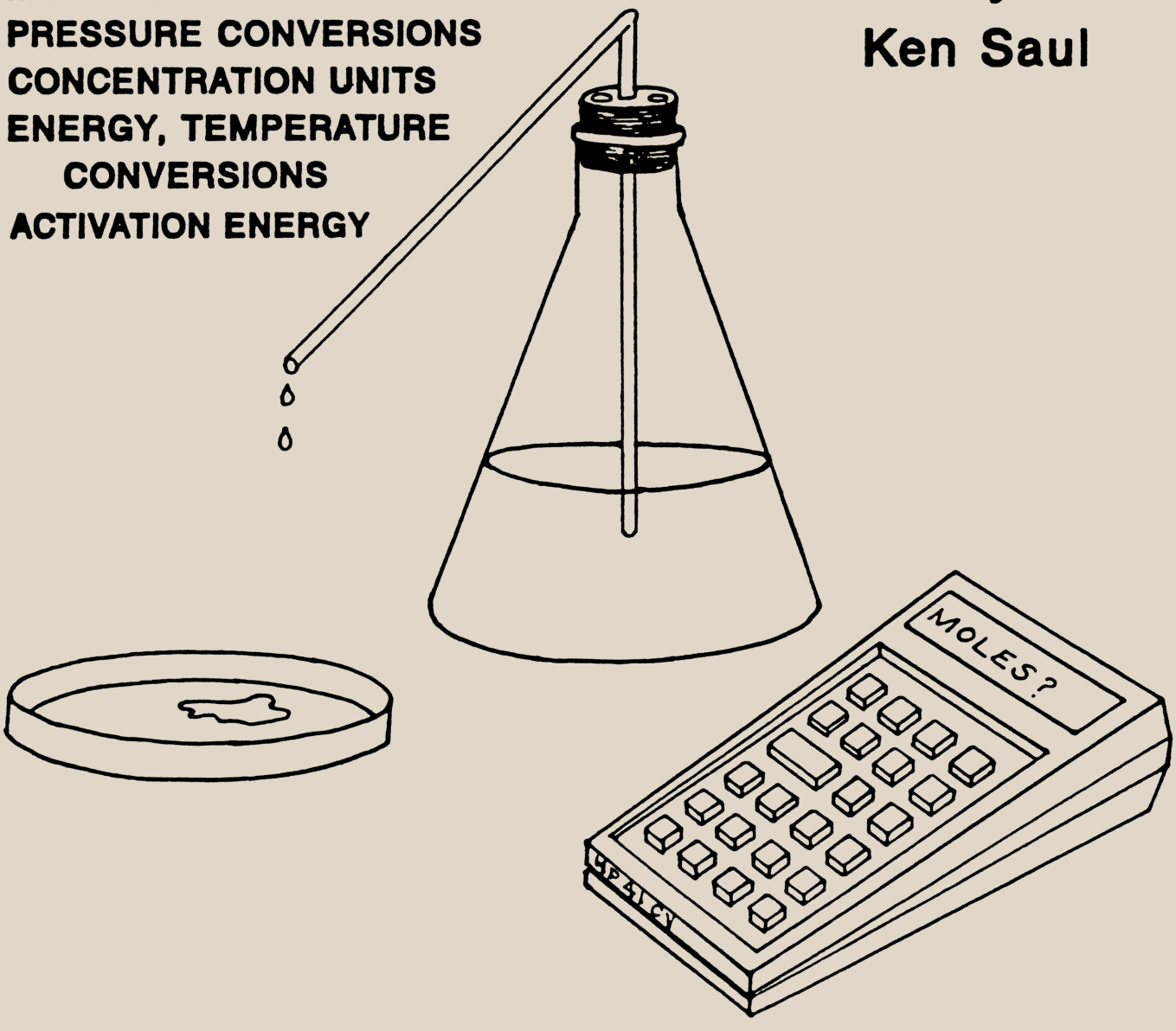
- INTRODUCTORY/REVIEW MATERIAL
- EXAMPLES AND ILLUSTRATIONS
- USER-FRIENDLY PROGRAMS
- COMPLETE PROGRAM LISTINGS
- BARCODE FOR EASY ENTRY

THE CHEMISTRY COLLECTION

RYDBERG EQUATION
MOLECULAR STRUCTURES
MOLARITY
PRESSURE CONVERSIONS
CONCENTRATION UNITS
ENERGY, TEMPERATURE CONVERSIONS
ACTIVATION ENERGY

by
Ken Saul



Seven HP-41C Programs for First-Year Chemistry Class

V7544-41

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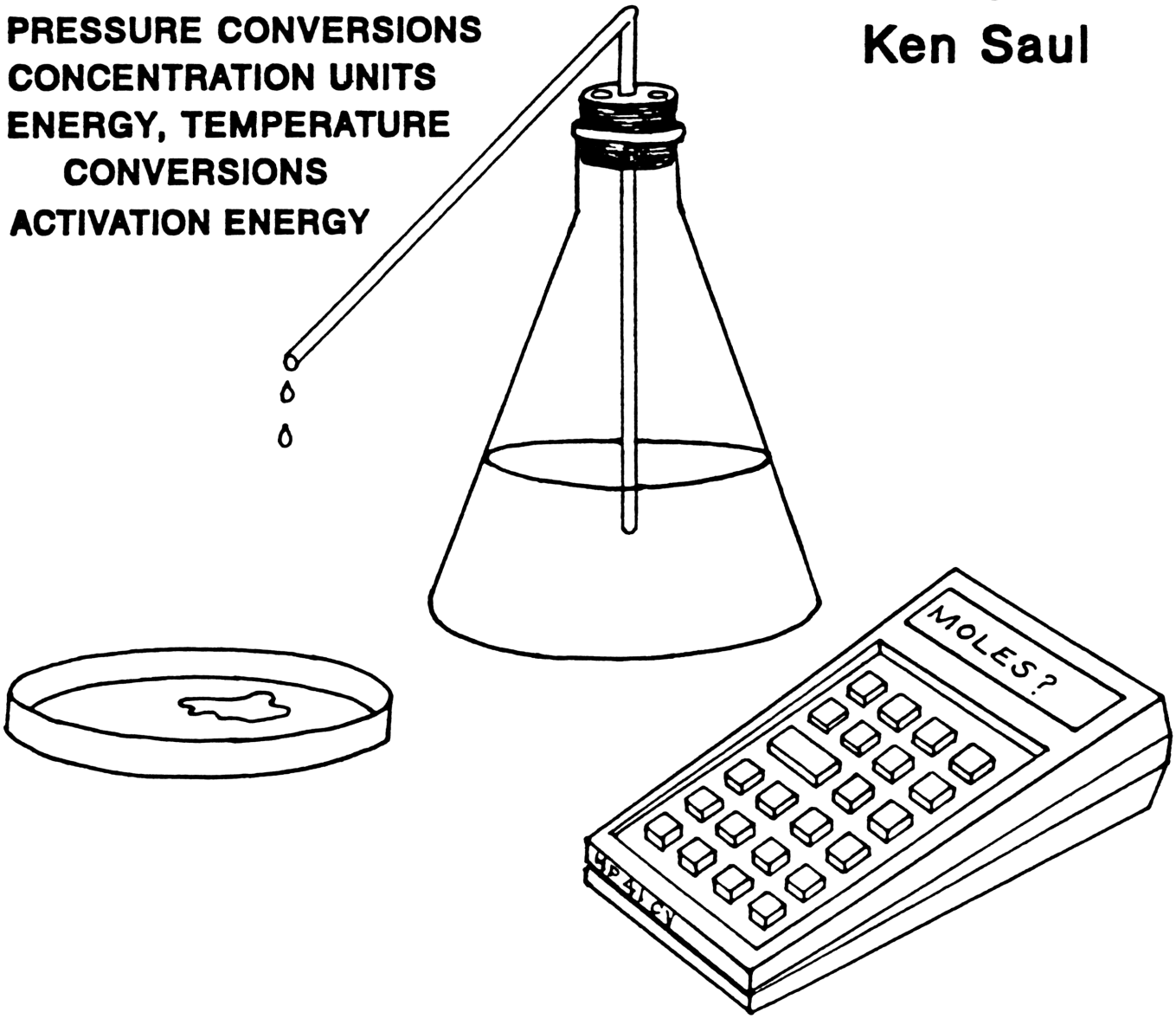

Seven HP-41C Programs for First-Year Chemistry Class

Printed in the United States of America.

Thank you for purchasing The Chemistry Collection. This group of HP-41C programs is part of a series of "Collections" written by Ken Saul especially for studies in first and second-year college science and engineering courses. All "Collections" come with complete introductory/review material, examples, instructions, program listings, and bar code. Recorded media (magnetic cards, mini-cassette, or HP-IL 3.5" disc) is available through the Hewlett-Packard User's Library.

