The PocketProfessionalTM

Chemistry Applications

Owner's Manual

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Notice

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1 Getting Started

In This Chapter

- Welcome
- Installing and Removing the Pocket Professional
- Using the Main Menu
- Using the Equation Library
- What you should know about the Solver
- GCHEMD Directory
- Equation Library Structure
- Summary of Softkeys

Welcome

Da Vinci Technology group's Pocket Professional software is the first of its kind, developed to provide speed, efficiency and portability to students and professionals in the technical fields. The PocketProfessionalTM Chemistry Application Pac instantly transforms the HP 48GX calculator into an electronic handbook. The information is organized into an six major sections: Equation Library, Periodic table, Stoichiometry, Species Library, Constants Library and Reference Library. These sections are organized in easily accessible, efficient menu driven format.

Installing, Removing the Pocket Professional

The HP 48GX has two ports for installing plug-in cards. You can install your Application Pac in either port. Be sure to **turn off the calculator** while installing or removing the card. Otherwise, user memory may be erased.

To Install the Card

- Turn off the calculator. Do not press on until you have completed the installation procedure.
- Remove the port cover. Press against the grip lines and push forward. Lift the cover to expose the two plug-in ports.
- Select either empty port for the Pocket Professional card.
- Position the card just outside the slot. Point the triangular arrow on the card toward the calculator port opening, as shown below.

- Slide the card firmly into the slot. After you feel resistance, push the card about 1/4" further, until it is fully seated.
- Replace the cover





To Remove the Card

- 1. Turn the calculator off. Do not press in until you have completed the procedure.
- 2. Remove the port cover. Press against the card's grip and slide the card out of the port.



3. Replace the port cover.

To Access the Chemistry Application Pac

After you turn your calculator $\overline{[m]}$, there are three ways to access the Chemistry Application Pac.

First Method: Press P Em to display all libraries available to the HP 48GX. Press the COAP, "softkey" to start the General Chemistry Application

{ HOME	3		
4:			10 MI # 12 01 4 19 19
3:			
2:			
1:			
GC MP D	CON MED		

Pac. Pressing the second softkey available at this level, **ABOUT**, displays the revision number of the software. Pressing the revision screen and returns you to the screen shown above. Second Method: Type in the letters GCAPP and press **EVER**.

Using the Main Menu

After you start the Application Pac, the main menu screen appears. The main menu lists the main categories

in a "browser" menu format. "Browser" refers to the ability to use the cursor keys 🔽 and 🛆 to move the pointer to the menu item you wish to select and to press ENTER to call that menu item to the screen.



The row of "softkeys" along the bottom of the screen may give you options that relate to the information displayed on any given screen.

Because the size of the calculator screen is limited, the names of constants and properties are usually abbreviated throughout the pac.

The items in the main menu are described briefly below, and discussed in detail in chapters to follow.

Equation Library	Allows you to solve, plot and analyze over 150 equations
Species Library	A list of chemical compounds to be used as reactants and products when building your own chemical equations.
Periodic Table	Lists properties of each element of the Periodic Table.
Stoichiometry	Allows you to enter your own chemical equation, checks Mass and charge balance (Does the balance the equation) and performs theoretical yield and limiting reagent calculations
Constants Library	Lists 29 commonly used constants
Reference library	Selected reference data

The "soft keys" located along the bottom of each screen gives the various options relating to that screen. A complete list of all the soft keys available is listed at the end of this chapter.

Moving Around the Screen

Use the \bigtriangledown and \bigtriangleup keys to move the pointer up and down in the menu list. Pressing \boxdot \bigtriangledown moves the pointer to the bottom of the screen, or pages down if the pointer is already at the bottom of the screen. Pressing \square \square moves to the top of the screen or pages up if the pointer is already at the top of the screen. Pressing \square \bigcirc moves the pointer to the bottom of the list or \square \square moves to the top of the list.

Viewing Items Too Wide for the Display

If the text of a topic or subtopic is too wide to fit within the display, an ellipsis (...) appears at the end of the line. Press the soft key $\bigvee I \subseteq W$ to display the rest of the text. To return the previous display, press \bigcirc key.

Changing the Font Size

The default font for the Application Pac displays information in condensed, uppercase letters only. Pressing the soft key **FONT** displays the information in a larger font, which is case-sensitive. The font size stays large until you press **FONT** key again.



