
A $K_1 \uparrow K_2 \rightarrow$	B C_a	C $C_{s,1}$	D $C_{s,2}$	E $[H_3O^+]$	0	FLAGS	TRIG	DISP
a INIT	b $b \rightarrow$	c $\equiv ?$	d pH	e $[OH^-]$	1 $\equiv ?$	ON OFF	DEG ☒	FIX ☐
0 Used	1 H_2A	2 $NaHA$	3 $H_2A + NaHA$	4 Na_2A	2 $b \rightarrow$	0 ☐ ☒	GRAD ☐	SCI ☒
5 Used	6 $NaHA + Na_2A$	7 Used	8	9 CF1	3	1 ☐ ☒	RAD ☐	ENG ☐
						2 ☐ ☒		n <u>2</u>
						3 ☐ ☒		

Program Description I

Program Title Weak Acid/Base Titration Curve

Contributor's Name Karl Marhenke

Address 1710 Wilshire Drive

City Aptos

State CA

Zip Code 95003

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:

$C = \frac{V_a M_a}{V_a + V_b}$, where V_a = the volume of H_4A taken at the outset

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 $Q = 1 + \frac{K_1}{[H^+]} + \frac{K_1 K_2}{[H^+]^2} + \frac{K_1 K_2 K_3}{[H^+]^3} + \frac{K_1 K_2 K_3 K_4}{[H^+]^4}$. For each acid ion concentration

in the equation above, we now substitute its fraction times C:

$$[H^+] + [Na^+] = \frac{K_w}{[H^+]} + \frac{CK_1}{Q[H^+]} + \frac{2CK_1 K_2}{Q[H^+]^2} + \frac{3CK_1 K_2 K_3}{Q[H^+]^3} + \frac{4CK_1 K_2 K_3 K_4}{Q[H^+]^4}.$$

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 **[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 **[A]**. But make sure 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 **[f]** **[P<S]** if necessary. (You may have pressed **[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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$$\begin{aligned}
& [H^+]^6 + (K_1 + [Na^+])[H^+]^5 + (K_1K_2 + [Na^+]K_1 - CK_1 - K_w)[H^+]^4 \\
& + (K_1K_2K_3 + [Na^+]K_1K_2 - 2CK_1K_2 - K_1K_w)[H^+]^3 \\
& + (K_1K_2K_3K_4 + [Na^+]K_1K_2K_3 - 3CK_1K_2K_3 - K_1K_2K_w)[H^+]^2 \\
& + ([Na^+]K_1K_2K_3K_4 - 4CK_1K_2K_3K_4 - K_1K_2K_3K_w)[H^+] - K_1K_2K_3K_4K_w = 0.
\end{aligned}$$

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:

$$\begin{aligned}
& [H^+]^5 + (K_1 + [Na^+])[H^+]^4 + (K_1K_2 + [Na^+]K_1 - CK_1 - K_w)[H^+]^3 \\
& + (K_1K_2K_3 + [Na^+]K_1K_2 - 2CK_1K_2 - K_1K_w)[H^+]^2 \\
& + ([Na^+]K_1K_2K_3 - 3CK_1K_2K_3 - K_1K_2K_w)[H^+] - K_1K_2K_3K_w = 0
\end{aligned}$$

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 $[f] [e]$ 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_3PO_4 titrated 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:

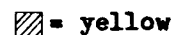
```
[f] [E] ----- 0.000
[C] ----- 1; Base mode
[C] ----- 0; Acid mode (correct)
7.5 [EEX] [CHS] 3[E] 6.2[EEX] [CHS] 8[E] [EEX] [CHS] 12[E]
50[ENTER] .2[ENTER] .5[D] ----- 3.000 (number of K's entered)
THEN:
```

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.

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[illegible]

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBL0	21 13	Reset FO to acid mode	057	RCL0	36 00	*K's +1 → R ₁ ; R ₁ now ready for step 90
002	SF0	16 21 00		058	STOI	35 46	K ₁
003	0	00		059	RCL1	36 01	[Na ⁺]
004	RTN	24		060	RCLA	36 11	
005	*LBLA	21 11		061	+	-55	
006	X=0?	16-43		062	FZS	16-51	
007	SF2	16 21 02		063	ST00	35 00	Store a in R ₅₀
008	FRTX	-14		064	FZS	16-51	
009	RCLB	36 12		065	RCL1	36 01	K ₁
010	XZY	-41		066	RCLC	36 13	C
011	x	-35	067	x	-35		
012	LSTX	16-63	068	JX	54	$\sqrt{K_1 C} = [H^+]_{\text{trial}}$ if Vol.=0	
013	RCLD	36 14	069	FZ?	16 23 02	Was Vol.=0?	
014	+	-55	070	GT01	22 01	Y: begin iterations	
015	=	-24	071	GT0B	22 12	N: use pH _{est} first	
016	STOA	35 11	072	*LBL0	21 00		
017	RCLC	36 15	073	RCL1	36 45		
018	LSTX	16-63	074	x	-35		
019	=	-24	075	GT0b	22 16 12	See p.4	
020	STOC	35 13	076	*LBLa	21 16 11		
021	R↑	16-31	077	2	02		
022	STOB	35 08	078	F0?	16 23 00	Change pH _{est} by ±2	
023	RCL0	36 00	079	CHS	-22		
024	STO7	35 07	080	ST+8	35-55 08		
025	*LBLc	21 16 13	081	*LBLB	21 12		
026	RCL7	36 07	082	RCL8	36 08		
027	STOI	35 46	083	GSBd	23 16 14		
028	ISZI	16 26 46	084	CHS	-22		
029	RCL1	36 45	085	10*	16 33	[H ⁺] = 10 ^{-pH}	
030	RCLA	36 11	086	*LBL1	21 01		
031	+	-55	087	FZS	16-51		
032	DSZI	16 25 46	088	ENT↑	-21		
033	RCL1	36 46	089	ENT↑	-21	Load stack with [H ⁺]	
034	RCLC	36 13	090	GT01	22 45	Use correct N-R routine	
035	x	-35	091	*LBL5	21 05	Routine for 4 K's	
036	-	-45	092	6	06		
037	RCL1	36 45	093	x	-35		
038	x	-35	094	RCL0	36 00		
039	EEK	-23	095	5	05		
040	CHS	-22	096	GSB6	23 06		
041	1	01	097	RCL1	36 01		
042	4	04	098	4	04		
043	-	-45	099	GSB6	23 06	Start forming f([H ⁺])	
044	*LBLb	21 16 12	100	RCL2	36 02		
045	DSZI	16 25 46	101	3	03		
046	GT00	22 00	102	GSB6	23 06		
047	RCL7	36 07	103	RCL3	36 03		
048	XZ1	16-41	104	2	02		
049	XZY	-41	105	GSB6	23 06		
050	FZS	16-51	106	RCL4	36 04		
051	STOI	35 45	107	GSB8	23 08		
052	FZS	16-51	108	RCL3	36 03		
053	7	07	109	GSB7	23 07		
054	STOI	35 46	110	RCL4	36 04	Continue forming f([H ⁺])	
055	DSZI	16 25 45	111	GSB7	23 07		
056	GT00	22 16 13	112	RCL5	36 05		

REGISTERS									
0 [#] K's + 1	1 ¹ K ₁	2 ² K ₂	3 ³ K ₃	4 ⁴ K ₄	5 ⁵ O	6 ⁶ O	7 ⁷ Counter	8 ⁸ pH _{est}	9 ⁹ [H ⁺] _{trial}
S0 a	S1 b	S2 c	S3 d	S4 e	S5 f	S6 g'([H ⁺])	S7	S8	S9
A [Na ⁺]	B N _b	C C	D V _a	E M _a V _a	I Control				

REGISTERS

0 #K's + 1	1 K ₁	2 K ₂	3 K ₃	4 K ₄	5 O	6 O	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 N _b	C C	D v _a	E M V _a	I Control				