Another Collection you may be interested in is The Physics Collection. The Physics Collection contains ten programs covering the following subjects:

1. Temperature Units Conversions (C, K, F, R)
2. Thermal Resistance Calculations
3. Simple Harmonic Waves
4. Speed of Sound
5. The Doppler Effect
6. Depth of a Well
7. Intensity of Diffraction Patterns
8. Bragg's Law for X-ray Diffraction
9. Relativistic and Newtonian Velocities
10. The Lorentz Transformation

More "Collections" will be released soon! Applications include Electronics, Mathematics, Statistics, and File Management. In order to receive information on these releases, as well as information on program updates and supplements, please fill in the form below and mail it to: Ken Saul, 3419 S.W. Long Ave., Corvallis, OR 97333..

========== Owner's Registration Form ==========

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_____

To order a "Collection" today, please use the order form enclosed.

The Chemistry Collection

Table of Contents

The Chemistry Collection

Introduction

The Chemistry Collection was developed while I was studying first-year chemistry at Oregon State University in Corvallis, Oregon. Many of my classmates found these programs to be of great value on their homework, in labs, and on exams. The problems of fast and accurate conversions between units of pressures, concentrations, temperatures, or energies are indispensable when problems are given in a variety of units, but the results are to be expressed in the MKS system.

The program on the structure of small molecules ("STRUCT") is terrific as an aid in learning about molecular bonding properties. I have confirmed the program's output with a professional chemist who assured me that the structures given by the program were correct for every small molecule she could think of.

These seven programs are intended to be easy to use and are fairly "bullet-proof". To become familiar with their operation, I would encourage you to follow through each example exactly as shown. Also, watch for the built-in default values that can save data entry time. You know as well as I do that on chemistry exams, you need all the time you can get! Good luck with these programs and let me know if you have any questions, comments, or requests.

I would like to give my special thanks to chemical engineers Carla Wykoff and Sadiq Bengali of Hewlett-Packard's Northwest Integrated Circuit Division, who provided reviews, criticism, and error-checking, to Kristy Sprinker who designed and drew the cover, and to many of my classmates who used these programs extensively in their chemistry classes. Finally, I would like to thank Colleen Johnson of the HP Users' Library for making these programs part of the Software Distribution Center.

Ken Saul
Corvallis, Oregon

Questions concerning these programs may be addressed directly to the author: Ken Saul, 3419 S.W. Long Ave., Corvallis, Oregon, 97330.

The Chemistry Collection

General Information

The seven programs are briefly described below:

1. "RYDBERG" Solves the wavelength of light absorbed or emmited when an electron goes from one orbital to another in the hydrogen atom.

2. "STRUCT" Gives the molecular type (ex: AX3E2), molecular shape, electronic structure shape, and type of hybrid orbitals for any small molecule.

3. "MOLAR" Solve interchangably for Molarity, Moles solute, and Liters solution.

4. "PRES" Pressure units conversion between Torr, Atmospheres, Pascals, and PSI.

5. "CONC" Concentration units conversion between mole fraction, weight fraction, molality, and molarity.

6. "C-J", "J-C" Calorie <-> Joule conversions and
   "C-F", "F-C" Fahrenheit <-> Celsius conversions.

7. "Ea" "K" Solve for the Activation Energy, proportionality constant, 'A', and 'k' for any temperature, T. Alternately, "K" solves for 'A' and 'k' at any temperature, when the activation energy is known.

Necessary Accessories: Card Reader or Wand is useful in loading programs. Periodic Table of the Elements.

Operating Limits and Warnings: See each program for individual limitations, if any.

Reference: Brady, James A. and Humiston, Gerard E. (1982). General Chemistry Principles and Structure, Third Edition, New York: John Wiley & Sons.

The Chemistry Collection:

1. The Rydberg Equation

In the Bohr theory of the hydrogen atom, there are discrete orbits where the single electron can exist. The orbits are numbered from 1 to infinity, starting at the level closest to the nucleus and having a certain amount of energy associated with them (the energy drops off with the square of the orbit number, n). All this was 'discovered' after scientists were baffled by the occurrence of the colored lines observed when a gas discharge from a hydrogen lamp was passed through slits and a prism. That is, unlike sunlight, which gives all the colors of the rainbow when passed through a prism, hydrogen light gives off only certain colors. The lines are produced when electrons fall from one discrete energy level to another.

Many physicists did experiments to identify the wavelengths of the emissions (Layman, Balmer, Paschen, and others) and Rydberg found that the equation $1/\lambda = 109{,}678 \text{ cm } [(1/n_1^2) - (1/n_2^2)]$ fit very well with the experimental evidence. In Bohr's theory, he found that the constant, derived from theory, was 109,730 cm , only 0.05% away from the equation derived from experiment.

In Rydberg's equation, n_2 is the 'from' level and n_1 is the 'to' level. If $n_2 > n_1$, then energy is <u>emitted</u> at the wavelength, lambda, and if $n_2 < n_1$, then energy is <u>absorbed</u> at the wavelength, lambda.

Example:

Find the wavelength of the emission when an electron goes from the fourth to the second orbital in the hydrogen atom. This would correspond to the second line in the Balmer series ($n_1 = 2$).

$1/\lambda = 109{,}678 \text{ cm } (1/2^2 - 1/4^2) \Longrightarrow \lambda = 48.63\text{E-}6 \text{ cm} = 486.3 \text{ nm}.$

Since $n_2 > n_1$, this wavelength of energy is <u>Emitted</u>.

The Chemistry Collection:

1. The Rydberg Equation

Program Description

To solve the example on page 3, follow the solution below.

Display	Input	Function	Comments
0.0000		[XEQ] [ALPHA] RYDBERG [ALPHA]	Run program.
FROM ↗ TO	4	[ENTER]	'From', Enter,
4.000 00	2	[R/S]	'To' , Run.
LAMBDA =			
48.63E-6 CM			Wavelength
		[R/S]	See if Emitted or Absorbed.
EMITTED			This wavelength is emitted.

Note that the solution is expressed in cm. 48.63E-6 cm is equal to 486.3 nm (nanometers = E-9 meters). The wavelength of the visible spectrum (visible light) is 400nm (violet) to 800 nm (red). Therefore, this emission lies in the visible spectrum. Infrared wavelengths are greater than 800nm and ultraviolet wavelengths are less than 400nm.

The Chemistry Collection:

2. Molecular Structures

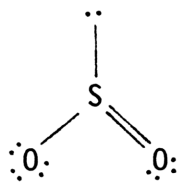
In chemistry, it is often important to know the shape of a molecule in order to determine other properties. There are basically five different geometries of small molecules (less than or equal to six electron pairs). They are represented in the program "STRUCT" as shown below:

Shape	41C Representation
Linear	LINEAR
Planar Triangular	PLATRI
Tetrahedral	TETRA
Trigonal bipyramidal	TRIBIP
Octahedral	OCTAHE

If there are one or more lone electron pairs, the molecular shape will differ from the electronic shape. The other molecular shapes that occur are variants of the five above:

Nonlinear	NONLINEAR
Pyramidal	PYRAM
Distorted Tetrahedral	DIST TETRA
T-shaped	T-SHP
Square pyramidal	SQU PYRAM
Square planar	SQU PLAN

Molecules can be described in generic types using the notation $AX_{\alpha}E_{\beta}$, where A is the central atom, X is a ligand (a branch), α is the number of ligands, E is a lone pair, and β is the number of lone pairs. For example, SO_2 is shown below:



This is an AX2E1 type molecule, since there are 2 ligands attached to the central atom, and one lone pair.

The molecular shape is decribed as nonlinear.

For each type of generic molecule, there is only one molecular structure (refer to your Chemistry textbook under 'Molecular Structure').

Another important aspect of molecular theory is the shape of the electronic structure and the type of hybrid orbital (hybrid orbitals are a combination of atomic orbitals as predicted by the Schrodinger wave equation). There are three types of atomic orbitals: s, p, and d, corresponding to the sub-shell designations. When these atomic orbitals combine, they form distinct shapes on a one-to-one basis.

The Chemistry Collection:

2. Molecular Structures

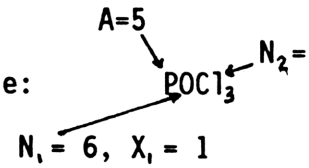
The common notation for the type of hybrid orbital is $sp^a d^b$, where the 'exponents' are the number of that particular type of atomic orbital involved. For example, the SO_2 diagram shown on page 5 is seen to have a planar triangular electronic structure with three orbitals. Therefore, the hybrid orbital type is sp^2.