Using the Search Mode

When the menu lists are long, it may be faster to locate an item using the

search mode. To initiate a search, press \square key, which displays the screen shown here. The calculator is now in the *alpha* entry mode, as indicated by the alpha (α) annunciator at the very top row of the calculator screen display. Alpha

RAD { Home gchemd }	PRG
Search for:	
+	
ESKIPSKIPS EDEL DELS I	NS 🗖 🕂 STK

entry mode overrides the function of the standard keyboard. This means that each key that has a white capital letter printed to it's lower right looses its original function and types that letter onto the command line when pressed. Type the first letter or letters of the name you wish to search for, to create a search string and press $\boxed{\text{EMEP}}$. The search function is case sensitive. To enter a lower case letter in the alpha entry mode press $\boxed{\text{EMEP}}$ key before typing the letter.

Editing Text Entries

The search mode soft keys along the bottom of the screen are command line editing keys. They are built into the HP 48GX and allow you to edit the search string. Their functions are outlined below:

< - SK I P	Moves the cursor to the beginning of the current word
SKIP->	Moves the cursor to the beginning of the next word
<-DEL	Deletes all characters in the current word to the left of
	the cursor
DEL->	Deletes all characters from the current position to the
	first character of the next word
INS	Toggles between insert and typeover modes
->STK	Accesse a version of the interactive stack inwhich only
	"ECHO" function is available.

Using the Equation Library

The Equation Library contains over 150 equations commonly used by today's chemist, and is organized into seven main categories. The Equation Library enables you to:

→ATDM SOLII GASE ACID: THER PREC KINE	Equa 157MDI 57LIQI 57BASE MD7EL IPITATI TICS	ation ECULES UIDS S ECTROCHE ON	Libran M	'n
			FONT	UP

- Select the equation category and topic from the main menu.
- List all the equations in a topic.
- Solve a specific equation or a set of equations.
- View a description of the variables.
- View a figure that illustrates the problem.
- Plot the equation.

Solving a Single Equation

Suppose, for example, you want to calculate the number of moles of iron (molecular weight =

At oms/Molecules Amass/Mole/atom Light Quantum Hydrogen S Dreitals P Dreitals D Dreitals D Dreitals F Dreitals MMIX EXXE MARE (IGURASOLVE)

55.847_g/mol) in a truck containing 1.5 metric tons of material.

Accessing Equations

The first step in solving this problem is to locate the necessary equation in the Equation Library. At the main menu, move the pointer to "EQUATION LIBRARY" and press ENER. This displays the list of categories available in the Equation Library, shown below:

Move the pointer to the category "ATOMS/MOLECULES", and press



ENTER to display the list of topics:

Selecting and Displaying Equations

Move the pointer to the topic "MASS/MOLE/ATOM" and press

INTER, or press the **EQNS** soft key, to display the equation set for mass-tomole conversions:

This screen lists all the equations in the current topic. In this case, there are only two. You may choose to solve all the equations in a set or solve only one equation. Solving multiple equations is discussed later in this



chapter. For this example, the number of moles of iron in the truck is given by the following equation (which is the first equation in the list):

$$n = \frac{ga}{MWT}$$

where n is the number of moles, ga is the mass of iron and MWT is the molecular weight of iron (55.847_g/mol). Any equation may be selected by moving the pointer to the desired equation and pressing the **SELECT** softkey. If no equation is selected, then all equations are solved. When an equation is selected, a triangular tag is placed in front of the equation:

If you want to view the equation in its full "textbook" form, move the pointer to the equation and press ENTER. This displays the equation on the screen:

When a chemical equation is lengthy, pressing \triangleright or \triangleleft scrolls the screen to the left or to the right to display the entire equation. Press $\boxed{\text{ENTER}}$ or $\boxed{\text{ME}}$ to return to the list of equations.

Viewing Variable Definitions

You can view a list that defines all the variables in the selected equation or

set of equations by pressing the **VARS** softkey at the equations screen. The screen below shows the definitions for each variable in the first equation of the MASS/MOLE/ATOM topic:



Using the Solver Function

The da Vinci "solver" is a software function that simplifies the job of

setting up equations to be calculated by the HP 48. The solver function is discussed in more detail later in this chapter, under "What You Need to Know About the Solver." To execute the solver, press **SOLVE** at the equations screen. The variables for the selected equation(s) now appear in the screen, waiting for you to enter values, as shown: To enter the mass of iron, move the pointer to **ga** and press **ME**. This displays the following screen:

Enter the mass of iron at the prompt.