97 Program Listing II

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
113	*LBL9	21 09	Finish forming $f([H^+])$	169	3	03	
114	+	-55		170	GSB6	23 06	
115	RCL6	36 06	RCL $f'([H^+])$	171	RCL2	36 02	
116	P2S	16-51		172	2	02	
117	÷	-24		173	GSB6	23 06	
118	-	-45	Forms $[H^+]_{n+1}$	174	RCL3	36 03	
119	X<0?	16-45	Is $[H^+]$ negative?	175	GSB6	23 06	
120	GT0a	22 16 11	Y: start over w. new pH_{est}	176	RCL3	36 03	
121	ST09	35 09	N: continue	177	GSB7	23 07	Continue forming $f([H^+])$
122	%CH	16 55		178	RCL4	36 04	
123	ABS	16 31		179	GT09	22 09	
124	1	01		180	*LBL3	21 03	Routine for 2 K's
125	X<Y?	16-35	Is $1\% \leq \%CH $?	181	4	04	
126	SF2	16 21 02	Y: set F2 N: leave it off	182	x	-35	
127	RCL9	36 09	RCL $[H^+]$	183	RCL0	36 00	Start forming $f'([H^+])$
128	F2?	16 23 02	Was $1\% \leq \%CH $?	184	3	03	
129	GT01	22 01	Y: do another iteration	185	GSB6	23 06	
130	LOG	16 32	N: $[H^+] \rightarrow pH$	186	RCL1	36 01	
131	CHS	-22		187	2	02	
132	GSBd	23 16 14		188	GSB6	23 06	
133	PRTX	-14		189	RCL2	36 02	
134	SPC	16-11	HP-67user should delete	190	GSB8	23 08	
135	RTN	24		191	RCL3	36 03	Continue forming $f([H^+])$
136	*LBLd	21 16 14		192	GT09	22 09	
137	F0?	16 23 00	Acid mode?	193	*LBL2	21 02	Routine for 1 K
138	RTN	24	Y: leave pH alone	194	3	03	
139	1	01	N: $14 - pH = pOH$ or	195	x	-35	Start forming $f'([H^+])$
140	4	04	$14 - pOH = pH$	196	RCL0	36 00	
141	X<Y	-41		197	2	02	
142	-	-45		198	GSB6	23 06	
143	RTN	24		199	RCL1	36 01	
144	*LBL6	21 06		200	SF2	16 21 02	Cause LBL 8 to exit to LBL 9
145	x	-35		201	GT08	22 08	
146	*LBL7	21 07	Steps repeatedly used	202	*LBLc	21 16 15	
147	+	-55	in polynomial	203	CLRG	16-53	
148	x	-35	evaluation	204	ISZi	16 26 45	
149	RTN	24		205	RTN	24	Initialize R_0 to 1
150	*LBL8	21 08		206	*LBLc	21 15	
151	+	-55		207	ISZi	16 26 46	
152	ST06	35 06	Steps common to all	208	ST0i	35 45	$K_i \rightarrow R_i$
153	CLX	-51	4 N-R routines;	209	RTN	24	
154	RCL0	36 00	completes and stores	210	*LBLd	21 14	$N_i \rightarrow R_0$
155	GSB7	23 07	$f'([H^+])$ in R_6 ; begins	211	ST0B	35 12	
156	RCL1	36 01	computation of $f([H^+])$	212	R+	-31	$V_e \rightarrow R_0$
157	GSB7	23 07		213	X<Y	-41	
158	RCL2	36 02		214	ST0D	35 14	$V_e M_e \rightarrow R_e$
159	F2?	16 23 02	F2 set in LBL 2 only	215	x	-35	* of K's
160	GT09	22 09		216	ST0E	35 15	* K's + 1 $\rightarrow R_0$
161	GT07	22 07		217	RCL1	36 46	
162	*LBL4	21 04	Routine for 3 K's	218	ST+0	35-55 00	
163	5	05		219	RTN	24	
164	x	-35		220	*LBLC	21 13	
165	RCL0	36 00	Start forming $f'([H^+])$	221	CF0	16 22 00	Clear F0 to base mode
166	4	04		222	1	01	
167	GSB6	23 06		223	RTN	24	
168	RCL1	36 01					

LABELS					FLAGS	SET STATUS		
A	B	C	D	E	0	FLAGS	TRIG	DISP
pH $\rightarrow$ V $\rightarrow$ pH	pH $\rightarrow$ N-R	Base?	V $\rightarrow$ M $\rightarrow$ N	$K_1; K_2 - K_4$	Acid mode	ON OFF	DEG ☒	FIX ☒
a $[H^+] < 0$ restart	b used	c used	d pH $\rightarrow$ pOH	e Start	1	1 ☐ ☒	GRAD ☐	SCI ☐
0 used	1 N-R start	2 mono.	3 di.	4 tri.	2 Used	2 ☐ ☒	RAD ☐	ENG ☐
5 quad.	6 x + x	7 + x	8 N-R mid.	9 N-R end	3	3 ☐ ☒		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 Description

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 are

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	Equations:
Contributor's Name	Ideal gas: $PV = nRT$
Address	Redlich-Kwong: $P = \frac{nRT}{(V - b)} - \frac{a}{T^{1/2} V (V + b)}$ $a = 4.934 b nRT_c^{1.5}$ $b = 0.0867 \frac{nRT_c}{P_c}$
City	

Program Description	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 R₀, R₁ 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 cm³ space at 1200 K. What is the pressure in bars? Assume an ideal gas.

Keystrokes:

Outputs:

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

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 (ft³/lb) of a gas at atmospheric pressure and at a temperature of 513°R? The molecular weight is 29. Assume an ideal gas.

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 cm³/g mole. The temperature will reach 400 K. What will the pressure be according to the Redlich-Kwong relation?

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

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

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

Keystrokes:

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)

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.

$$T_c = 304.2 \text{ K}$$

$$P_c = 72.9 \text{ atm}$$

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

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)

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

5000 B C →	6.39 (g moles)
-------------------	----------------

Sample Problem

Solution(s)

Reference(s)

21

[illegible]

REGISTERS

0	1	2	3	4	5	6	7	8	9
		$a/T^{1/2}$	$(V+b)$	$(V-b)$	P	V	n	R	T
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
A	B	C	D	E	F	G	H	I	J
a	b	T_C	P_C	nR	Control				

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
113	RCL1	36 45	Display result of iteration $\frac{\partial P}{\partial V}$	169	X ²	53	Display P. Calculate a and b.
114	RTN	24		170	=	-24	
115	*LBL6	21 06		171	RCL2	36 02	
116	RCL6	36 06		172	x	-35	
117	ENT1	-21		173	-	-45	
118	+	-55		174	RCL5	36 15	
119	RCL8	36 12		175	x	-35	
120	+	-55		176	RCL1	36 45	
121	RCL2	36 02		177	=	-24	
122	x	-35		178	RTN	24	
123	RCL3	36 03	$\frac{\partial P}{\partial T}$	179	*LBL5	21 05	
124	RCL6	36 06		180	LSTX	16-63	
125	x	-35		181	+	-55	
126	X ²	53		182	STO5	35 05	
127	=	-24		183	R/S	51	
128	RCL5	36 15		184	*LBL1	21 01	
129	RCL9	36 09		185	RCL7	36 07	
130	x	-35		186	RCL8	36 08	
131	RCL4	36 04		187	x	-35	
132	X ²	53		188	STOE	35 15	
133	=	-24	$\frac{\partial P}{\partial n}$ or $\frac{\partial P}{\partial R}$	189	.	-62	
134	-	-45		190	0	00	
135	RTN	24		191	8	08	
136	*LBL9	21 09		192	6	06	
137	RCL5	36 15		193	7	07	
138	RCL4	36 04		194	RCLD	36 14	
139	=	-24		195	=	-24	
140	RCL2	36 02		196	X ² Y	-41	
141	2	02		197	RCLC	36 13	
142	=	-24		198	x	-35	
143	RCL9	36 09		199	x	-35	
144	=	-24		200	STOB	35 12	
145	RCL6	36 06		201	LSTX	16-63	
146	=	-24		202	x	-35	
147	RCL3	36 03		203	RCLC	36 13	
148	=	-24		204	IX	54	
149	+	-55		205	x	-35	
150	RTN	24		206	4	04	
151	*LBL7	21 07		207	.	-62	
152	*LBL8	21 08		208	9	09	
153	RCL9	36 09		209	3	03	
154	RCL6	36 06		210	4	04	
155	x	-35		211	x	-35	
156	RCL4	36 04		212	STOA	35 11	
157	X ²	53		213	RTN	24	
158	=	-24					
159	RCL6	36 06					
160	ENT1	-21					
161	+	-55					
162	RCL8	36 12					
163	+	-55					
164	RCL5	36 15					
165	=	-24		220			
166	RCL6	36 06					
167	=	-24					
168	RCL3	36 03					

LABELS					FLAGS		SET STATUS			
A ↔P	B ↔V	C ↔n	D ↔R	E ↔T	0 R-K		FLAGS		TRIG	DISP
a R-K?	b T _C	c P _C	d	e	1 a,b		ON OFF			
0 Used	1 a,b	2 Iter	3	4	2		0 ☐ ☒	DEG ☒	FIX ☒	
5 P	6 V	7 n	8 R	9 T	3 Calc		1 ☐ ☒	GRAD ☐	SCI ☐	
							2 ☐ ☒	RAD ☐	ENG ☐	n <u>2</u>
							3 ☐ ☒			

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

$$\left(P + \frac{a}{\bar{V}^2}\right) (\bar{V} - b) = RT \text{ where } \bar{V} = \frac{V}{n}$$

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

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

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 $\bar{V}_c = 3b$, $P_c = \frac{a}{27b^2}$, $T_c = \frac{8a}{27bR}$

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 $^{\circ}K$, 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 $a = .2444$ and $b = .2661$