My general formula for the number of lone pairs, B, is given below:

$$B' = [(A-Q) - (\sum_{i=1}^{N} NiXi)] \text{ MOD } 8 \qquad \text{where } Ni = (8-Ni) \text{ for Groups 3 to 8.}$$

$$B = [(B' \text{ MOD } 2) + B'] / 2$$

Where A = Group number of the central atom
Q = ionic charge (may be positive or negative)
N = number of additional elements in the molecule
Ni = group number of an attached atom
Xi = subscript of an attached atom

For example: 

Q = 0 (no ionic charge)

The electronic shape is then found by the total number of branches, including the number of lone pairs, that is, there are only 5 defined shapes, each with a unique hybrid orbital type.

For example:

$POCl_3$: $B' = [(5 - 0) - (8 - 6)*(1) - (8 - 7)*(3)] \text{ MOD } 8$

$B' = (5 - 2 - 3) \text{ MOD } 8 = 0$

Then, $B = (B' \text{ MOD } 2 + B') / 2 = (0 \text{ MOD } 2 + 0)/2 = 0.$

$POCl_3$ = AX(1 + 3)E0 = AX4 (Tetrahedral)

Because there are no lone pairs, the electronic structure is the same as the molecular structure. There are four orbitals, so the hybrid type is sp^3.

Note: My formula for B is not found in the Chemistry text cited on page 2, but works for every molecule that I could try it on, including those that appeared on the exams!

The Chemistry Collection:

2. Molecular Structures

Program Description

To try the $POCl_3$ example shown on page 6, get out your periodic table and follow the instructions below.

Display	Input	Function	Comments
0.0000	Load the program "STRUCT" from cards, wand, etc.		
0.0000	[XEQ] [ALPHA] STRUCT [ALPHA]		Run program.
GP CTR ATM	5	[R/S]	Phosphorus is Group 5.
IONIC CHG	0	[R/S]	No ionic charge
N. ADTL. ELEM.	2	[R/S]	Two more elements.
GP NO. ATM 1	6	[R/S]	Oxygen is Gp. 6
SUBSCRIPT 1	1	[R/S]	Only one Oxygen atom.
GP NO. ATM 2	7	[R/S]	Chlorine is Group 7.
SUBSCRIPT 2	3	[R/S]	3 Cl atoms.
TYPE: AX4		[R/S]	Generic type.
M: TETRA		[R/S]	Molecular shape is tetrahedral.
e:TETRA, SP3			Electronic shape is also tetra., and the hybrid orbital is sp3.
		[R/S]	Restart program or press [<--] to end program.

The Chemistry Collection:

2. Molecular Structures

User Instructions

This page describes how to run the program in general terms, showing all the different features and expected data entries.

Step	Instructions	Input	Function	Display
1.	Enter the program.			
2.	Begin program.		[XEQ] [ALPHA] STRUCT [ALPHA]	
3.	Enter the group number of the central atom (from a periodic table).	A	[R/S]	GP CTR ATM
4.	Enter the ionic charge of the molecule, which may be positive, negative, or zero.	Q	[R/S]	IONIC CHG
5.	Enter the number of additional elements in the molecule.	N	[R/S]	N. ADTL. ELEM.
6.	Enter the group number of the atom requested. Additional atoms may be entered in any order.	Ni	[R/S]	GP NO. ATM 1
7.	Enter the subscript of the atom requested. Enter a '1' if there is no subscript.	Xi	[R/S]	SUBSCRIPT 1
8.	Repeat steps 6-7 for each additional atom.			
9.	View the generic type.		[R/S]	TYPE: AX_xE_e
10.	View the Molecular Shape.		[R/S]	M: shape
11.	View the Electronic Structure and the type of hybrid orbitals.			e: shape, SP^ad^b

The Chemistry Collection:

2. Molecular Structures

User Instructions Concluded

Step	Instructions	Input	Function	Display
12.	Restart the program		[R/S]	GP CTR ATM
12a.	or End program.		[<--]	0.0000

Notes: None of the entries are optional. If you do not enter a number in response to a prompt, you will be requested to enter the value again. If you enter values that result in greater than six 'branches' on the molecule (including lone pairs), you will get a 'NONEXISTENT' response to the molecular shape, although the 'generic type' will be shown. You will need to restart the program (you may type [XEQ] 22 to restart from this point).

The Chemistry Collection:

3. Molarity Calculations

There are many ways to express the concentration of a solute in a solution, but one of the most common is in terms of moles solute per liter of solution, called molarity. Molarity is useful, since moles are directly linked to the weight of the substance:

Weight of substance = (Number of moles) * (Total molecular weight)

Molarity is expressed in a formula as:

$$M = \frac{\text{moles solute}}{\text{liters solution}}$$

Here are three examples to demonstrate the types of problems associated with this formula.

Examples

Example 1: Find molarity, given moles solute and liters solution.

What is the molarity of 0.30 moles of NaOH in a total of 400 ml of solution?

This is a straight plug-in: M = 0.30 mol / 0.400 l = 0.75 M.

This is read as 0.75 molar.

Example 2. Find an amount of substance to prepare a certain solution.

Find the amount, by weight, of NaOH that is required to prepare 100 ml of 0.632 M solution.

To solve this problem, we must first find how many moles of NaOH are required, and then we can translate this amount into the weight.

From the formula for molarity, we see that moles = molarity * liters.

mol NaOH = 0.632 M * 0.100 l = 0.0632 mol NaOH.

Next, the molecular weight of NaOH is the sum of the atomic weights of the individual constituents of NaOH: from the periodic table, the atomic weights are Na = 23, O = 16, and H = 1, making a total of 40 grams/mol.

Finally, grams NaOH = 0.0632 mol NaOH * 40 grams/mol NaOH = 2.528 g.

The Chemistry Collection:

3. Molarity Calculations

Examples, concluded

Example 3: Find the amount of liters solution, given molarity and moles solute.

How many liters of 0.5 M NaOH solution are required to provide 0.2 mol NaOH?

From the formula for molarity, we see that liters = moles/molarity

Therefore, liters solution = 0.2 mol / 0.5 M = 0.4 l = 400 ml.

The program to do all these calculations is called "MOLAR". Try following the instructions on the next page to check the three examples just shown.

The Chemistry Collection:

3. Molarity Calculations

Program Description

Display	Input	Function	Comments
0.0000	Load "MOLAR" from cards, wand, etc.		
0.0000	[XEQ] [ALPHA] MOLAR [ALPHA]		Run program.
MOLES?	0.3	[R/S]	number of moles
LITERS?	0.4	[R/S]	liters solution
MOLAR?	(no input)	[R/S]	solve for Molar
MOLAR=0.7500			ans. 1: 0.75 M
		[R/S]	Run ex. 2.
MOLES?	(no input)	[R/S]	solve for moles
LITERS?	0.1	[R/S]	liters solution
MOLAR?	0.632	[R/S]	molarity
MOLES=0.0632			here's the no. of moles.
	40	*	weight = MW*mol
2.528			ans. 2: 2.528 g
		[R/S]	Run ex. 3.
MOLES?	0.2	[R/S]	number of moles
LITERS?	(no input)	[R/S]	solve for liters
MOLAR?	0.5	[R/S]	molarity
LITERS=0.4000			ans. 3: 0.4 l

The Chemistry Collection:

3. Molarity Calculations

User Instructions

Below is a general description of how to run the program "MOLAR".

Step	Instructions	Input	Function	Display
1.	Enter the program.			
2.	Begin program.		[XEQ] [ALPHA] MOLAR [ALPHA]	
3.	Enter the number of moles solute if known, else just press [R/S].	(mols)	[R/S]	MOLES?
4.	Enter the number of liters of solution if known, else press [R/S].	(liters)	[R/S]	LITERS?
5.	Enter the molarity if known, else press [R/S].	(M)	[R/S]	MOLAR?

NOTE: You must enter two of the three variables for a valid answer. Variables may not be reused without re-entering them.

6.	Press [R/S] to view the solution to the unknown variable.		[R/S]	answer.
7.	To restart program, press [R/S].		[R/S]	MOLES?
8.	To end the program, press [<--].		[<--]	answer is in X-reg.

The Chemistry Collection:

4. Pressure Conversions

A common problem that comes up on homework and exams involves the conversion of various units of gas pressures. A problem will be stated in, say, so many atmospheres, but the solution must be in torr or Pascals. All pressures are in units of force per unit area, and the system of units must match that used in the rest of the problem. For example, pounds per square inch, or psi, is used when the problem is in the English system involving inches or pounds. Pascals are the common SI units (Newtons per square meter), but the torr, or millimeter of mercury, is often seen. The standard atmosphere, or atm, is defined in terms of torr, where 1 atm = 760 torr (at 0 degrees C, sea level). This is also the same as 14.7 psi. The program that manages all these conversions is called "PRES".