Mass/Mole/Atom KG' '-KG/MOL' CALC LEONS VARS UNITE HOST K 11:

RAD { Home gchemd }			PRG		
Set	9a,	Mass	1		
4					
_KG	_6	_MG	_11	LE	_T

After the mass has been entered, you may assign units to your entry by

RAD PRG { HOME GCHEMD }	RAD PRG
Set ga, Massi	set ga, nass.
	1.5_t .kg _g _mg _u _ls _t

pressing the appropriate unit soft key. If you choose not to add units and press will be assumed. In some cases, more units are available than the six softkeys displayed in the first screen. In these cases, press will to display the next page of additional units. For a complete description of units available in the HP 48 manual.

In this example, press **E** to add units of metric tons to this entry.

Press to store this value into **ga.** This returns you to the solver screen with 1.5_t of iron stored into the variable, **ga**:



is a known variable. Repeat this procedure for the other known variable, **MWT**, which for iron is 55.847_g/mol. This results in the following screen:

PMWT: '55.847_G/MOL'
CALC LEONS VARS UNIT + + STK UP

With two of the three variables known in this equation, you can now solve the equation for the number of moles by pressing **CALC**. After a few moments, the calculator returns to this screen with the calculated value of n: The * by n indicates that this value was calculated and was not user specified.

Converting Data to Different Units

Suppose you want to convert the mass



of iron just computed to pounds. First press is to view a new page of softkeys:

→_KG _G _MG _U _LB _T _TZ	Co	onve	rt 1	to	
_921					EXIT

Mass/Mole/Atom XN: '26959.0971762_M0L' +>FGA: '3306.93393277_LB' >MWT: '55.847_G/M0L'	
KNOW WANT CLEAR FURGE CONV	UP

Move the pointer to the variable ga and press \bigcirc . This lists all the possible units for **ga**:

Move the pointer to **-LB** and press **ENTER**.

This converts the mass in metric tons to pounds. If you want to use the data for further calculations, move the pointer to the data item and press EMENT to place it on the calculator stack.

Options After Solving the Equation

Pressing exits the Chemistry Application Pac and places you in the calculator operating environment. Pressing **CLEAR** resets all entries in the current topic to zero. Pressing **PURGE** eliminates each variable in the current topic from calculator memory. To return to the main menu screen press **UP** multiple times. At the main menu, a new "RESUME SOLVING..." entry will have been added to the list, as shown:

Selecting the RESUME SOLVING function returns you directly to the equation set you were working with, with all previous entries still intact.

Managing Units

When solving an equation, **UNITES** (a toggle key) controls whether the calculations are performed in your choice of units, or in Systeme Internationale d'Unites (SI) units. When the **UNITES** softkey appears, it means that all entries are converted to SI units and the unit designations are removed. **UNITED** indicates that the software is managing units, and that all values will contain the unit designations that you specify. All values entered without unit designations are assumed to be in (SI) units. Be aware that **using designated units increases the processing time substantially.**

Solving Multiple Equations

For many problems, the result of one calculation acts as the input to another. The Chemistry Application Pac is capable of solving multiple equations, sequentially and systematically.



Selecting the Equation Set

Suppose you want to calculate the concentration in moles per liter (molarity) of HCl in water in a 100_ml solution that is a 36% by weight HCl with a density of 1.19_g/ml (a standard concentrated HCl solution).

To solve this problem, move to the "CONCENTRATION" topic under the "SOLIDS/LIQUIDS" category. This topic contains 12 equations which relate the various forms of concentration of solute (labeled a) in the solvent (labeled



b) to the fundamental parameters of the solution. These equations are listed below:

$$gs = ga + gb \qquad ma = \frac{na}{gb}$$

$$na = \frac{ga}{MWTa} \qquad xa = \frac{na}{na + nb}$$

$$ga = ga \cdot \frac{gs}{100} \qquad wa + wb = 100$$

$$gb = wb \cdot \frac{gs}{100} \qquad nb = \frac{gb}{MWTb}$$

$$gs = vs \cdot \rho s \qquad ppma = \frac{ga \cdot 1E6}{gb}$$

$$Ma = \frac{na}{vs} \qquad gb = vb \cdot \rho b$$

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These equations are displayed on the screen when you select the CONCENTRATION topic, shown below:

To view the variables for this equation set, press **VARS**. All the variables for the CONCENTRATION topic, and their (SI) units are listed in the following table:

Variable	Description	Units
ga	mass solute	kg
gb	mass solvent	kg
na	moles solute	mol
nb	moles solvent	mol
MWTa	molecular weight solute	kg/mol
MWTb	molecular weight solvent	kg/mol
wa	weight % solute	-
wb	weight % solvent	
ρ b	pure solvent density	kg/m^3
vb	volume of solvent	m^3
gs	mass solution	kg
vs	volume solution	m^3
ρ s	density solution	kg/m^3
Ма	molarity solution	mol/m^3
ma	molality solution	mol/kg
ха	mole fraction solution	63
ррта	solute concentration	83

Solving the Equation Set

Press **SOLVE** to execute the solver function. Enter all the information pertaining to the problem at one time, including any unit conversions you wish to make,

Concentration	
XNA: '1.17495728301_MOL' XNA: '4.22754118745_MOL'	
PMWTA: '96,4609_G/MOL' PMWTB: '18.0152_G/MOL'	
XWB: 64.000000002	
CALC EONS VARS UNIT = +STK	ЦP

using the procedure described previously. Press **CALC** to start the solver. The solver then steps through each equation in the list, solving those equations that contain sufficient information to calculate a solution.

When all variables are found, or all remaining equations have more than one unknown variable, the solver stops. It then lists the variables it can't find, and returns to the solver screen. The given variables and calculated results for this example are shown below:

Concentration *KGA: '.0576_KG' *KGA: '.0576_KG' *KGA: '.0576_KG' *MA: '.52808219178_MBL' *MMTA: '36.5_G/MGL' *MMTB: '18.05_G/MGL' *MMTB: '18.05_G/MGL' *MMTB: '18.05_G/MGL' *MMTB: '18.0000000001 *F: '0.KG/M^3' VB: '0.KG/M^3' *KGA: '15.400 *Y5: '16_KG' *Y5: '16_KG' *Y5: '16_KG' *Y5: '15.400 *Y5: '15.400 *Y5: '15.400 *Y6: '15.400 *Y6: '25.400 *Y76 *Y6: '25.400 *Y76 *

Given		Result	
MWTa	=	1	LANSING LOMLAN
	36.4609	_g/mol (HCl)
Ma	2	11.7_mol/l	
MWTb	=	18.0152_g/1	mol (H ₂ O)
wa		36.0	
vs	25	100ml	
ρ s	22	1.19_g/ml	

With the information given, the solver found all variables but two, $\rho \mathbf{b}$ and \mathbf{vb} (no asterisk *). The solver also calculated the solution concentration in molality, in mole-fraction, and in parts-per-million, as the screen below shows:

The screen above has been graphically expanded to reveal the entire list. To see all 17 variables on the calculator screen, you must scroll through the variable list.

Tagging Variables

If you want to solve for only one variable in the list, you can "tag" it: Move the pointer to the variable you want to tag, press to display the additional softkeys for this screen, and press **WANT**. This places a "?" tag in front of the variable you want to solve for:

If you tag Ma (molarity) and press CALC the solver calculates for Ma only, rather than solving for the entire set. It is possible to tag more than one variable in the list.

Plotting One Equation

Any equation in the equation library that is of the form: y=f(a,b,...) can

be easily plotted using the General Chemistry Application Pac. To plot an

equation, the dependent variable, y (on the left), and the desired independent variable, a or b or c, etc. (on the right), must be unknown (no triangular tag). However, all other variables must be known.

Finding and Selecting the Equation

As an example, plot the titration curve (the pH versus the volume of added

base) of the titration: 25_ml of a 0.1_mol/l strong acid with a 0.1_mol/l strong base at 25 °C. The equations that describe strong acid/strong base titrations are filed in the ACIDS/BASES category of the Equation Library, under the topic



TITRATION (SA/SB). The equation screen for this topic is shown below:

Select the second equation in the list. This equation is written out below:

$$pH = -LOG\left[\frac{-(Vb \cdot Cb - Va \cdot Ca)}{2 \cdot (Va + Vb)} + \frac{1}{2} \cdot \sqrt{\left(\left(\frac{Vb \cdot Cb - Va \cdot Ca}{Va Vb}\right)^{2} + 4 \cdot Kw\right)}\right]$$

where

Ca	acid concentration	mol/m^3
СЬ	base concentration	mol/m^3
Va	volume of acid solution	m^3
Vb	volume of base titrant	m^3
Kw	water dissociation constant	mol^2/m^6
pН	pH value	65

Tagging and Entering the Variables

To plot the titration curve (**pH** versus **Vb**), **Ca, Cb, Va,** and **Kw** must be tagged as known variables. Move the pointer to the second equation and press **SELECT**. Then press **SOLVE** to enter the values for the following known variables:

Ca = 0.1 mol/lCb = 0.1 mol/lVa = 25 mlKw = $1.01 \times 10^{-14} \text{mol}^{2/l^{2}}$

Use the **CONV** softkey to change the units of Vb to ml for the plot.