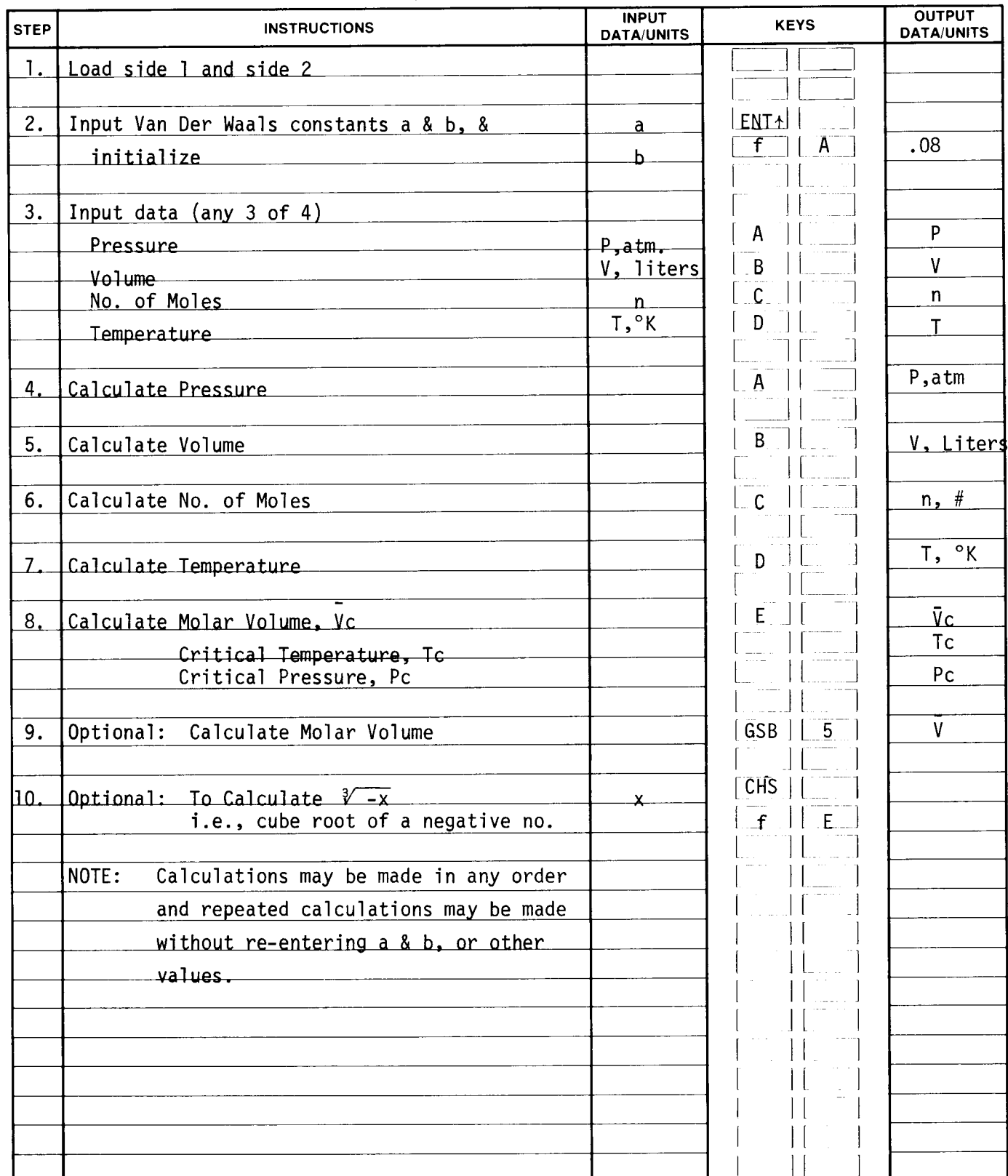
Solution(s)

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

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. Stegun, Handbook of Mathematical Functions, Nat'l Bureau of Standards, 1964, p 17.



97 Program Listing I

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBLa	21 16 11	Initialize:	057	3	03	
002	ST02	35 02		058	=	-24	
003	R↓	-31	Store a,b & R	059	ST00	35 00	
004	ST01	35 01		060	RCL5	36 05	
005	.	-62		061	3	03	
006	0	00		062	=	-24	
007	8	08		063	RCL0	36 00	
008	2	02		064	X²	53	
009	0	00		065	-	-45	
010	5	05		066	ENT↑	-21	
011	6	06		067	ENT↑	-21	
012	2	02		068	X	-35	
013	ST03	35 03		069	X	-35	
014	RTN	24	Pressure	070	ST07	35 07	
015	*LBLA	21 11	Data entry?	071	RCL5	36 05	
016	F3?	16 23 03		072	RCL0	36 00	
017	GT01	22 01	Calculate P	073	X	-35	
018	GSB5	23 05		074	RCL4	36 04	
019	RCL3	36 03	.	075	-	-45	
020	RCLD	36 14	.	076	2	02	
021	X	-35	.	077	=	-24	
022	RCL9	36 09	.	078	RCL0	36 00	
023	RCL2	36 02		079	ENT↑	-21	
024	-	-45		080	X²	53	
025	=	-24		081	X	-35	
026	RCL1	36 01		082	-	-45	
027	RCL9	36 09		083	ST08	35 08	
028	X²	53		084	ENT↑	-21	
029	=	-24		085	X	-35	
030	-	-45		086	RCL7	36 07	
031	ST0A	35 11		087	+	-55	
032	PRTX	-14		088	JX	54	
033	RTN	24	Store P	089	ST07	35 07	
034	*LBL1	21 01		090	RCL8	36 08	
035	ST0A	35 11		091	+	-55	
036	RTN	24	Volume	092	GSBe	23 16 15	
037	*LBLB	21 12	Date entry?	093	RCL8	36 08	
038	F3?	16 23 03		094	RCL7	36 07	
039	GT02	22 02	Calculate V	095	-	-45	
040	RCL2	36 02		096	GSBe	23 16 15	
041	RCL1	36 01		097	+	-55	
042	RCLA	36 11		098	RCL0	36 00	
043	=	-24		099	-	-45	
044	ST05	35 05		100	RCLC	36 13	
045	X²Y	-41		101	X²Y	-41	
046	X	-35		102	X	-35	
047	CHS	-22		103	ST0B	35 12	
048	ST04	35 04		104	PRTX	-14	
049	LSTX	16-63		105	RTN	24	
050	RCL3	36 03		106	*LBL2	21 02	Store V
051	RCLD	36 14		107	ST0B	35 12	
052	X	-35		108	RTN	24	
053	RCLA	36 11		109	*LBLC	21 13	Moles
054	=	-24		110	F3?	16 23 03	Data entry?
055	+	-55		111	GT04	22 04	
056	CHS	-22		112	RCLB	36 12	

REGISTERS

0	Used	1	a	2	b	3	R	4	Used	5	Used	6		7	Used	8	Used	9	-	V
S0		S1		S2		S3		S4		S5		S6		S7		S8		S9		
A	P	B	V	C	n	D	T	E		F		G		H		I		J		

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
113	RCL9	36 09	Calculate n	169	PRTX	-14	Calculate $\sqrt[3]{-x}$
114	=	-24		170	X $\div$ Y	-41	
115	STOC	35 13	Store n	171	LSTX	16-63	
116	PRTX	-14		172	=	-24	
117	RTN	24	Temperature	173	PRTX	-14	
118	*LBL4	21 04		174	RTN	24	
119	STOC	35 13	Data entry?	175	*LBL _e	21 16 15	
120	RTN	24		176	X<0?	16-45	
121	*LBLD	21 14	Calculate T	177	SF1	16 21 01	
122	F3?	16 23 03		178	ABS	16 31	
123	GT03	22 03	Calculate T	179	3	03	
124	GSB5	23 05		180	1/X	52	
125	RCLA	36 11	Store T	181	Y*	31	
126	RCL1	36 01		182	F1?	16 23 01	
127	RCL9	36 09	Calculate $\bar{V}$	183	CHS	-22	
128	X $\div$	53		184	CF1	16 22 01	
129	=	-24	Calculate $\bar{V}$, Pc, Tc	185	RTN	24	
130	+	-55					
131	RCL9	36 09	Calculate $\bar{V}$				
132	RCL2	36 02					
133	-	-45	Calculate $\bar{V}$				
134	x	-35					
135	RCL3	36 03	Calculate $\bar{V}$				
136	=	-24					
137	STOD	35 14	Calculate $\bar{V}$				
138	PRTX	-14					
139	RTN	24	Calculate $\bar{V}$				
140	*LBL3	21 03					
141	STOD	35 14	Calculate $\bar{V}$				
142	RTN	24					
143	*LBL5	21 05	Calculate $\bar{V}$				
144	RCLB	36 12					
145	RCLC	36 13	Calculate $\bar{V}$				
146	=	-24					
147	STO9	35 09	Calculate $\bar{V}$				
148	RTN	24					
149	*LBL _e	21 15	Calculate $\bar{V}$				
150	8	08					
151	RCL1	36 01	Calculate $\bar{V}$				
152	x	-35					
153	9	09	Calculate $\bar{V}$				
154	=	-24					
155	RCL3	36 03	Calculate $\bar{V}$				
156	=	-24					
157	RCL1	36 01	Calculate $\bar{V}$				
158	9	09					
159	=	-24	Calculate $\bar{V}$				
160	RCL2	36 02					
161	=	-24	Calculate $\bar{V}$				
162	RCL2	36 02					
163	3	03	Calculate $\bar{V}$				
164	x	-35					
165	DSP5	-63 05	Calculate $\bar{V}$				
166	PRTX	-14					
167	DSP2	-63 02	Calculate $\bar{V}$				
168	=	-24					

LABELS										FLAGS	SET STATUS					
A	P	B	V	C	n	D	T	E	$\bar{V}_C, P_C, T_C$	0	FLAGS		TRIG		DISP	
a	Initialize	b		c		d		e	$\sqrt[3]{-X}$	1	$\sqrt[3]{-X}$	ON	OFF	DEG	TRIG	FIX
0		1	Sto P	2	Sto V	3	Sto T	4	Sto n	2		0	☐	☒	☒	☒
												1	☐	☒	GRAD	☐
												2	☐	☒	RAD	☐
5	V	6		7		8		9		3	Data Entry	3	☐	☒		ENG
																n <u>2</u>

Program Description I

Program Title Beer's Law/Absorbivity 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 absorbivity, a , by the least squares method:

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

Initialization (Key A) clears all registers and sets b equal to 1 cm. Either conc., absorbance (Key D) or conc., $\%T$ (Key C) data may be entered. In the latter case $\%T$ is automatically converted to absorbance: $A = 2 - \log \%T$

Corrections to C, A or $C, \%T$ may be made by pressing 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 absorbivity 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).