Here are the conversion factors used in the program:

Pa	atm	psi	torr
1	9.8692E-6	1.4503E-4	7.5008E-3
101325	1	14.7	760
6895	6.8027E-2	1	51.717
133.32	1.3158E-3	1.9336E-2	1

Examples:

1. Convert 123000 Pa into atm.

   From the conversion table, 1 atm = 101325 Pa.

   123000 Pa * (1 atm / 101325 Pa) = 1.2139 atm

2. Convert 320 torr into psi.

   From the conversion table, 1 psi = 51.717 torr.

   320 torr * (1 psi / 51.717 torr) = 6.1875 psi.

The Chemistry Collection:

4. Pressure Conversions

Program Description

Try the following instructions to check the two examples just shown and to become familiar with the program.

Display	Input	Function	Comments
0.0000	Load "PRES" from cards, wand, etc.		
0.0000	[XEQ] [ALPHA] PRES [ALPHA]		Run program.
PRESSURE?	123000	[R/S]	pressure to convert from.
FROM :			"FROM :" is briefly displayed
TORR,ATM,Pa,PSI		[D] (LOG key)	Press the key under the units "Pa".
TO :			"TO :" is briefly displayed
TORR,ATM,Pa,PSI		[C] ($\sqrt{x}$ key)	Press the key under the units "ATM"
1.2139			ans. 1: 1.2139 atm
		[R/S]	Run ex. 2.
PRESSURE?	320	[R/S]	known pressure
FROM :			
TORR,ATM,Pa,PSI		[A] (or [B])	Press key A or B for torr.
TO :			
TORR,ATM,Pa,PSI		[E] (ln key)	Press key under units "PSI".
6.1875			ans. 2: 6.1875 psi

The Chemistry Collection:

5. Concentration Units

Concentration units are all ratios that in some way express the relative proportions of various components of a a solution. The units that are used in the program "CONC" are mole fraction, weight fraction, molality, and molarity.

The mole fraction is defined as the number of moles one substance in the solution, divided by the total number of moles of all the substances in the solution. The mole fraction is represented by the symbol 'X'.

$$Xa = \frac{Na}{Na + Nb + \ldots} \qquad \text{[Mole Fraction, X]}$$

The weight fraction is defined as the weight of one component, divided by the total weight of the mixture. A related unit is the weight percent and is equal to the weight fraction multiplied by 100.

$$Wa = \frac{Wt.a}{Wt.a + Wt.b + \ldots} \qquad \text{[Weight Fraction, W]}$$

Molarity, as defined back in program 3, "MOLAR", is the ratio of the number of moles solute to the total volume of solution and has the units of moles per liter.

$$M = \frac{\text{moles solute}}{\text{liters solution}} \qquad \text{[Molarity, M, mol/l]}$$

Molality is defined as the number of moles of solute per kilogram solvent. It has the units of moles per kg.

$$m = \frac{\text{moles solute}}{\text{1 kilogram solvent}} \qquad \text{[Molality, m, mol/kg]}$$

In the case of water, the density is about 1 kg per liter at room temperature so there is little or no difference between molarity and molality. However, other solvents have much higher densities and the difference between molarity and molality may be great. You will need to know the density of the solvent in order to do some conversions between these units of concentration. The other data that you will need is the molecular weights of the solute and of the solvent.

The Chemistry Collection:

5. Concentration Units

Example

1. A solution of Epsom salts in water is 10% magnesium sulfate by weight. What is the molality and molarity of the solution, and the mole fraction of magnesium sulfate (MgSO4) in the water? (Aren't you glad the 41-C will do this for you?)

First, get the basic information from the periodic table. The molecular weight of MgSO4 is 24.3+32+(4*16) = 120.3 grams/mol. The molecular weight of water, H2O, is 18. The density of the solvent, in this case, water, is 1.

Now, we convert the weight percent into a weight fraction. That's just 10/100 = 0.10. From this, we know that there are 10 grams of MgSO4 in every 100 grams of the mixture.

mol solute = (10 g / 120.3 g/mol) = 0.08313 mol MgSO4
kg solvent = (90 g * 1kg/1000 g) = 0.0900 kg H2O

Then, molality, m = 0.08313/0.0900 = 0.9236 m MgSO4.

The molarity is the moles solute/liter solution. In this case, we will assume that the solution has a density near 1 (mostly water).

From the weight fraction, we know there are 100 g MgSO4 in 1000 g solution (remember that with the density = 1, 1000 g = 1 liter).

M = mol solute/liters solution = (100 g / 120.3 g/mol) / 1 = 0.8313 M

For the mole fraction, we take the number of moles of MgSO4 and divide it by the total number of moles in the mixture:

mol solvent = (90 g / 18 g/mol) = 5.0000 mol H2O.

X = (0.0831) / (0.0831 + 5.0000) = 0.0164 (for MgSO4)

If the density of the solution was given as 1.100 g/ml, then there would be a change in the molarity by a factor of 1.1:

M, with density = 1.10 g/ml = 0.8313 * 1.1 = 0.9144 M.

The Chemistry Collection:

5. Concentration Units

Program Description

Try the following instructions to check the example just shown and to become familiar with the program.

Display	Input	Function	Comments
0.0000	Load "CONC" from cards, wand, etc.		
0.0000	[XEQ] [ALPHA] CONC [ALPHA]		Run program.
MW SOLUTE?	120.3	[R/S]	molecular weight of MgSO4.
MW SOLVENT?	18	[R/S]	molecular wt. of H2O.
DENSITY?G/ML	1	[R/S]	enter the density in g/ml
VALUE?	.1	[R/S]	we know the weight fraction
UNITS?			"UNITS" briefly displayed.
X, WT/,ML, MR		[B] (1/x key)	press key below "WT/" for units.
MOL/=0.0164		[R/S]	Mole fraction displayed.
MLTY=0.9236		[R/S]	Molality displayed.
MRTY=0.8313		[R/S]	Molarity displayed.
0.8313			End of program. Press [R/S] to restart.

Please see the note concerning "defaults" on the User Instructions on the next page.

The Chemistry Collection:

5. Concentration Units

User Instructions

Below is a general description of how to run the program "CONC", as well as some of the special features that you will want to know about.

Step	Instructions	Input	Function	Display
1.	Enter the program.			
2.	Begin program.		[XEQ] [ALPHA]	CONC [ALPHA]
3.	Enter the molecular weight of the solute.	MW	[R/S]	MW SOLUTE?
	Note: This is not an optional entry. If you do not enter a value, you will be re-prompted.			
4.	Enter the molecular weight of the solvent.	MW	[R/S]	MW SOLVENT?
	** DEFAULT: If the solvent is <u>water</u>, you can just press [R/S] and the value of 18 will be automatically entered.			
5.	Enter the density in units of g/ml.	d	[R/S]	DENSITY?G/ML
	** DEFAULT: If the density is equal to 1, you can just press [R/S] and the value of 1 will be automatically entered.			
6.	Enter the known value: mole fraction, weight fraction, molarity, or molality.	X, Wt/ M, m	[R/S]	VALUE?
7.	"UNITS" is displayed briefly.			UNITS?
8.	Press the key directly below the correct units in the menu.	[A] for X (mol frac) [B] for WT/(wt. frac) [C] for ML (molality) [D] for MR (molarity)		X,WT/,ML, MR
9.	First solution		[R/S]	(solution 1)
10.	Second solution		[R/S]	(solution 2)
11.	Third solution		[R/S]	(solution 3)
12.	Press [R/S] to restart		[R/S]	(value of solu. 3)

The Chemistry Collection:

6. Calorie - Joule Conversion and Fahrenheit - Celsius Conversion

This short set of four subroutines may seem strange to be including in this set of longer programs, but the problem of converting units properly under pressure was always a problem for me and many of my classmates. Rather than try to memorize the conversion factors, I wrote these special little programs to do the job and assigned their labels to keys for quick execution.

First, a quick review of the units and conversion factors:

The SI unit for energy is the Joule (J) and is defined as 1 $kg*m^2/s$. Nearly all chemical reactions, however, discuss energy in terms of calories (cal). A calorie is the amount of heat needed to raise one gram of water at 15 degrees celsius by one degree.

The conversion factor between them is 1 cal = 4.1840 J.

The SI temperature scale is in degrees Celsius (C). The English unit of degrees Fahrenheit is often seen as a 'confusion factor' in problems that are intended to be worked out in SI units only.