With these four variables entered, return to the equations screen by pressing **EQNS**. Move the pointer to the second equation and press **PLOT**. Since this equation is of the proper form, and all but Vb has been specified on the right hand side, it may be plotted.

Entering the X and Y Coordinates

The first prompt asks whether you want to erase the previous plot and reset the axes, **MES**, or whether you want the new plot drawn over any existing graphics already on the screen, **NO**. To continue with this



example, at the prompt enter **MES** to clear all previous plots from the screen.

Now enter the minimum and maximum x coordinates for the graph, starting with the x range as x1 x2. Type the coordinates for the plot on the same line, separated by a space (use the sec key). Plot between 0 and 50

milliliters of added base, since this is approximately twice the equivalent volume:

At the next prompt, enter the y axis limits in the same format. For this example, plot from -3 to 16,



to ensure that all portions of the plot are visible. If you press $\overline{\text{MER}}$ without typing in the y axis limits, the calculator autoscales the plot. Once the x and y axes limits are entered, press $\overline{\text{MER}}$. After several minutes of working time, the calculator draws the following plot:

Plotting Speed

The calculator takes approximately 10 minutes to draw this plot (plus an additional three minutes if autoscaling is desired). The plotting speed is limited by the HP 48 unit manager. If the units are turned off (by pressing UNITE at the solver screen) the plot takes only 40 seconds (plus 10 seconds for autoscaling). However, as described earlier in this chapter under "Managing Units," when you turn off units, all user entered values are converted to SI units. Therefore, when you enter the x-axis coordinates, you need to enter them as "0 0.000050" to account for

concentration units of m^3 instead of _ml. The plot will also be displayed in SI units.

Softkeys for the Plot Function

The softkeys shown in the above plot are plot function keys in the HP 48. For example, pressing **COORD** displays the (x,y) coordinates of any point on the screen indicated by the cursor. For a description of the behavior of the plot function softkeys, see the HP 48 Owner's Manual. Note that the **SLOPE** and **E** keys, inside the HP 48 **EON** submenu, are supported by the Chemistry Application Pac only when SI units are used (units are off). You can remove the softkeys from the plot to expose more of the graph by pressing **NATION** and **KEYS**. Press **DE** to interrupt the plotting of an equation or to return to the equation screen.

Plotting Multiple Equations

For comparison purposes, you may want to plot the same variables in an equation to a new parameter. To do this, simply answer \mathbf{NO} to the "clear plot first?" prompt after you have pressed **PLOT**.

For example, suppose you're interested in plotting a family of titration curves on the previous graph, except with lower concentrations of acid and base solutions (**Ca=**0.001_mol/l and

PH	CNO	UNITS)	PH=	TRAT	ON (-(YB	SA/SB) ECB-YA
ŀ			F			
[5			etan a
E-		+++	+-+		4 Y D	
200	M	6 YD TRA	CE F	CN	EDIT	CANCL

Cb=0.001_mol/l). First, return to the solver screen and enter the new values for Cb and Ca. Then, go to the equations screen, move the pointer to the pH titration equation, and press **PLOT**. At the prompt, press **NO**. The new graph will plot over the previous one, as shown:

There is no limit to the number of times your equation can be plotted on the current axis. However, the HP 48 plot/graphics function keys support only the most recent plot.

What You Should Know About the Solver

As you have seen in the examples in this chapter, the Sparcom solver allows you to easily specify the values and units of your equation or set of equations before sending the data to the HP 48 numerical root-finder. For the selected equations(s), the solver screen lists all the variables, shows whether they are known (triangular tag), unknown (no tag), wanted ("?" tag), or already calculated (*); and whether units are on or off. Once you set these parameters, pressing **CALC** activates the HP 48GX root-finder to calculate the solution(s). The root-finder requires an initial value on which to base its search. You can provide a "guess" for the calculator to use, or the solver will provide the root-finder "guess" value of 1. The rootfinder then generates pairs of intermediate values and interpolates between them to find the solution. The time required to find the root depends on how close the initial guess is to the actual solution.

Speeding Up Computing Time

You can speed up computing time by providing the calculator a "guess" value close to the expected solution. At the variables screen, enter your guess value into the "unknown" variable. The variable will then be tagged as "known" (triangle). Press the **KNOW** softkey to toggle the variable back to "unknown" (no tag). Now press **CALC**.