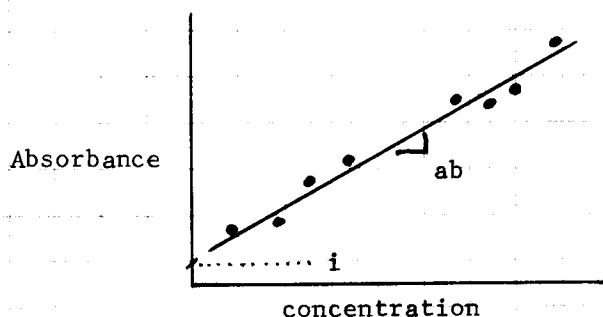
Operating Limits and Warnings Unless b is 1 cm, then a new value must be entered (f, A) each time the program is initialized. Initialization also removes molecular weight from memory. The least squares program requires at least two C, A data pairs to calculate a . Enter 0,0 into Key D if only one pair 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

	<u>%T</u>	<u>mg/l as P</u>
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

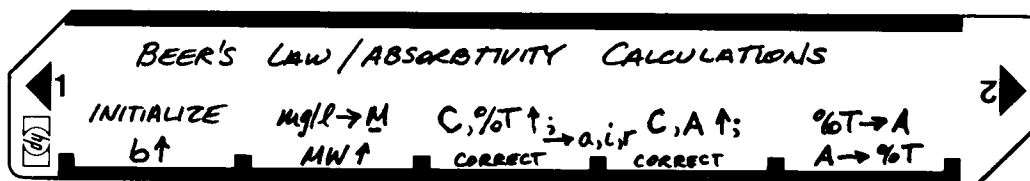
Solution(s)

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

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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 $b \neq 1$	b	f	A	b
4	(optional) enter molecular weight	MW	f	B	MW
5	Enter molar conc. and absorbance	C_i, A_i	$\uparrow$	D	n_i
	or				
5	Enter mg/l and absorbance	C_i, A_i	$\uparrow$	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	$C_i, \%T_i$	$\uparrow$	C	n_i
	or				
5	Enter mg/l and percent transmittance	$C_i, \%T_i$	$\uparrow$	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	$\uparrow$	d	n-1
	or correct an entry	$C_k, \%T_k$	$\uparrow$	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 from mg/l values	MW	f	B	MW
		mg/l	B		$\underline{M}$
	To calculate A from %T	%T	E		A
	To calculate %T from A	A	f	e	%T

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	f LBL A	31 25 11	INITIALIZE		-	51	
	f CL REG	31 43	Clear all reg.		CHS	42	
	f PPS	31 42	Set b=1		g 10 ^x	32 53	
	f CL REG	31 43		060	f FIX	31 23	
	I	01			DSP I	23 01	
	STO A	33 11			h RTN	35 22	→ %T
	f FIX	31 23			f LBL 1	31 25 01	
	DSP I	23 01			f PPS	31 42	CALCULATE
	h RTN	35 22			RCL 9	34 09	absorbivity
010	g LBL A	32 25 11	ENTER b		RCL B	34 08	intercept
	STO A	33 11			X	71	Correlation Coef.
	h RTN	35 22			RCL 4	34 04	
	f LBL B	31 25 12	mg/l → M		RCL 6	34 06	
	RCL B	34 12		070	X	71	
	÷	81			-	51	
	EE X	43			STO C	33 13	
	3	03			RCL 9	34 09	
	÷	81			RCL 7	34 07	
	DSP 2	23 02			X	71	
020	g SCI	32 23			RCL 6	34 06	
	h RTN	35 22			g X ²	32 54	
	g LBL b	32 25 12	ENTER MW		-	51	
	STO B	33 12			STO D	33 14	
	h RTN	35 22		080	÷	81	
	f LBL D	31 25 14	ENTER C _i , A _i		RCL A	34 11	
	Σ+	21			÷	81	
	f FIX	31 23			f FIX	31 23	
	DSP 0	23 00			DSP 0	23 00	
	R/S	84			f -X-	31 84	DISPLAY a
030	GTO 1	22 01	→ a, i, r		RCL 7	34 07	
	g LBL d	32 25 14	CORRECT C _i , A _i		RCL 4	34 04	
	h Σ-	35 21			X	71	
	R/S	84			RCL 6	34 06	
	GTO 1	22 01	→ a, i, r	090	RCL B	34 08	
	f LBL C	31 25 13	ENTER C _i , %T _i		X	71	
	f GSBE	31 22 15			-	51	
	Σ+	21			RCL D	34 14	
	f FIX	31 23			÷	81	
	DSP 0	23 00			DSP 4	23 04	
040	R/S	84	→ a, i, r		f -X-	31 84	DISPLAY i
	GTO 1	22 01			RCL C	34 13	
	g LBL C	32 25 13	CORRECT C _i , %T _i		RCL D	34 14	
	f GSBE	31 22 15			f √x	31 54	
	h Σ-	35 21		100	÷	81	
	R/S	84	→ a, i, r		RCL 9	34 09	
	GTO 1	22 01			RCL 5	34 05	
	f LBL E	31 25 15	ENTER %T		X	71	
	f LOG	31 53			RCL 4	34 04	
	Z	02			g X ²	32 54	
050	-	51			-	51	
	CHS	42			f √x	31 54	
	f FIX	31 23			÷	81	DISPLAY r
	DSP 4	23 04	→ A		f PPS	31 42	
	h RTN	35 22	ENTER A	110	R/S	84	
	g LBL E	32 25 15			GTO 1	22 01	
	2	02			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 ΣA	S5 ΣA ²	S6 ΣC	S7 ΣC ²	S8 ΣAC	S9 n
A	b	B	MW	C	n ΣAC - ΣA ΣC	D	n ΣC ² - (ΣC) ²	E	I

67 Program Listing II

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[illegible]

Program Description I

Program Title Activity Coefficients from Potentiometric Data

Contributor's Name John R. Joyce

Address 1825 S. 71st E. Avenue

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 involved 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.

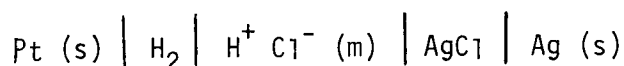
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Program Description II

Sketch(es)

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

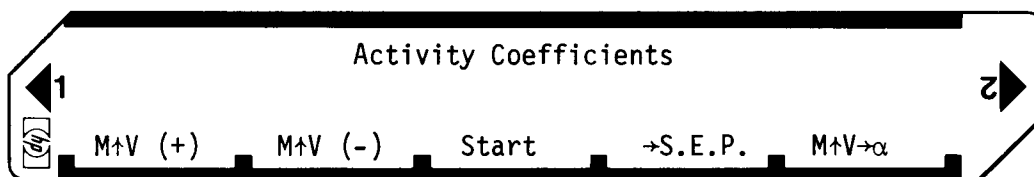
Concentration (M)	Potential (V)	F = 1
0.003215	0.52053	$v = 2$
0.004488	0.50384	$E_{\text{REF}} = 0.000$
0.005619	0.49257	$n = 1$
0.007311	0.47948	
0.009138	0.46860	
0.011195	0.45861	



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
 .009138 [ENTER] .46860[A] .011195[ENTER] .45861[A] --> 6
 [D] --> .9338 (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.

[illegible]

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

REGISTERS									
0	1 M	2 V	3 Y	4	5	6	7	8	9
S0	S1	S2	S3	S4 ΣM	S5 ΣM^2	S6 Σy	S7 Σy^2	S8 ΣMy	S9 n
A f	B v	C Ref. Electrode(v)	D #e ⁻	E S.E.P.	I				

Program Description I

Program Title Crystallographic to cartesian coordinate transformations

Contributor's Name Craig G. Shaeter

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:

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

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

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

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

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

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

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

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

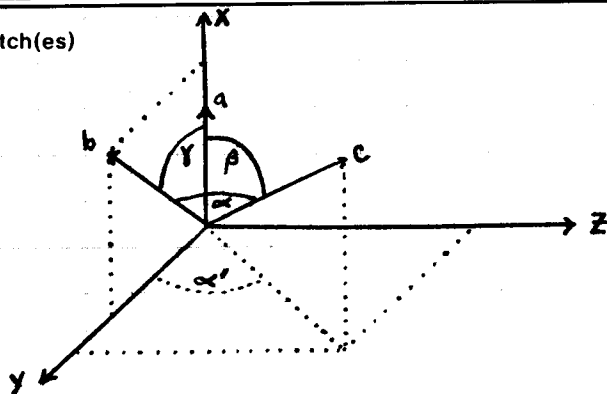
Operating Limits and Warnings One of the distances, D_{ij} , must be calculated before calculating the angle between three points. Input a, b, c before α, β, γ .

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:

$$a = 11.716 \text{ \AA}$$

$$\alpha = 90.00^\circ$$

$$b = 8.102 \text{ \AA}$$

$$\beta = 106.14^\circ$$

$$c = 11.166 \text{ \AA}$$

$$\gamma = 90.00^\circ$$

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

$$N_2 \quad 0.508 \quad 0.259 \quad 0.170$$

$$C_1 \quad 0.585 \quad 0.410 \quad 0.189$$

$$C_3 \quad 0.430 \quad 0.249 \quad 0.034$$

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.) $11.716 \uparrow 8.102 \uparrow 11.166 \quad [A] \rightarrow 0.000$

2.) $90.00 \uparrow 106.14 \uparrow 90.00 \quad [F][A] \rightarrow 0.000$

3.) $0.585 \uparrow 0.410 \uparrow 0.189 \quad [B] \rightarrow 6.267 \quad x_1$

4.) $0.508 \uparrow 0.259 \uparrow 0.170 \quad [C] \rightarrow 5.424 \quad x_2 \quad 3.322 \quad y_1$

5.) $0.430 \uparrow 0.249 \uparrow 0.034 \quad [D] \rightarrow 2.098 \quad y_2 \quad 2.027 \quad z_1$

$\rightarrow 4.932 \quad x_3 \quad 1.823 \quad z_2 \quad 1.000 \quad \text{atom \#1}$

$2.017 \quad y_3 \quad 2.000 \quad \text{atom \#2}$

$0.365 \quad z_3$

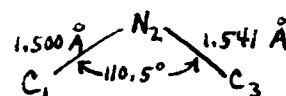
$3.000 \quad \text{atom \#3}$

Reference(s) 6.) $12 \quad [F][D] \rightarrow 1.500 \quad \text{Distance from atoms 1 to 2}$

$[RCLB] \rightarrow 1.541 \quad \text{Distance from atoms 2 to 3}$

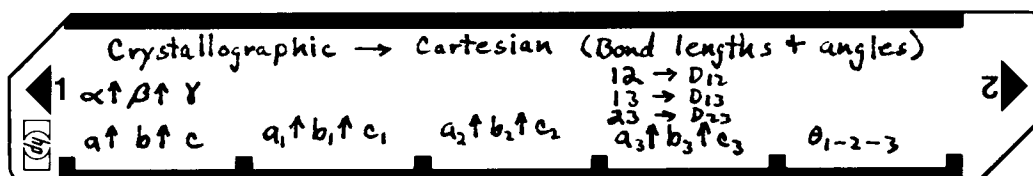
$[RCLC] \rightarrow 2.499 \quad \text{Distance from atoms 1 to 3}$

7.) $[E] \rightarrow 110.536 \quad \text{Angle from 1-2-3}$



User Instructions

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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.				