The conversion factors between them are:

$^{\circ}C = (5/9)*(^{\circ}F - 32)$ ($^{\circ}F - ^{\circ}C$)

$^{\circ}F = [(9/5)*^{\circ}C] + 32$ ($^{\circ}C - ^{\circ}F$)

The Chemistry Collection:

6. Calorie - Joule Conversion and Fahrenheit - Celsius Conversion

User Instructions

The following instructions are a reference on how to run the programs. No examples are necessary for them.

Input	Functions	Comments
0.0000	Load "C-J" from cards, wand, etc. Program "C-J" has all four conversions under the same general main title.	
entry in cal	[XEQ] [ALPHA] C-J [ALPHA]	Convert Cal to Joules.
answer in Joules.		
entry in Joules	[XEQ] [ALPHA] J-C [ALPHA]	Convert Joules to Cal.
answer in Cal.		
entry in deg. C	[XEQ] [ALPHA] C-F [ALPHA]	Convert deg. C to deg. F.
answer in deg. F.		
entry in deg. F	[XEQ] [ALPHA] F-C [ALPHA]	Convert deg. F to deg. C.
answer in deg. C.		

The Chemistry Collection:

7. Activation Energy

In a chemical reaction, molecules are colliding with a kinetic energy sufficient for them to overcome electron repulsions that tend to force them apart. The minimum amount of energy that is required is called the activation energy, and is given the symbol Ea.

The rate at which the reaction takes place depends on the activation energy, the temperature of the process (in Kelvin), and a proportionality constant related to the collision frequency and the the effect of molecular orientations during a collision. These factors are related by the Arrhenius equation as shown below:

[1] $k = A \exp(-Ea/RT)$

where k = rate constant
A = proportionality constant
exp = base of natural logarithm
Ea = activation energy
R = gas constant
T = temperature

This equation gives you a way of determining the activation energy and the proportionality constant, A, from measurements of the rate constant at two different temperatures. Once these values are known, the rate constant may be found for any other temperature.

With two values of k and T, we use the equation:

[2] $\ln (k1/k2) = (Ea/R) * [(1/T2) - (1/T1)]$

since the value of A is the same for both sets of data.

This gives us only one unknown, the activation energy:

[3] $Ea = [R*\ln (k1/k2)] / [(1/T2) - (1/T1)]$

Similarly, if k, T, and Ea are known (one temperature only), we can solve for the proportionality constant, A, and then solve for further values of k at selected temperatures.

The Chemistry Collection:

7. Activation Energy

Example:

Given that k1 = 0.180 s^{-1} at 220°C and 0.344 s^{-1} at 245°C, find the values of A and Ea.

First, convert the degrees C into Kelvin: 220°C + 273 = 493 K and 245°C + 273 = 518 K. Use R = 8.314 J mol K so that Ea will be in Joules.

(Note: if Ea was in calories, you would use R = 1.987 cal mol K.)

Putting our numbers into equation [3], we have:

$$Ea = \frac{[8.314 * \ln (0.180/0.344)]}{(1/518) - (1/493)}$$

Ea = 55,006 J.

Now we can use one of the sets of data and the value of Ea to solve for the proportionality constant, A:

[4] $A = k1 / [\exp (-Ea/RT1)]$

$A = 0.18 / [\exp \{ -55006.043 / (8.314 * 493)\}]$

A = 121,204 s^{-1} . (Note that A has the same units as k).

Finally, a new rate constant at a third temperature, T3, may be predicted from equation [1]:

If T3 = 260 C = 533 K, to find k3 we use Ea and A found above:

$k3 = A \exp (-Ea/RT3) = 121204 \exp (-55006 / (8.314*533))$

k3 = 0.4928 s^{-1}.

The Chemistry Collection:

7. Activation Energy

Program Description

Try the following instructions to check the example just shown and to become familiar with the program.

Display	Input	Function	Comments
0.0000	Load "Ea" from cards, wand, etc.		
0.0000	[XEQ] [ALPHA] E [shift] a [ALPHA]		Run program.
K1, K2=?	0.18 0.344	[ENTER] [R/S]	k1, [ENTER], k2, [R/S]
T1, T2=?	493 518	[ENTER] [R/S]	T1, [ENTER] T2, [R/S] (in Kelvin)
Ea= 55,006.0427		[R/S]	Activation Energy in J.
A= 121,204.0561		[R/S]	Proportionality Constant in s^{-1}.
T3?	533	[R/S]	Find k3 at T3.
K=0.4928		[R/S]	k3 in s^{-1}.
T3?	---	---	You can continue to solve for k at selected temperatures.

Similarly, if you know just one set of k and T but also Ea, perform the following instructions:

0.0000	[XEQ] [ALPHA] K [ALPHA]		Run program.
K, T, Ea?	0.18 493 55006	[ENTER] [ENTER] [R/S]	k1, [ENTER], T1, [ENTER] Ea, [R/S]
A= 121,202.7936		[R/S]	Proportionality Constant.
T3?	533	[R/S]	A new temp.
K=0.4928			k3 shown.

The Chemistry Collection:

7. Activation Energy

User Instructions

Below is a general description of how to run the programs "Ea" and "K" for your reference.

Step	Instructions	Input	Function	Display
1.	Enter the program "Ea". (Also contains "K".)			
2.	If you know k1 and k2 at their corresponding temperatures in Kelvin, then do the following:			
			[XEQ] [ALPHA] E [shift] a [ALPHA]	
3.	Enter the first k value, [ENTER], then the second k value, then [R/S].	k1 k2	[ENTER] [R/S]	K1, K2?
4.	Enter the first temp in Kelvin, [ENTER], then the second temp, then [R/S].	T1 T2	[ENTER] [R/S]	T1, T2?
5.	View the value of Ea.		[R/S]	(Ea value)
6.	View the value of A.		[R/S]	(A value)
7.	Enter a new temperature.	T3	[R/S]	T3?
8.	View the rate constant, k3.			(k3 value)
9.	Repeat steps 7 and 8 to solve for more rate constants at selected temperatures.		[R/S]	(k3 value)
10.	End program by clearing the display.		[<--]	(k3 value)

The Chemistry Collection:

7. Activation Energy

User Instructions, concluded.

Similarly, if k1, T1, and Ea (in Joules) are known, do the following:

Step	Instructions	Input	Function	Display
11.			[XEQ] [ALPHA] K [ALPHA]	
12.	Enter k1, [ENTER], T1, [ENTER], and Ea, then [R/S]	k1 T1 Ea	[ENTER] [ENTER] [R/S]	K, T, Ea?
13.	Same as steps 6 - 10.			

Note: If Ea is given in calories, you must first convert it to Joules! (See program 6, "C-J").

The Chemistry Collection:

Registers, Flags, and Status

This section lists the registers and flags used in the programs as well as the minimum SIZE, the total registers required, and the number of bytes.

"RYDBERG"

Registers	Flags	Size	Total Reg.	# of Bytes
none	none	000	12	83

"STRUCT"

Registers		Flags		Size	Total Reg.	# of Bytes
00	A - (±q)	00	0 lone pairs	017	80	440
01	Loop ctr.	01	1 lone pair			
02	sum of ni	02	2 lone pairs			
03	sum(8-n)* sum(ni)	03	3 lone pairs			
04	# lone pairs	22	digit entry			
05	"NON"	29	controls display format.			
06	"LINEAR"					
07	"PLATRI"					
08	"TETRA"					
09	"PYRAM"					
10	"TRIBIP"					
11	"DIST"					
12	"T-SHP"					
13	"OCTAHE"					
14	"SQU"					
15	"PLAN"					
16	", SP"					

"MOLAR"

Registers		Flags		Size	Total Reg.	# of Bytes
00	#moles solute	00	solve for Moles	007	24	118
01	#liters solu.	01	solve for Liters			
02	molarity	02	solve for Molarity			
03	loop counter	22	digit entry			
04	"MOLES"					
05	"LITERS"					
06	"MOLAR"					

Registers, Flags, and Status

"PRES"

Registers	Flags		Size	Total Reg.	# of Bytes
none	Set	Clear	000	38	262
	00 "FROM" pass	"TO" pass			
	01 from Torr	not from Torr			
	02 from Atm	not from Atm			
	03 from Pa	not from Pa			
	04 from psi	not from psi			
	22 digit entry				
	27 USER on				

"CONC"

Registers	Flags	Size	Total Reg.	# of Bytes
00 mw solute	22 digit entry	004	41	252
01 mw solvent	27 User ON			
02 density				
03 value (known)				

"C-J", "J-C", "F-C", "C-F"

Registers	Flags	Size	Total Reg.	# of Bytes
none	none	000	9	60

"Ea", "K"

Registers	Flags	Size	Total Reg.	# of Bytes
00 8.314 (gas const.)	01 skip "K, T, Ea" prompt.	005	24	130
01 k2 in "Ea" or k in "K"				
02 T2 in "Ea" or T in "K"				
03 Ea				
04 A				