"Bad Guess" Message

If the calculator displays the message, "Bad Guess(es)," after you press the **CALC** softkey, it indicates an error has been made in setting up the problem. Go back through the set up process and check for errors in specifying data.

Equations with Multiple Roots

It is advisable to provide "guesses" for the unknown variables in equations containing multiple roots. For example, the positive root of a cubic equation is desired when solving for the H^+ concentration in a weak acid. A guess near the desired solution will minimize the chance that the positive root will be missed in lieu of one of the negative roots.

See the *HP 48GX Owner's Manual* for a detailed discussion on using the root finder or HP's solver function.

Loading Values from the Stack

There are two methods of entering a value into the Sparcom solver directly from the calculator stack:

First Method: At the HOME screen make sure the value you want is on level one of the stack. Press **CCAP**, then select RESUME SOLVING to return to the equation set you're working with. At the variables screen, move the pointer to the variable that will incorporate the value currently on the stack and press INTER. A prompt message asks you to enter the value. Press INTER: to reveal the command line editing keys. Pressing INSTIK displays the value in a limited version of the HP 48GX's interactive stack. Press ICHO then INTER. This takes you back to the "enter value" prompt message. Press INTER again to reveal the solver screen, showing the value incorporated into the selected variable and tagged as "known."

Second Method: Alternatively, store the desired value into a global variable in the GCHEMD directory under the same name as the equation variable. When the solver is entered, it will automatically recall the value and load it into the selected equation variable.

da Vinci's GCAPPD Directory

When you plug in the Chemistry Application Pac for the first time, the software creates its own directory, GCHEMD, in the HOME directory of the HP 48GX. ALL operations performed by the software take place in the GCHEMD directory. It is, therefore, the only place where global variables are created or purged by the solver level. If you purge this directory by mistake, it will be recreated in its entirety. However, all the values that you have stored in the software memory will be lost.

The variables created in the GCHEMD directory and their functions are described below:

Gcpar	The parameter GCpar is utilized to provide a direct path from the main menu to the solver level. GCpar is created (or rewritten) whenever the equation, solver, or variable levels of the Equation Library is exited. The three possible exit routes that trigger a GCpar update are:		
-			
	1) Pressing we to quit the General Chemistry Pac and		
	exit to the calculator stack,		
	2) Pressing UP to return to the topic level, or		
	3) Pressing MAIN to return to the main menu level		
RXNS	Contains user defined reactions. To eliminate all		
	reactions, this variable may be purged. It is recreated		
	whenever a new reaction is built		
SPEC	Contains user-defined species stored in the Species		
	Library. To eliminate all species, this variable may be		
	purged. It is recreated whenever a new species is added		
SPECCODE	Contains the index of the last species added to the		

Species Library. User modification or deletion of this
variable will corrupt the reaction and species librariesUSRSYMBSContains user-defined chemical symbols

USRATWTS Contains user-defined atomic weights

Summary of Softkeys

Stores all variable values and iterates through the set of selected equations in an attempt to find values for all wanted variables. After completion of the solver process, the user is returned to the solver level, where newly found variables are marked with "*"
Denote the vertice of the summer verticable set to more
Resets the values of the current variable set to zero.
Enters the equation level of the current topic.
Displays a figure for the currently selected topic or displays "No figure".
Toggles between small and medium display fonts of the HP 48GX.
Toggles the currently selected variable between known and unknown, adding or removing the triangular tag.
Returns to the main menu.
Prompts the user for x-axis and y-axis values (with
option for autoscale v). This feature only works for
equations of the form $y=f(a,b,)$ where y and one
variable on the right are unknown.
Purges the global copies (in the GCHEMD directory) of
the current variable set displayed in the solver level.
Exits the Chemistry Application Pac.
Marks or unmarks the currently selected equation with
the triangular tag. Only variables in the marked
7 requations will appear in the solver and variable levels.
If no equations are selected all will be used
Enters the solver level of the current tonic
Copies selected entry to calculator stack
Toggle key. Indicates that units are on.
Toggle key. Indicates units are off. When off. all
variables are assumed to be SI if entered with no units or
are converted to S1 units.
Noves up one level in the software menu structure.
Enters the variable level for the current topic.
Displays the full text entry for a variable description or
value if the description is too wide to fit on the screen.
Toggles the currently selected variable between wanted

and not wanted, adding or removing the symbol "?". If no variables are marked "wanted," all variables are assumed to be wanted.