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBL A	31 25 11	store a, b, c		1	01	i = 2
	STO 7	33 07			RTN	35 22	
	STO 8	33 08			*LBL C	31 25 13	
	STO 9	33 09		060	1	01	
	R↓	35 53			4	04	
	STO 4	33 04			STOE	33 15	
	STO 5	33 05			R↓	35 53	
	R↓	35 53			G S B 0	31 22 00	
	STO 1	33 01			2	02	
010	CLX	44			RTN	35 22	
	RTN	35 22	store α, β, γ calculate transformation matrix		*LBL D	31 25 14	i = 3
	*LBL a	32 25 11			1	01	
	STOC	33 13			7	07	
	R↓	35 53		070	STOE	33 15	
	STOB	33 12			R↓	35 53	
	R↓	35 53			G S B 0	31 22 00	
	COS	31 63			3	03	
	STOA	33 11			RTN	35 22	
	RCLC	34 13			*LBL O	31 25 00	
020	COS	31 63			STOB	33 12	
	STOD	33 14	cos γ		R↓	35 53	store a; b; c;
	STOX 4	33 71 04			STOA	33 11	
	RCLC	34 13			R↓	35 53	
	SIN	31 62		080	STO O	33 00	
	STOE	33 15			1	01	
	STOX 5	33 71 05			STOI	35 33	
	RCLB	34 12			G S B 1	31 22 01	
	COS	31 63			2	02	
	STO 0	33 00			STOI	35 33	
030	STOX 7	33 71 07			G S B 1	31 22 01	
	RCLB	34 12	sin β		3	03	multiply oblique coordinate by matrix element and add
	SIN	31 62			STOI	35 33	
	STOX 8	33 71 08			G S B 1	31 22 01	
	STOX 9	33 71 09		090	RTN	35 22	
	RCL E	34 15			*LBL I	31 25 01	
	X	71			0	00	
	RCL D	34 14			RCL O	34 00	
	RCL O	34 00			G S B 2	31 22 02	
	X	71			RCL A	34 11	
	RCL A	34 11			G S B 2	31 22 02	
040	X ≡ Y	35 52	$\frac{\cos \alpha - \cos \gamma \cos \beta}{\sin \gamma \sin \beta}$ sin α'		G S B 2	31 22 02	display rectangular coordinate store cartesian coordinates
	-	51			PSE	35 72	
	X ≡ Y	35 52		100	RCL E	34 15	
	÷	81			X ≡ I	35 24	
	STOX 8	33 71 08			R↓	35 53	
	COS ⁻¹	32 63			STO(i)	33 24	
	SIN	31 62			ISE	31 34	
	STOX 9	33 71 09			R↑	35 54	
	CLX	44			X ≡ I	35 24	
050	RTN	35 22			STOE	33 15	
	*LBL B	31 25 12	a; b; c; → x; y; z; i = 1		RTN	35 22	perform matrix multiplication
	1	01			*LBL 2	31 25 02	
	1	01		110	RCL(i)	34 24	
	STOE	33 15			X	71	
	R↓	35 53			+	61	
	G S B 0	31 22 00					

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	

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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			*LBL7	31 25 07	subtract 6 from I	
	RTN	35 22			RCL I	35 34		
	*LBL4	32 25 14	calculate distances		6	06		
	STO 0	33 00	between points		-	51		
	I	01			STO I	35 33		
120	I	01			R↓	35 33		
	STO I	35 33			RTN	35 22		
	0	00			*LBL9	31 25 09	which distance	
	GSRB3	31 22 03	$(x_i - x_j)^2$		I	01	should be	
	GSRB3	31 22 03	$(y_i - y_j)^2$	180	2	02	displayed?	
	GSRB3	31 22 03	$(z_i - z_j)^2$		RCL 0	34 00		
	√X	31 54			X=Y?	32 51		
	STOA	33 11	D ₁₂		GTO I	22 01		
	0	00			I	01		
	GSRB3	31 22 03			3	03		
130	GSRB3	31 22 03			X=Y?	32 51		
	GSRB3	31 22 03			GTO 3	22 03		
	√X	31 54			RCLB	34 12	D ₂₃	
	STOB	33 12	D ₂₃		RTN	35 22		
	0	00		190	*LBL3	31 25 03	D ₁₃	
	GSRB4	31 22 04			RCLC	34 13		
	GSRB4	31 22 04			RTN	35 22		
	GSRB4	31 22 04			*LBL1	31 25 01	D ₁₂	
	√X	31 54			RCLA	34 11		
	STOC	33 13	D ₁₃		RTN	35 22		
140	GTO 9	22 09			*LBL5	31 25 15	calculate angle from	
	*LBL3	31 25 03	$(x_i - x_j)^2$		P=S	31 42	1-2-3	
	RCL(i)	34 24			0	00		
	GSRB5	31 22 05	ISZ, ISZ, ISZ		STOI	35 33		
	RCL(i)	34 24		200	GSRB5	32 22 15	$(x_1 - x_2)(x_3 - x_2) +$	
	-	51			GSRB5	32 22 15	$(y_1 - y_2)(y_3 - y_2) +$	
	X ²	32 54			GSRB5	32 22 15	$(z_1 - z_2)(z_3 - z_2)$	
	+	61			RCLA	34 11	D ₁₂	
	DSZ	31 33			÷	81		
	DSZ	31 33			RCLB	34 12	D ₂₃	
150	RTN	35 22			÷	81		
	*LBL4	31 25 04	D ₁₃		COS ⁻¹	32 63	θ ₁₋₂₋₃	
	RCL(i)	34 24			P=S	31 42		
	GSRB7	31 22 07	add -6 to I		RTN	35 22		
	RCL(i)	34 24		210	*LBL5	32 25 15		
	-	51			ISZ	31 34		
	X ²	32 54			RCL(i)	34 24		
	ISZ	31 34			GSRB5	31 22 05	ISZ, ISZ, ISZ	
	ISZ	31 34			RCL(i)	34 24		
	ISZ	31 34			STOE	33 15		
160	ISZ	31 34			-	51		
	ISZ	31 34			GSRB5	31 22 05		
	ISZ	31 34			RCL(i)	34 24		
	+	61			RCL5	34 15		
	ISZ	31 34		220	-	51		
	RTN	35 22			X	71		
	*LBL5	31 25 05	add 3 to I		+	61		
	ISZ	31 34			GSRB7	31 22 07	subtract 6 from I	
	ISZ	31 34			RTN	35 22		
LABELS				FLAGS		SET STATUS		
A a↑b↑c	B a ₁ ↑b ₁ ↑c ₁	C a ₂ ↑b ₂ ↑c ₂	D a ₃ ↑b ₃ ↑c ₃	E θ ₁₋₂₋₃	0	FLAGS	TRIG	DISP
a α↑β↑γ	b	c	d D _{ij}	e dot product	1	ON OFF		
0 store a _i b _i c _i	1 store Cartesian coord.	2 matrix multiplication	3 (x _i - x _j) ²	4 D ₁₃	2	0 ☐ ☒	DEG ☒	FIX ☒
5 I+3=I	6	7 I-6=I	8	9 which distance?	3	1 ☐ ☒	GRAD ☐	SCI ☐
						2 ☐ ☒	RAD ☐	ENG ☐
						3 ☐ ☒		n <u>3</u>

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

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

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

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

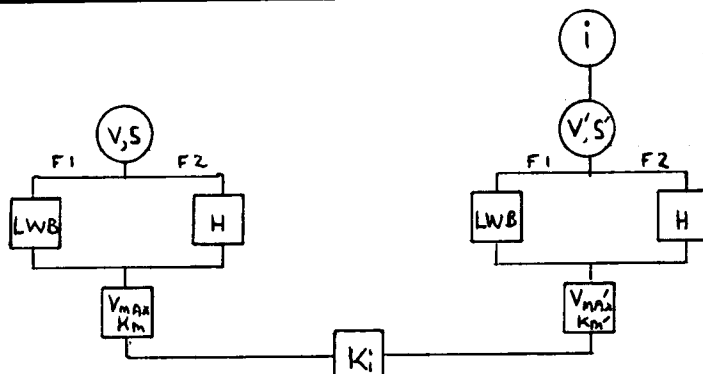
Operating Limits and Warnings Because registers are cleared when selecting an operating mode, do not attempt to change from one type of curve fit to another during data entry. The methods of Lineweaver-Burk and Hofstee will give similar, but not necessarily identical results. For one discussion of the 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 K_m and V_{max} for product formation with and without the inhibitor. What is the K_i ?