==========

Collection Totals:

Maximum Size	Total Registers	Total Bytes
017	228	1345

PROGRAM LISTING

☐ 67 ☐ 97 ☒ 41C "RYDBERG"

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
01	LBL "RYDBERG"		
02	ENG 3		Set ENG 3 mode
03	"FROM ↑ TO"		
04	PROMPT		
05	"LAMBDA ="		Display "LAMBDA="
06	AVIEW		
07	X↑2		$1/n_1^2$
08	1/X		
09	X<>Y		
10	X↑2		$1/n_2^2$
11	1/X		
12	-		
13	109678		$109678\,cm^{-1}\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right)$
14	*		
15	1/X		λ
16	ENTER↑		copy λ
17	ABS		
18	CLA		
19	ARCL X		Form display
20	RDN		
21	" CM"		
22	AVIEW		
23	STOP		
24	"EMITTED"		For $\lambda > 0$, show EMITTED, else show ABSORBED.
25	X<0?		
26	"ABSORBED"		
27	AVIEW		
28	END		
40			
50			
51			
60			
70			
80			
90			
00			

Note: Refer to HP-41C OWNER'S HANDBOOK AND PROGRAMMING GUIDE for specific information on keystrokes. The Function Index is found at the very back of the Handbook. Refer to Appendix E in 67 or 97 OWNER'S HANDBOOK AND PROGRAMMING GUIDE for exact keystrokes.

PROGRAM LISTING

☐ 67 ☐ 97 ☒ 41C

"STRUCT"

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
01	LBL "STRUCT"		
02	LBL 22		
03	CF 00		Initialize Flags
04	CF 01		
05	CF 02		
06	CF 03		
07	CF 04		
08	CF 29		
09	FIX 0		Set FIX 0 display
10	0		
11	STO 02		Clear 02, 03
12	STO 03		
13	"NON"		Store "Shapes"
14	ASTO 05		
15	"LINEAR"		
16	ASTO 06		
17	"PLANRI"		
18	ASTO 07		
19	"TETRA"		
20	ASTO 08		
21	"PYRAM"		
22	ASTO 09		
23	"TRIBIP"		
24	ASTO 10		
25	"DIST "		
26	ASTO 11		
27	"T-SHP"		
28	ASTO 12		
29	"OCTAHE"		
30	ASTO 13		
31	"SQU "		
32	ASTO 14		
33	"PLAN "		
34	ASTO 15		
35	". SP"		
36	ASTO 16		
37	"GP CTR ATM"		Prompt for A
38	XEQ 60		
39	"IONIC CHG"		Prompt for Q
40	XEQ 60		
41	-		
42	STO 00		00 = A - Q
43	"N. ADTL. ELEM."		Prompt for N
44	XEQ 60		
45	.001		
46	*		Form Loop Control
47	1		in 01
48	+		
49	STO 01		
50	LBL 00		Additional Elements Loop
51	"GP NO. ATM "		
52	ARCL 01		
53	XEQ 60		Get Group No., N_i
54	2		
55	X<>Y		
56	X<=Y?		Group 1 or 2?
57	GTO 01		Yes. Goto LBL 01
58	8		No. N_i =
59	X<>Y		$8 - N_i$.
60	-		
61	LBL 01		
62	"SUBSCRIPT "		Get Subscript, x_i
63	ARCL 01		
64	XEQ 60		$\sum_{i=1}^{N} x_i \rightarrow 02 = \alpha$
65	ST+ 02		
66	*		$\sum_{i=1}^{N} N_i \cdot \sum_{i=1}^{N} x_i \rightarrow 03$
67	ST+ 03		
68	ISG 01		
69	GTO 00		
70	RCL 00		Calculate # of Lone Pairs, β.
71	RCL 03		
72	-		
73	8		$\beta' = 04 = [(A-Q) - (\sum_{i=1}^{N} N_i x_i)]$ MOD 8
74	MOD		
75	STO 04		
76	2		
77	MOD		
78	RCL 04		
79	+		$\beta = 04 = \frac{\beta' \text{ MOD } 2 + \beta'}{2}$
80	2		
81	/		
82	STO 04		Set Flag = β
83	SF IND 04		
84	"TYPE: AX"		Display Type:
85	ARCL 02		
86	RCL 04		$A X_\alpha E_\beta$
87	X=0?		
88	GTO 09		
89	"E"		
90	ARCL 04		

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PROGRAM LISTING

"STRUCT"

☐ 67 ☐ 97 ☐ 41C

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
91	LBL 09		
92	AVIEW		
93	STOP		
94	CLA		Set up Molecular Shape Directed by χ_α and found from E_β
95	"M: "		
96	XEQ IND 02		
97	LBL 02		
98	FS? 01		
99	ARCL 05		
100	FS? 02		
101	ARCL 05		
102	ARCL 06		AX_2
103	XEQ 20		
104	LBL 03		AX_3
105	FS? 00		E_0
106	ARCL 07		
107	FS? 01		E_1
108	ARCL 09		
109	FS? 02		E_2
110	ARCL 12		
111	XEQ 20		
112	LBL 04		AX_4
113	FS? 02		E_2
114	GTO 41		
115	FS? 01		E_1
116	ARCL 11		
117	ARCL 08		
118	GTO 42		
119	LBL 41		
120	ARCL 14		
121	ARCL 15		
122	LBL 42		
123	XEQ 20		
124	LBL 05		AX_5
125	FS? 01		E_1
126	ARCL 14		
127	FS? 01		
128	ARCL 09		
129	FS? 00		E_0
130	ARCL 10		
131	XEQ 20		
132	LBL 06		AX_6
133	ARCL 13		
134	LBL 20		Set up Elec. Shape & Hybrids. $\alpha + \beta$ = # of branches. Add 10 & execute that subroutine. Leave calculator in Fix 4 mode.
135	AVIEW		
136	STOP		
137	CLA		
138	"e:"		
139	RCL 02		
140	RCL 04		
141	+		
142	10		
143	+		
144	XEQ IND X		
145	FIX 4		
146	SF 29		
147	AVIEW		
148	STOP		
149	GTO 22		End of Program
150	LBL 12		
151	ARCL 06		
152	ARCL 16		
153	RTN		
154	LBL 13		
155	ARCL 07		
156	ARCL 16		
157	"↓2"		
158	RTN		
159	LBL 14		
160	ARCL 08		
161	ARCL 16		
162	"↓3"		
163	RTN		
164	LBL 15		
165	ARCL 10		
166	ARCL 16		
167	"↓3d"		
168	RTN		
169	LBL 16		
170	ARCL 13		
171	ARCL 16		
172	"↓3d2"		
173	RTN		
174	LBL 60		
175	CF 22		
176	LBL 61		Input Subroutine
177	PROMPT		
178	FC?C 22		
179	GTO 61		
180	RTN		
181	END		

00

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PROGRAM LISTING

"MOLAR"

☐ 67 ☐ 97 ☒ 41C

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
01	LBL "MOLAR"		
02	CF 00		Initialize flags
03	CF 01		
04	CF 02		
05	CF 22		
06	.002		
07	STO 03		Loop Counter→03
08	"MOLES"		Store Vocabulary
09	ASTO 04		
10	"LITERS"		
11	ASTO 05		
12	"MOLAR"		
13	ASTO 06		
14	LBL 10		Data Entry Loop
15	CLA		
16	RCL 03		
17	4		
18	+		
19	ARCL IND X		Form Prompt
20	"↳?"		
21	PROMPT		
22	FC? 22		Number entered?
23	SF IND 03		No. Set "Solve" flag
24	FS?C 22		
25	STO IND 03		Yes. Store entry in 00, 01, or 02
26	ISG 03		
27	GTO 10		
28	.002		
29	STO 03		
30	CLA		
31	LBL 11		Which flag was set? Solve accordingly
32	FS?C IND 03		
33	GTO IND 03		
34	ISG 03		
35	GTO 11		
36	RTN		
37	LBL 00		Flag 00 was set: Solve for moles: moles = M · l
38	RCL 01		
39	RCL 02		
40	*		
41	ARCL 04		
42	GTO 12		
43	LBL 01		Flag 01 was set: solve for l: $l = \frac{mol}{M}$
44	RCL 00		
45	RCL 02		
46	/		
47	ARCL 05		
48	GTO 12		
49	LBL 02		Flag 02 was set: solve for M: $M = \frac{mol}{l}$
50	RCL 00		
51	RCL 01		
52	/		
53	ARCL 06		
54	LBL 12		Display result.
55	"↳="		
56	ARCL X		
57	AVIEW		
58	END		

50 00 80 90

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PROGRAM LISTING

"PRES"