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

Solution(s) 4

40 69 88 10 160 15 185

6.00

24 44 60 10 126 15 158

1.0000

6.0000

.9996 (r^2), .0042 (a), .0209 (b)

240.8340 (V_{max}), 5.0275 (K_m)

1.0000

6.0000

.9999 (r^2), .0040 (a), .0377 (b)

249.7286 ($V_{max'}$), 9.4028 (K_m')

6.8943 (K_i)

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

1

←
(d)

Compet Lineweaver Hofstee V→S S→V

2
→

S ↑ V (+)
S ↑ V (-)
r², a, b
Vmax, Km
Ki

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 h R↓ then B .				
	A set of data may be deleted by entering the set as in steps 3 and 4 and pressing B .				

67 Program Listing I

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*Lb1 b	32 25 12	LINEWEAVER-BURK		*Lb1 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	
	*Lb1 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 42	register		x	71	
	Cl Reg	31 43			F? 1	35 71 01	
	P↔S	31 42		070	1/X	35 62	
	1	01			P↔S	31 42	
	Rtn	35 22			Rtn	35 22	
	*Lb1 A	31 25 11	SUMMATION		*Lb1 e	32 25 15	PROJECT S → V
	CF 3	35 61 03	clear Σ - flag		STO A	33 11	
	*Lb1 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	
	*Lb1 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			*Lb1 C	31 25 13	COMPUTE b
	Σ +	21	compute sums		P↔S	31 42	
	*Lb1 7	31 25 07		090	Rcl 8	34 08	
	Ent	41			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	
	*Lb1 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	
	*Lb1 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	
	X↔Y	35 52			Rcl 6	34 06	COMPUTE r ²
	GTO 2	22 02			x ²	32 54	
	*Lb1 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	STEP	KEY ENTRY	KEY CODE	COMMENTS	
	Rcl 7	34 07						
	+	61		170				
	*	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		180				
	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,	190				
	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	200				
	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	210				
	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		220				
	-	51						
	+	81						
	STO E	33 15						
	Rtn	35 72						
LABELS				FLAGS		SET STATUS		
A	B	C	D	E	0	FLAGS	TRIG	DISP
S↑V(+)	S↑V(-)	r ² , a, b	Vmax, Km	Ki	Linewea	ON OFF		
a competit	b Linewea	c Hofstee	d V→S	e S→V	1 Hofstee	0 ☐ ☒	DEG ☒	FIX ☒
0 Σ-	1	2 V/S	3	4 Km (LWB)	2	1 ☐ ☒	GRAD ☐	SCI ☐
5	6	7 Display	8 Σ-	9 V/S	3 Σ-	2 ☐ ☒	RAD ☐	ENG ☐
						3 ☐ ☒		n 2

Program Description I

Program Title

Mixture Viscosities

Contributor's Name

Richard D. Hyman

Address

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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.

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

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

X_i = Mole fraction of component i

μ_i = Viscosity " " i

M_i = Molecular weight 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 weight 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 1 atm + 293°K.

Component	X_i	M_i	$\mu_i \left(\frac{g}{cm \cdot sec} \right)$
1: CO ₂	.133	44.01	1462 $\times 10^{-7}$
2: O ₂	.039	32.000	2031 $\times 10^{-7}$
3: N ₂	.828	28.016	1754 $\times 10^{-7}$

Solution(s)

$$\begin{aligned}
 &44.01 [A] \quad 32.0 [A] \quad 28.016 [A] \quad 1 [A] \rightarrow 44.01 \\
 &1462 [A] \quad 2031 [A] \quad 1754 [A] \quad 1 [B] \rightarrow 1462 \\
 &.133 [A] \quad .039 [A] \quad .828 [A] \quad 0 [C] \rightarrow .133
 \end{aligned}$$

$$[D] \rightarrow 1714.29912$$

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

Reference(s)

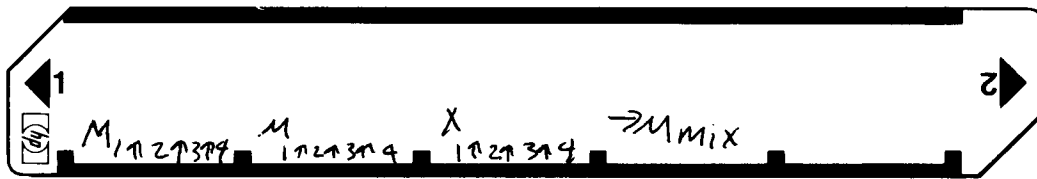
R. Byron Bird, Warren E. Stewart, Edwin N. Lightfoot.

Transport Phenomena 1st Edition

John Wiley + Sons Inc. 1960

User Instructions

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STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS	OUTPUT DATA/UNITS
1	Load Side 1+2 of card			
2	Input Molecular weight of Component 1 (M_1) must be a non zero #	M_1		
3	Enter			
4	Input M_2 (must be $\neq 0$)	M_2		
5	Enter			
6	Input M_3 "	M_3		
7	Enter			
8	Input M_4 "	M_4		
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		
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 $\neq 0$ 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		
23	Solve for μ_{mix}			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	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	*LBLA	21 11		057	RCLA	36 11	
002	CLRG	16-53		058	ST+0	35-55 00	
003	PZS	16-51		059	RCL5	36 05	
004	CLRG	16-53		060	RCLA	36 11	
005	PZS	16-51		061	x	-35	
006	ST04	35 04		062	RCL0	36 00	
007	R4	-31		063	=	-24	
008	ST03	35 03		064	ST09	35 09	
009	R4	-31		065	RCL6	36 06	
010	ST02	35 02		066	RCL8	36 08	
011	R4	-31		067	RCL2	36 02	
012	ST01	35 01		068	RCL4	36 04	
013	RTN	24		069	GSBE	23 15	
014	*LBLB	21 12		070	RCLD	36 14	
015	ST08	35 08		071	x	-35	
016	R4	-31		072	ST00	35 00	
017	ST07	35 07		073	RCL6	36 06	
018	R4	-31		074	RCL7	36 07	
019	ST06	35 06		075	RCL2	36 02	
020	R4	-31		076	RCL3	36 03	
021	ST05	35 05		077	GSBE	23 15	
022	RTN	24		078	RCLC	36 13	
023	*LBLC	21 13		079	x	-35	
024	ST0D	35 14		080	ST+0	35-55 00	
025	R4	-31		081	RCLB	36 12	
026	ST0C	35 13		082	ST+0	35-55 00	
027	R4	-31		083	RCL6	36 06	
028	ST0B	35 12		084	RCL5	36 05	
029	R4	-31		085	RCL2	36 02	
030	ST0A	35 11		086	RCL1	36 01	
031	RTN	24		087	GSBE	23 15	
032	*LBLD	21 14		088	RCLA	36 11	
033	RCL5	36 05		089	x	-35	
034	RCL8	36 08		090	ST+0	35-55 00	
035	RCL1	36 01		091	RCL6	36 06	
036	RCL4	36 04		092	RCLB	36 12	
037	GSBE	23 15		093	x	-35	
038	RCLD	36 14		094	RCL0	36 00	
039	x	-35		095	=	-24	
040	ST00	35 00		096	ST+9	35-55 09	
041	RCL5	36 05		097	RCL7	36 07	
042	RCL7	36 07		098	RCL8	36 08	
043	RCL1	36 01		099	RCL3	36 03	
044	RCL3	36 03		100	RCL4	36 04	
045	GSBE	23 15		101	GSBE	23 15	
046	RCLC	36 13		102	RCLD	36 14	
047	x	-35		103	x	-35	
048	ST+0	35-55 00		104	ST00	35 00	
049	RCL5	36 05		105	RCLC	36 13	
050	RCL6	36 06		106	ST+0	35-55 00	
051	RCL1	36 01		107	RCL7	36 07	
052	RCL2	36 02		108	RCL6	36 06	
053	GSBE	23 15		109	RCL3	36 03	
054	RCLB	36 12		110	RCL2	36 02	
055	x	-35		111	GSBE	23 15	
056	ST+0	35-55 00		112	RCLB	36 12	

REGISTERS

0	1	2	3	4	5	6	7	8	9
	M_1	M_2	M_3	M_4	M_1	M_2	M_3	M_4	
S0	S1	S2	S3	S4	S5	S6	S7	S8	S9
	M_i	M_j	M_i	M_j					
A	X_1	B	X_2	C	X_3	D	X_4	E	I

97 Program Listing II

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
113	x	-35		169	ST02	35 02	
114	ST+0	35-55 00		170	R↓	-31	
115	RCL7	36 07		171	ST01	35 01	
116	RCL5	36 05		172	RCL4	36 04	
117	RCL3	36 03		173	RCL3	36 03	
118	RCL1	36 01		174	=	-24	
119	GSBE	23 15		175	4	04	
120	RCLA	36 11		176	1/X	52	
121	x	-35		177	YX	31	
122	ST+0	35-55 00		178	RCL1	36 01	
123	RCL7	36 07		179	RCL2	36 02	
124	RCLC	36 13		180	=	-24	
125	x	-35		181	√X	54	
126	RCL0	36 00		182	x	-35	
127	=	-24		183	1	01	
128	ST+9	35-55 09		184	+	-55	
129	RCLD	36 14		185	X²	53	
130	ST00	35 00		186	RCL3	36 03	
131	RCL8	36 08		187	RCL4	36 04	
132	RCL7	36 07		188	=	-24	
133	RCL4	36 04		189	1	01	
134	RCL3	36 03		190	+	-55	
135	GSBE	23 15		191	√X	54	
136	RCLC	36 13		192	=	-24	
137	x	-35		193	8	08	
138	ST+0	35-55 00		194	√X	54	
139	RCL8	36 08		195	=	-24	
140	RCL6	36 06		196	P↔S	16-51	
141	RCL4	36 04		197	RTN	24	
142	RCL2	36 02					
143	GSBE	23 15		200			
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		210			
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	*LBL E	21 15					
164	P↔S	16-51		220			
165	ST04	35 04					
166	R↓	-31					
167	ST03	35 03					
168	R↓	-31					