☐ 67 ☐ 97 ☒ 41C

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
01	LBL "PRES"		
02	LBL 00		
03	SF 27		Initialize flags
04	CF 22		
05	CF 00		
06	CF 01		
07	CF 02		
08	CF 03		
09	CF 04		
10	"PRESSURE?"		
11	PROMPT		Get Pressure.
12	FC?C 22		
13	GTO 00		
14	"FROM :"		Display "FROM:"
15	AVIEW		
16	SF 00		
17	LBL 01		
18	"TORR,ATM,Pa,PSI"		Display Menu
19	AVIEW		
20	STOP		
21	RTN		
22	LBL 02		
23	"TO :"		Display "TO:"
24	AVIEW		
25	GTO 01		
26	LBL A		TORR
27	LBL B		
28	FS? 00		
29	SF 01		Set "FROM TORR" flag.
30	FS?C 00		
31	GTO 02		
32	ENTER↑		
33	*		
34	LASTX		
35	FS? 02		ATM → TORR
36	1.3158 E-3		
37	FS? 03		Pa → TORR
38	133.32		
39	FS? 04		PSI → TORR
40	1.9336 E-2		
41	/		
42	CF 27		
43	STOP		
44	GTO 00		
45	LBL C		ATM
46	FS? 00		
47	SF 02		Set "FROM ATM" flag.
48	FS?C 00		
49	GTO 02		
50	ENTER↑		
51	*		
52	LASTX		
53	FS? 01		TORR → ATM
54	760		
55	FS? 03		Pa → ATM
56	101325		
57	FS? 04		PSI → ATM
58	14.7		
59	/		
60	CF 27		
61	STOP		
62	GTO 00		
63	LBL D		Pa
64	FS? 00		
65	SF 03		Set "FROM Pa" flag
66	FS?C 00		
67	GTO 02		
68	ENTER↑		
69	*		
70	LASTX		
71	FS? 01		
72	7.5008 E-3		
73	FS? 02		
74	9.8692 E-6		
75	FS? 04		
76	1.4503 E-4		
77	/		
78	CF 27		
79	STOP		
80	GTO 00		
81	LBL E		PSI
82	FS? 00		
83	SF 04		"FROM PSI"
84	FS?C 00		
85	GTO 02		
86	ENTER↑		
87	*		
88	LASTX		
89	FS? 01		
90	51.717		
91	FS? 02		
92	6.8027 E-2		
93	FS? 03		
94	6895		
95	/		
96	CF 27		
97	END		

00

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PROGRAM LISTING

☐ 67 ☐ 97 ☒ 41C

"CONC"

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
01	LBL "CONC"		
02	"MW SOLUTE?"		Get mw of Solute
03	XEQ 60		
04	STO 00		
05	18		
06	"MW SOLVENT?"		Get mw solvent;
07	PROMPT		Default is 18.
08	STO 01		
09	1		
10	"DENSITY?G/ML"		Get density;
11	PROMPT		Default is 1.
12	STO 02		
13	"VALUE?"		Get a value.
14	XEQ 60		
15	"UNITS?"		
16	AVIEW		
17	SF 27		USER on
18	STO 03		
19	"X, WT/, ML, MR"		Display menu.
20	AVIEW		
21	STOP		
22	LBL A		X (mole fraction)
23	CF 27		USER OFF
24	1		
25	RCL 03		
26	-		
27	RCL 00		
28	RCL 03		
29	*		
30	X<>Y		
31	RCL 01		
32	*		
33	GTO 01		
34	LBL B		Wt/
35	CF 27		
36	GTO 03		
37	LBL C		Molality
38	CF 27		
39	RCL 00		
40	RCL 03		
41	*		
42	1 E3		
43	GTO 01		
44	LBL D		Molarity
45	CF 27		
46	RCL 02		
47	1 E3		
48	*		
49	RCL 00		
50	RCL 03		
51	*		
52	X<>Y		
53	/		
54	GTO 02		
55	LBL 01		Calculate
56	X<>Y		weight fraction.
57	+		
58	LASTX		
59	X<>Y		
60	/		
61	LBL 02		
62	STO 03		
63	"WT/="		
64	XEQ 70		

50

80

CONTINUED

90

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Note: Refer to HP-41C OWNER'S HANDBOOK AND PROGRAMMING GUIDE for specific information on keystrokes. The Function Index is found at the very back of the Handbook. Refer to Appendix E in 67 or 97 OWNER'S HANDBOOK AND PROGRAMMING GUIDE for exact keystrokes.

PROGRAM LISTING

☐ 67 ☐ 97 ☒ 41C

"CONC"

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
65	LBL 03		Calculate mole fraction, X.
66	RCL 03		
67	1 E2		
68	*		
69	LASTX		
70	X<>Y		
71	-		
72	LASTX		
73	RCL 00		
74	/		
75	X<>Y		
76	RCL 01		
77	/		
78	X<>Y		
79	+		
80	LASTX		
81	X<>Y		
82	/		
83	"MOL/="		
84	XEQ 70		
85	RCL 03		Calculate Molality, m.
86	1 E2		
87	*		
88	LASTX		
89	X<>Y		
90	-		
91	LASTX		
92	RCL 00		
93	/		
94	X<>Y		
95	1 E3		
96	/		
97	/		
98	"MLTY="		
99	XEQ 70		
100	RCL 02		Calculate Molarity, M.
101	1 E3		
102	*		
103	RCL 03		
104	*		
105	RCL 00		
106	/		
107	"MRTY="		
108	GTO 70		
50			

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
109	LBL 60		Input Subroutine
110	CF 22		
111	LBL 61		
112	PROMPT		
113	FC?C 22		
114	GTO 61		
115	RTN		
116	LBL 70		Output Subroutine
117	ARCL X		
118	AVIEW		
119	STOP		
120	END		
70			
80			
90			
00			

Note: Refer to HP-41C OWNER'S HANDBOOK AND PROGRAMMING GUIDE for specific information on keystrokes. The Function Index is found at the very back of the Handbook. Refer to Appendix E in 67 or 97 OWNER'S HANDBOOK AND PROGRAMMING GUIDE for exact keystrokes.

PROGRAM LISTING

☐ 67 ☐ 97 ☒ 41C

"C-J", "J-C", "F-C", "C-F"

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
01	LBL "C-J"		
02	4.184		J = 4.184 Cal
03	*		
04	RTN		
05	LBL "J-C"		
06	4.184		Cal = J / 4.184
07	/		
08	RTN		
09	LBL "F-C"		
10	32		°C = $\frac{5}{9}$ (°F - 32)
11	-		
12	5		
13	*		
14	9		
15	/		
16	RTN		
17	LBL "C-F"		
18	9		°F = $\frac{9}{5}$ °C + 32
19	*		
20	5		
21	/		
22	32		
23	+		
24	END		
40			
50			
51			
60			
70			
80			
90			
00			

Note: Refer to HP-41C OWNER'S HANDBOOK AND PROGRAMMING GUIDE for specific information on keystrokes. The Function Index is found at the very back of the Handbook. Refer to Appendix E in 67 or 97 OWNER'S HANDBOOK AND PROGRAMMING GUIDE for exact keystrokes.

PROGRAM LISTING

"Ea" and "K"

☐ 67 ☐ 97 ☒ 41C

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
01	LBL "Ea"		
02	SF 01		
03	8.314		R = 8.314 J/mol/K
04	STO 00		
05	"K1, K2=?"		Enter rate constants
06	PROMPT		
07	STO 01		
08	/		$\ln \frac{k_1}{k_2}$
09	LN		
10	"T1, T2=?"		Get Temp's.
11	PROMPT		
12	STO 02		
13	1/X		Calculate Ea:
14	X<>Y		
15	1/X		$\frac{1}{T_2} - \frac{1}{T_1}$
16	-		
17	/		$Ea = \frac{R \ln (k_1/k_2)}{\frac{1}{T_2} - \frac{1}{T_1}}$
18	RCL 00		
19	*		
20	STO 03		
21	"Ea= "		
22	ARCL X		
23	AVIEW		
24	STOP		
25	FS? 01		
26	GTO 01		
27	LBL "K"		"K" entry point when k, T, and Ea are known.
28	"K, T, Ea?"		
29	PROMPT		
30	STO 03		
31	RDN		
32	STO 02		
33	RDN		
34	STO 01		
35	LBL 01		
36	8.314		R
37	STO 00		
38	RCL 02		
39	*		
40	RCL 03		
41	X<>Y		$A = k e^{(Ea/RT)}$
42	/		
43	E^X		
44	RCL 01		
45	*		
46	STO 04		
47	"A="		Display A
48	ARCL X		
49	AVIEW		
50	STOP		
51	LBL 02		Solve for k at another Temp.:
52	"T3?"		
53	PROMPT		
54	RCL 00		
55	*		
56	RCL 03		$k_3 = A e^{-(Ea/RT_3)}$
57	CHS		
58	X<>Y		
59	/		
60	E^X		
61	RCL 04		
62	*		
63	"K="		
64	ARCL X		
65	AVIEW		
66	STOP		
67	GTO 02		Repeat for next Temp.
68	END		