LABELS					FLAGS	SET STATUS		
A	B	C	D	E		FLAGS	TRIG	DISP
0	1	2	3	4	5	ON OFF		
0	1	2	3	4	5	0 ☐ ☒	DEG ☒	FIX ☒
0	1	2	3	4	5	1 ☐ ☒	GRAD ☐	SCI ☐
0	1	2	3	4	5	2 ☐ ☒	RAD ☐	ENG ☐
0	1	2	3	4	5	3 ☐ ☒		n <u>5</u>

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)

$$\text{LOG } P_v = A/T + B \quad \text{WHERE } P_v = \text{VAPOR PRESSURE,}$$

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 $\Rightarrow$

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

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 $\sum y_i$ FOR THE FIRST BUBBLE. SIMILARLY FOR DEW POINTS, THE PROGRAM DECREMENTS FROM SEED (USU. HIGHEST CONDENSING POINT) CHECKING $\sum x_i$ FOR THE FIRST DROP. THE DECREMENTS OR INCREMENTS ARE CHOSEN BY USER, AS IS THE ACCURACY WITH WHICH THE PROGRAM COMPARES ITS $\sum x_i$, $\sum y_i$ TO THE IDEAL 1.0. THE PRESENT TEMP AND $\sum x_i$ OR $\sum y_i$ 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 REPRESENTATIVE 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 $\approx$ 0.196 H₂O $\approx$ 0.804. Also the vapor pressure of EG at 350°F (855°R) is needed. The following is given
 AT 338°F P_v EG = 310 mm Hg P_v H₂O = 5942 mm Hg
 AT 320°F P_v EG = 220 mm Hg P_v H₂O = 4636 mm Hg

Boiling Points Pure Components (Condensing Points Same)
 AT 760 mm Hg

EG = 338°F H₂O = 212°F

Find bubble and dew points to correspond with 0.1% of vapor and liquid mole fraction sums (ie $\sum x_i$ or $\sum y_i \leq 1.001$)

Solution(s) Follow Instructions

KEYSTROKES

2[H][ST I] 310 [ET] 338 [ET] 220 [ET] 320 [AT] $\rightarrow$ -5150.31

5942 [ET] 338 [ET] 4636 [ET] 320 [R/S] [R/S] $\rightarrow$ -3727.35

760 [STD] [B] 1.001 [STD] [C] 2 [STD] [D] [STD] [E] [F] [P/S] .196 [STD] [Z] .804 [STD] [G] [G] [P/S] $\rightarrow$ 0.80

212 [ET] 460 [F] [STD] [AT] [B] $\rightarrow$ RUNS $\approx$ 100 SEC 221.12 BUBBLE POINT OF

2 [STD] [D] 338 [ET] 460 [F] [STD] [AT] [D] $\rightarrow$ RUNS $\approx$ 130 SEC 308.8 DEW POINT OF

2 [H] [ST I] 395 [ET] 460 [F] [STD] [AT] [C] $\rightarrow$ 834.89 mm Hg LITERATURE GIVES US

848 mm Hg AT 395°F so error is 1.55% FOR P_v CALCULATION

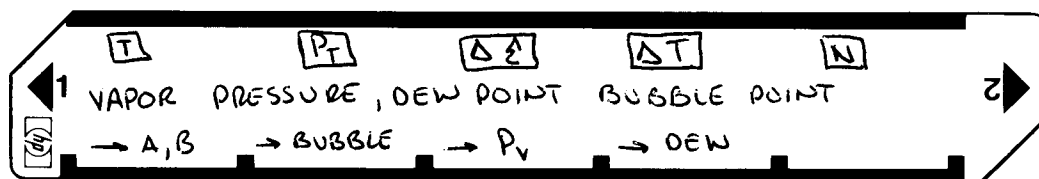
Reference(s)

"INTRODUCTION TO CHEMICAL ENGINEERING THERMODYNAMICS" SMITH & VANNES
 2ND ED. COPYRIGHT 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) STOI	
3	LOAD STACK WITH P_v VS T DATA N TH COMPONENT FIRST, ABS. PRESS MM H_g AND OF PRESS A	N TH COMP.	P_N E↑ T_N E↑ P'_N E↑ T'_N A	mm Hg OF mm Hg OF
4	LOAD STACK WITH P_v VS T DATA FOR N-1 TH COMPONENT NEXT, PRESS R/S TWICE FOLLOW STEP 4 UNTIL ALL COMPONENT DATA HAS BEEN ENTERED.	N-1 TH COMP	P_{N-1} E↑ T_{N-1} E↑ P'_{N-1} E↑ T'_{N-1} R/S R/S	
5	STORE R_A WITH SEED GUESS TEMP.	T OR	(T) STOA	
6	STORE R_B WITH TOTAL PRESSURE	P_T mmHg	(P_T) STOB	
7	STORE R_C WITH ΔE , ie IF YOU WANT Δy_i OR $\Delta y_i \leq 1.001$ STORE 0.001		0.001 STOC	
8	STORE R_D WITH ΔT OR INTERVAL	OR	(ΔT) STOD	
9	STORE R_E WITH N	N	(N) STOE	
10*	FOR BUBBLE POINT STORE X_N IN R_{10+N}	MOLE FRACT	$P \rightarrow S$ STON $P \rightarrow S$	
11*	FOR DEW POINT STORE y_N IN R_{10+N}	MOLE FRACT	$P \rightarrow S$ STON $P \rightarrow S$	
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) STOI	
15*	STORE T IN R_A	OR	(T) STOA	
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

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STEP	KEY ENTRY	KEY CODE	COMMENTS	STEP	KEY ENTRY	KEY CODE	COMMENTS
001	* LBL A	31 25 11	LOADING FOR COEFFICIENT SOLUTIONS		STO 0	33 00	BEGIN LOOP DO N CALCULATE K_i, X_i CALCULATE Y_i ΔY_i LOOP UNTIL N COMPARE Δ WITH 1. CHECK FOR DIRECT APPROACH, IF NOT CHANGE DT COMPARE ACCURACY DISPLAY BUBBLE TRY NEW T START AGAIN CALC. P_V
	STO A	33 11			* LBL 0	31 25 00	
	R↓	35 53			GSD 1	31 22 01	
	STO B	33 12		060	X	71	
	R↓	35 53			GSD 2	31 22 02	
	STO C	33 13			DSZ	31 33	
	R↓	35 53			GTO 0	22 00	
	STO D	33 14			RCL 0	34 00	
	LOG	31 53			1	01	
010	RCL C	34 13			-	51	
	4	04	CONVERTING °F → °R		X>0	31 81	CHECK FOR DIRECT APPROACH, IF NOT CHANGE DT COMPARE ACCURACY DISPLAY BUBBLE TRY NEW T START AGAIN CALC. P_V
	6	06			GTO 3	22 03	
	0	00			ABS	35 64	
	+	61		070	RCL C	34 13	
	STO C	33 13			X↔Y	35 52	
	X	71			X≤Y	32 71	
	RCL B	34 12			GTO 4	22 04	
	LOG	31 53			GSD 5	31 22 05	
	RCL A	34 11			GTO B	22 12	
020	4	04		* LBL C	31 25 13		
	6	06	SOLVED FOR COEFF. B STORE IN RN		RCL A	34 11	CHECK FOR DIRECT APPROACH, IF NOT CHANGE DT COMPARE ACCURACY DISPLAY BUBBLE TRY NEW T START AGAIN CALC. P_V
	0	00			X↔I	35 24	
	+	61			5	05	
	STO A	33 11		080	+	61	
	X	71			X↔I	35 24	
	-	51			RCL(i)	34 24	
	RCL C	34 13			X↔Y	35 52	
	RCL A	34 11			÷	81	
	÷	51			X↔I	35 24	
030	÷	81			5	05	
	STO(i)	33 24	SOLVED FOR COEFF. A		-	51	CHECK FOR DIRECT APPROACH, IF NOT CHANGE DT COMPARE ACCURACY DISPLAY BUBBLE TRY NEW T START AGAIN CALC. P_V
	RCL D	34 14			X↔I	35 24	
	LOG	31 53			RCL(i)	34 24	
	RCL C	34 13		090	+	61	
	X	71			10*	32 53	
	RCL(i)	34 24			RTN	35 22	
	RCL C	34 13		* LBL D	31 25 14		
	X	71			RCL E	34 15	
	-	51			STO I	35 33	
040	X↔I	35 24			CL X	44	
	5	05	STORE IN RN+5		STO 0	33 00	BEGIN DO LOOP CALCULATE K_i, Y_i CALCULATE X_i ΔX_i LOOP UNTIL N COMPARE Δ WITH 1. CHECK FOR CORRECT APPROACH, IF NOT CHANGE DT COMPARE ACCURACY
	+	61			* LBL 6	31 25 06	
	X↔I	35 24			GSD 1	31 22 01	
	STO(i)	33 24		100	X↔Y	35 52	
	X↔I	35 24			÷	81	
	5	05			GSD 2	31 22 02	
	-	51			DSZ	31 33	
	X↔I	35 24			GTO 6	22 06	
	DSZ	31 33			RCL 0	34 00	
050	RIS	84			1	01	
	RIS	84	STOP AT N COMPONENTS		-	51	CHECK FOR CORRECT APPROACH, IF NOT CHANGE DT COMPARE ACCURACY
	GTO A	22 11			X>0	31 81	
	* LBL B	31 25 12			GTO 7	22 07	
	RCL E	34 15		110	ABS	35 64	
	STO I	35 33			RCL C	34 13	
	CL X	44			X↔Y	35 52	