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RYDBERG
PROGRAM NUMBER: V7544

ROW 1 (1-2)

ROW 2 (3-5)

ROW 3 (5-11)

ROW 4 (12-19)

ROW 5 (19-24)

ROW 6 (24-26)

ROW 7 (26-28)

STRUCT
PROGRAM NUMBER: V7544-

ROW 1: LINES 1-3

ROW 2: LINES 3-9

ROW 3: LINES 10-15

ROW 4: LINES 15-18

ROW 5: LINES 18-21

ROW 6: LINES 21-24

ROW 7: LINES 25-27

ROW 8: LINES 27-31

ROW 9: LINES 31-34

ROW 10: LINES 34-37

ROW 11: LINES 37-39

ROW 12: LINES 39-43

STRUCT
PROGRAM NUMBER: V7544-

ROW 13: LINES 43-43

ROW 14: LINES 44-51

ROW 15: LINES 51-52

ROW 16: LINES 53-62

ROW 17: LINES 62-64

ROW 18: LINES 64-71

ROW 19: LINES 72-83

ROW 20: LINES 84-87

ROW 21: LINES 88-95

ROW 22: LINES 95-101

ROW 23: LINES 102-108

ROW 24: LINES 108-114

STRUCT
PROGRAM NUMBER: V7544-

ROW 25: LINES 114-120

ROW 26: LINES 120-126

ROW 27: LINES 127-133

ROW 28: LINES 133-142

ROW 29: LINES 142-149

ROW 30: LINES 150-157

ROW 31: LINES 157-164

ROW 32: LINES 165-170

ROW 33: LINES 171-176

ROW 34: LINES 176-181

MOLAR
PROGRAM NUMBER: V7544

ROW 1: LINES 1-3

ROW 2: LINES 4-8

ROW 3: LINES 8-11

ROW 4: LINES 12-18

ROW 5: LINES 19-25

ROW 6: LINES 25-32

ROW 7: LINES 32-41

ROW 8: LINES 41-50

ROW 9: LINES 51-58

ROW 10: LINES 58-58

PRES
PROGRAM NUMBER: V7544

ROW 1: LINES 1-4

ROW 2: LINES 5-10

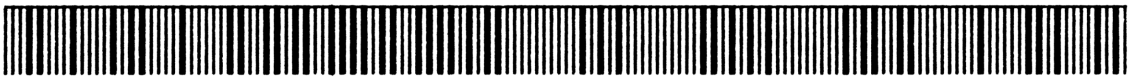
ROW 3: LINES 10-14

ROW 4: LINES 14-18

ROW 5: LINES 18-18

ROW 6: LINES 19-26

ROW 7: LINES 26-33

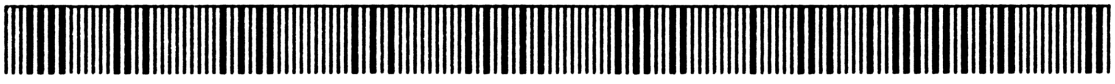


ROW 8: LINES 34-37

ROW 9: LINES 37-40

ROW 10: LINES 40-45

ROW 11: LINES 46-53

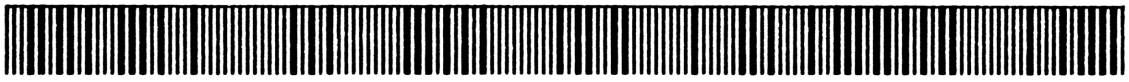


ROW 12: LINES 54-57

PRES
PROGRAM NUMBER: V7544

ROW 13: LINES 58-64

ROW 14: LINES 64-72



ROW 15: LINES 72-74

ROW 16: LINES 74-76

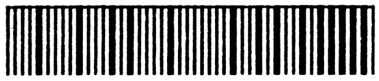
ROW 17: LINES 76-82

ROW 18: LINES 82-90

ROW 19: LINES 90-92

ROW 20: LINES 92-97

ROW 21: LINES 97-97



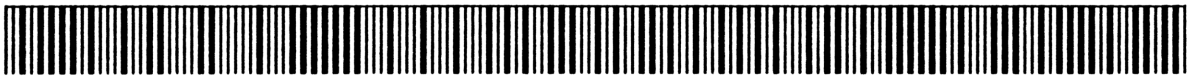
CONC
PROGRAM NUMBER: V7544-

ROW 1: LINES 1-2

ROW 2: LINES 2-6

ROW 3: LINES 6-8

ROW 4: LINES 9-10



ROW 5: LINES 10-14

ROW 6: LINES 15-19

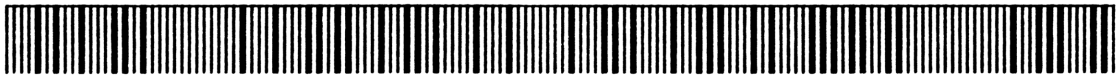
ROW 7: LINES 19-20

ROW 8: LINES 21-31

ROW 9: LINES 32-38

ROW 10: LINES 39-46

ROW 11: LINES 47-56



ROW 12: LINES 57-64

CONC
PROGRAM NUMBER: V7544-

ROW 13: LINES 64-74

ROW 14: LINES 75-83

ROW 15: LINES 83-91

ROW 16: LINES 92-98

ROW 17: LINES 98-106

ROW 18: LINES 107-110

ROW 19: LINES 111-117

ROW 20: LINES 118-120

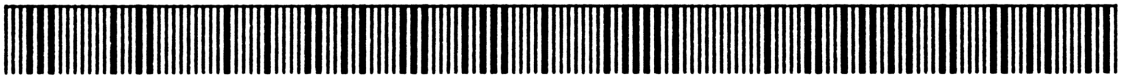
C-J
PROGRAM NUMBER: V7544

ROW 1: LINES 1-3

ROW 2: LINES 4-6

ROW 3: LINES 7-12

ROW 4: LINES 13-19



ROW 5: LINES 20-24

Ea
PROGRAM NUMBER: V7544

ROW 1: LINES 1-3

ROW 2: LINES 4-8

ROW 3: LINES 9-13

ROW 4: LINES 14-22

ROW 5: LINES 22-28

ROW 6: LINES 28-32

ROW 7: LINES 33-41

ROW 8: LINES 42-51

ROW 9: LINES 52-61

ROW 10: LINES 62-68

Ordering Information

Program Title	Program Number
The Physics Collection	V7543-41
The Chemistry Collection	V7544-41

Prices

For documentation and barcode only $25.00

For documentation, barcode, and your choice of magnetic recorded media (cards, cassette, or 3.5" HPIL disc) $45.00

For recorded media alone (you must include proof of purchase of documentation - please enclose a copy of your sales receipt) $20.00

Use the enclosed order form to order directly from the Hewlett-Packard Users' Library Software Distribution Center.

USERS' LIBRARY ORDER FORM

After completing this Users' Library Order form, return to: Hewlett-Packard
Dept. 39UL
1000 NE Circle Blvd
Corvallis, OR 97330 (503) 757-2000

Make checks payable to Hewlett-Packard; check or money order must be in U.S. dollars, drawn on a U.S. bank and enclosed with the order. Please include state and local taxes if appropriate.

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–Multiple programs can be recorded on an HP-IL 3.5″ disc or mini data cassette for $19.50 plus the cost of each program requested.

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Company _____

Address _____

City _____ **State** _____ **Zip** _____

Country _____ **Daytime telephone number** _____

Method of payment:

☐ Cash, check or money order enclosed ☐ Master Card ☐ VISA ☐ Purchase order ($20 minimum)

Card Number _____ Exp. Date _____

PLEASE NOTE
When ordering programs with media, remember to specify media type for each item.

PROGRAM NUMBER	QTY	DOC ONLY	MEDIA CHOICE			PRICE
			w/mag cards	✱w/mini cassette	✱w/3.5″ disc	

☐ This order is tax exempt

_____

Program Total _____
25% Discount† _____
Subtotal _____
Software Distribution Center _____
(Mini cassette/3.5″ disc) **$19.50 ea** _____
State & Local **Taxes** _____
(Postage & handling–outside the USA)**10%** _____
TOTAL _____

✱ ***May be*** an additional $19.50 Please read pricing information included in the Introduciton.

† Discount applies to 6 or more Library PROGRAMS only (cassettes discs. SDC programs or other products are not discounted) Prices subject to change without notice

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