REGISTERS

0 $\Delta X_i, Y_i$	1 A_N	2 A_{N-1}	3 A_{N-2}	4 A_{N-3}	5 A_{N-4}	6 B_N	7 B_{N-1}	8 B_{N-2}	9 B_{N-3}
S0 B_{N-4}	S1 X, Y	S2 X, Y	S3 X, Y	S4 X, Y	S5 X, Y	S6	S7	S8	S9
A SEED T	B TOTAL PRESS	C Δ	D DT	E N	I				

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 K:				
	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 X1 OR Y1				
	RTN	35 22					
*	LBL 2	31 25 02	Δ X1 OR Y1				
	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 DT FOR DEW				
	GSB b	32 22 12					
	GSB a	32 22 11					
	GTO B	22 12					
140	* LBL 4	31 25 04	CONVERT OR TO OF DISPLAY T				
	RCL A	34 11					
	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 DT FOR BUBBLE	210			
	GSB 5	31 22 05					
	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		220			
	RCL A	34 11					
	RCL D	34 14					
	-	51					
	STO A	33 11					
	RTN	35 22					

LABELS					FLAGS	SET STATUS		
A CALL A, B	B CALL BUB.	C CALL P _v	D CALL DEW	E	0	FLAGS		
a CHANGE DT	b CHANGE DT	c	d	e	1	TRIG		
0 DO LOOP	1 CALC K _i	2 Δ X1 OR Y1	3 CHANGE DT	4 DISP T	2	DISP		
5 CHANGE DT	6 DO LOOP	7 CHANGE DT	8	9	3			

ON	OFF
0 ☐	☒
1 ☐	☒
2 ☐	☒
3 ☐	☒

DEG ☒	FIX ☒
GRAD ☐	SCI ☐
RAD ☐	ENG ☐
n <u>2</u>	

Program Description I

Program Title SINGLE STAGE EQUILIBRIUM FLASH CALCULATION

Contributor's Name Kerry R. Kelly

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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}).

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

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

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

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

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

Operating Limits and Warnings

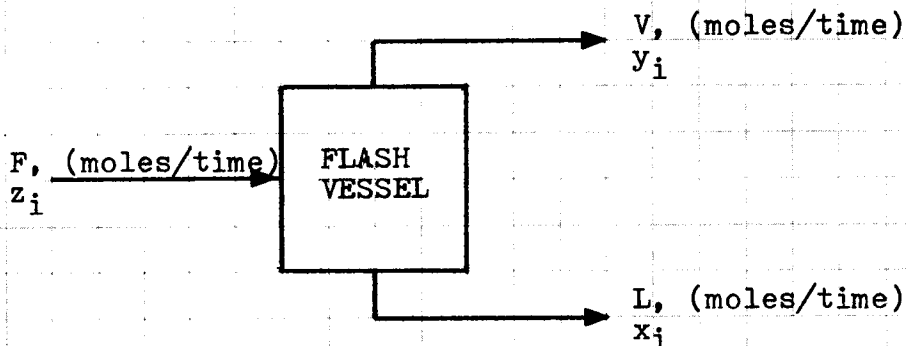
Maximum number of components = 10

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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:

<u>Component</u>	<u>z_i</u>	<u>K_i @ 270°F & 50 psia</u>
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

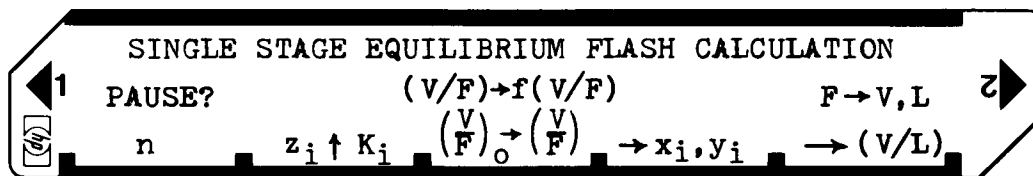
Calculate (V/F) and the composition of both the vapor and the liquid product streams.

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

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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			z_i
4	Input equilibrium ratio between phases for component i.	K_i			
5	Repeat steps 3 and 4 for i = 1 to n		B		n - i
6	Input a first guess for the mole ratio (V/F) and compute and output the actual ratio.*	$(V/F)_0$			
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 **		C		(V/F)
			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} .				
	* 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.		f	A	1.00/0.00
	** This step can be performed only after step 6.				

67 Program Listing I

STEP	KEY ENTRY	KEY CODE	COMMENTS	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)		RCL E	34 15	Set flag 0 so that subroutine c will calc. f'(V/F).
	1	01			+	61	
	-	51			STO E	33 15	
	h ST I	35 33		060	h RTN	35 22	
	STO D	33 14			f LBL 2	31 25 02	
	1	01			RCL A	34 11	
	+	61			h SF 0	35 51 00	
	h RTN	35 22	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)		g GSB c	32 22 13	Must constrain trials to $0 \leq (V/F) \leq 1$
010	f LBL B	31 25 12			CHS	42	
	STO (i)	33 24			h CF 0	35 61 00	
	h x $\geq$ y	35 52			h RTN	35 22	
	f P $\geq$ S	31 42			f LBL C	31 25 13	
	STO (i)	33 24		070	STO A	33 11	
	f P $\geq$ S	31 42			h ABS	35 64	
	f DSZ	31 33	Prepare for calculation of f(V/F) or f'(V/F).		g FRAC	32 83	Calc. f(V/F)
	GTO 0	22 00			g GSB c	32 22 13	
	f LBL 0	31 25 00			STO C	33 13	
	h RC I	35 34			h F1?	35 71 00	
	1	01			h PAUSE	35 72	
020	+	61			h ABS	35 64	
	h RTN	35 22			EEX	43	Is $ f(V/F) < 10^{-6}$?
	g LBL c	32 25 13	Calculate f(V/F)		6	06	
	STO A	33 11		080	CHS	42	
	RCL D	34 14			g x>y	32 81	
	h ST I	35 33			GTO 4	22 04	
	0	00			f GSB 2	31 22 02	
	STO E	33 15			RCL C	34 13	
	f LBL 6	31 25 06	If flag 0 is set Calc. f'(V/F)		h x $\geq$ y	35 52	Adjust (V/F) by Newton's method and check the new value by returning to C.
030	f GSB 1	31 22 01			+	81	
	f DSZ	31 33			RCL A	34 11	
	GTO 6	22 06			h x $\geq$ y	35 52	
	f GSB 1	31 22 01			-	51	
	RCL E	34 15			GTO C	22 13	
	h RTN	35 22		090	f LBL 4	31 25 04	Return with the latest value of (V/F) in dsply.
	f LBL 1	31 25 01	or Compute the value of x_i then y_i for $i=1$ to n .		RCL A	34 11	
	RCL A	34 11			h RTN	35 22	
	RCL (i)	34 24			f LBL D	31 25 14	
	1	01			f GSB E	31 22 15	
	-	51			RCL D	34 14	
040	X	71			h ST I	35 33	
	1	01	REGISTERS		f LBL 7	31 25 07	Compute the value of x_i then y_i for $i=1$ to n .
	+	61			f GSB 5	31 22 05	
	h F0?	35 71 00			f DSZ	31 33	
	g x 2	32 54		100	GTO 7	22 07	
	RCL (i)	34 24			f GSB 5	31 22 05	
	f P $\geq$ S	31 42			h RTN	35 22	
	RCL (i)	34 24			f LBL 5	31 25 05	
	h x $\geq$ y	35 52	REGISTERS		RCL (i)	34 24	Compute the value of x_i then y_i for $i=1$ to n .
	1	01			RCL E	34 15	
050	-	51			X	71	
	h F0?	35 71 00			1	01	
	g x 2	32 54			+	61	
	X	71			RCL E	34 15	
	h x $\geq$ y	35 52		110	1	01	
	+	81			+	61	
	f P $\geq$ S	31 42			h x $\geq$ 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				

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NOTES

NOTES

NOTES

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Small Business
Antennas
Butterworth and Chebyshev Filters
Thermal and Transport Sciences
EE (Lab)
Industrial Engineering
Aeronautical Engineering
Control Systems
Beams and Columns
High-Level Math
Test Statistics
Geometry
Reliability/QA

Medical Practitioner
Anesthesia
Cardiac
Pulmonary
Chemistry
Optics
Physics
Earth Sciences
Energy Conservation
Space Science
Biology
Games
Games of Chance
Aircraft Operation
Aviation
Calendars
Photo Dark Room
COGO-Surveying
Astrology
Forestry

CHEMISTRY

A variety of general physical chemical programs including equations-of-state and acid-base equilibria are included. Several programs on gas mixtures and vapor liquid equilibrium are also of interest to chemical engineers.

pH OF WEAK ACID/BASE SOLUTIONS

ACID-BASE EQUILIBRIUM (DIPROTIC)

WEAK ACID/BASE TITRATION CURVE

EQUATIONS OF STATE

VAN DER WAALS GAS LAW

BEER'S LAW AND ABSORBTIVITY CALCULATIONS

ACTIVITY COEFFICIENTS FROM POTENTIOMETRIC DATA

CRYSTALLOGRAPHIC TO CARTESIAN COORDINATE
TRANSFORMATIONS

KINETICS USING LINEWEAVER-BURK OR HOFSTEE PLOTS

MIXTURE VISCOSITIES

VAPOR PRESSURE, BUBBLE AND DEW POINT CALCULATION

SINGLE-STAGE EQUILIBRIUM CALCULATION



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Reorder No. 00097-14006 Printed in U.S.A. 00097-90181
Revision C 7-78