ENTER

CHICE.

Prompts for the value of the currently selected variable. If the selected variable already contains a value, that Value is copied to the command line for editing. Pressing we clears the command line, or returns you to the variables screen if the command line is already empty.

Generally used to exit a function or application.

2 Equation Library

In This Chapter

The Equation Library for the General Chemistry Application Pac contains over 150 equations organized into seven main categories, each containing one or more topics. Each topic includes a description, an equation or set of equations, a complete list of variables, a set of units for all variables, and a working example. The examples in this chapter often give results in units different from the SI units used by the software. To match the printed results with those shown on the calculator, convert the units using the procedure described in Chapter 1. Some of the equation sets also include a figure to illustrate the topic more fully.

- Atoms/Molecules
- Thermo/Electrochemistry
- Solids/Liquids

- Gases
- Kinetics
- Aids/Bases

• Precipitation

In the Equation Library, the following constantshave been built-in and the values need not be entered.

pi	π
g	Acceleration due to gravity
R	Universal gas constant
NA	Avogadro's number
с	Velocity of light
h	Planck's constant
k	Boltzmann's constant
q	Electron charge
Rω	Rydberg's constant
ao	Bohr radius
σ	Stefan-Boltzmann
F	Faraday constant

Atoms Molecules

In this category, equations relating to the fundamental relationships of elements and molecules are contained in the following topics:

- Mass/Mole/Atom .
- p, d and f Orbitals
- Light
- Diatomic Moment

Mass/Mole/Atom

number of $m = \frac{ga}{MWT}$

These equations relate the mass of a sample to its number of moles and

 $Natoms = NA \cdot n$

Quantum

- Symmetrical Moment
- Hydrogen Energy



Variable	Description	Units
n	number of moles	mol
ga	mass of sample	kg
MWT	molecular weight of sample	kg/mol
Natoms	number of atoms	-

Example: How many atoms and moles are contained in a 45 lb. sample of iron (molecular weight=55.847 g/mol)?

Given	Result
ga = 45_lb	n = 365.5 mol
MWT = 55.847 g/mol	Natoms = 2.201E26

Light

These equations relate the frequency, wavelength, photon energy, and wavenumber of light.

$\lambda =$	$\frac{c}{\gamma} \qquad E = h \cdot \gamma$	$nubar = \frac{1}{\gamma}$
Variable	Description	Units
λ	wavelength	m
γ	frequency	Hz
E	photon energy	J
nubar	wave number	1/m

Quantum

Two fundamental equations of quantum mechanics included here relate the de Broglie wavelength of a particle to its momentum, and the particle mass to its inherent energy.

$$\lambda l = \frac{h}{m \cdot \nu} \qquad \qquad E = m \cdot c^2$$

Variable	Description	Units
λ1	de Broglie wavelength	m
m	mass	kg
v	velocity	m/s
E	energy	J
h	Plank's constant	J.s
С	velocity of light	m/s

Example: What is the de Broglie wavelength of a 1.0_oz bullet moving at 600 ft/s? What is the bullet's inherent energy ?

Hint - You do not need enter values for h and c. They are extracted from internal tables.

Given m = 1.0_oz v = 600_ft/s **Result** λ1 = 1.28 E-25_nm **E**=2.55 E15_J

Hydrogen Energy

These equations relate the energy, wavelength, and frequency of transition to their initial and final quantum numbers in a one-electron atom.



PRESS CENTERI TO RETURN TO LIST ...

$$E = \frac{-R\infty \cdot Z^2}{ni^2} \qquad \Delta E = -R\infty \cdot Z^2 \cdot \left(\frac{1}{nl^2} - \frac{1}{ni^2}\right)$$
$$\gamma = \frac{\Delta E}{h} \qquad \lambda l = \frac{c}{\gamma}$$

Variable	Description	Units
E	energy	J
Z	nuclear charge	-
ni	initial quantum number	-

nf	final quantum number	-
ΔE	energy change	J
γ	frequency	Hz
λ1	wavelength	m

s,p,d and f Orbitals

These equations describe the angular and radial portions of the Schroedinger one-electron atom. They are grouped by azimuthal quantum number (s, p, d or f). Note that the wavefunction, φ nlm, is given by:

$$\varphi_{nml} = R_{nl} \cdot X_{lm}$$



The normalization constant given below

is provided for reference only and guarantees that the integrated probability over all space is unity.

$$\rho = \frac{2 \cdot Z \cdot r}{ao}$$

Radial Functions:

(1s) $Rnl = R10 = Z^{\frac{3}{2}} \cdot e^{-\frac{\rho}{2}}$ constant $= \frac{2}{ao^{\frac{3}{2}}}$ (2s) $R20 = Z^{\frac{3}{2}} \cdot (2-\rho)e^{-\frac{\rho}{2}}$ constant $= \frac{2}{ao^{\frac{3}{2}} \cdot 2 \cdot \sqrt{2}}$ (3s) $R30 = Z^{\frac{3}{2}} \cdot (6-6 \cdot \rho + \rho^{2}) \cdot e^{-\frac{\rho}{2}}$ constant $= \frac{2}{ao^{\frac{3}{2}} \cdot 9 \cdot \sqrt{3}}$

(4s)
$$R40 = Z^{\frac{3}{2}} \cdot (24 - 36 \cdot \rho + 12 \cdot \rho^{2} - \rho^{3}) \cdot e^{-\frac{\rho}{2}}$$

constant $= \frac{2}{ao^{\frac{3}{2}} \cdot 96}$
(2p) $R21 = Z^{\frac{3}{2}} \cdot \rho \cdot e^{-\frac{\rho}{2}}$
constant $= \frac{1}{ao^{\frac{3}{2}} \cdot 2 \cdot \sqrt{6}}$
(3p) $R31 = Z^{\frac{3}{2}} \cdot (4 - \rho) \cdot \rho \cdot e^{-\frac{\rho}{2}}$
constant $= \frac{1}{ao^{\frac{3}{2}} \cdot 9 \cdot \sqrt{6}}$
(4p) $R41 = Z^{\frac{3}{2}} \cdot (20 - 10 \cdot \rho + \rho^{2}) \cdot \rho \cdot e^{-\frac{\rho}{2}}$
constant $= \frac{1}{ao^{\frac{3}{2}} \cdot 32 \cdot \sqrt{15}}$
(3d) $R32 = Z^{\frac{3}{2}} \cdot \rho^{2} \cdot e^{-\frac{\rho}{2}}$
constant $= \frac{1}{ao^{\frac{3}{2}} \cdot 9 \cdot \sqrt{30}}$
(4d) $R42 = Z^{\frac{3}{2}} \cdot (6 - \rho) \cdot \rho^{2} \cdot e^{-\frac{\rho}{2}}$
constant $= \frac{1}{ao^{\frac{3}{2}} \cdot 96 \cdot \sqrt{5}}$
(4f) $R43 = Z^{\frac{3}{2}} \cdot \rho^{2} \cdot e^{-\frac{\rho}{2}}$
constant $= \frac{1}{ao^{\frac{3}{2}} \cdot 9 \cdot \sqrt{30}}$

Chemistry Application

24

Angular Wave Functions

(s)
$$Xml = X00 = \frac{1}{2} \cdot \sqrt{2}$$

(p)
$$X10 = COS(\theta)$$

constant $= \frac{1}{2} \cdot \sqrt{6}$

(p)
$$X = SIN(\theta)$$

constant $= \frac{1}{2} \cdot \sqrt{3}$

(d)
$$X20 = 3 \cdot COS^2(\theta) - 1$$

constant $= \frac{1}{4} \cdot \sqrt{10}$

(d)
$$X21 = SIN(\theta) \cdot COS(\theta)$$

constant $= \frac{1}{2} \cdot \sqrt{15}$

(d)
$$X22 = SIN^2(\theta)$$

constant = $\frac{1}{4} \cdot \sqrt{15}$

(f)
$$X30 = \frac{5}{3} \cdot COS^{3}(\theta) - COS(\theta)$$

constant $= \frac{3}{4} \cdot \sqrt{14}$

(f)
$$X = SIN(\theta) \cdot (5 \cdot COS^{2}(\theta) - 1)$$

$$constant = \frac{1}{8} \cdot \sqrt{42}$$

(f)
$$X = SIN^{2}(\theta) \cdot COS(\theta)$$

constant =
$$\frac{1}{4} \cdot \sqrt{105}$$

(f)
$$X33 = SIN^3(\theta)$$



constant =
$$\frac{1}{8} \cdot \sqrt{70}$$

Variable	Description	Units
ρ	normalized distance	-
r	distance from nuclei	m
Z	nuclear charge	-
R10	1s radial function	-
R20	2s radial function	-
R30	3s radial function	-
R40	4s radial function	-
R21	2p radial function	-
R31	3p radial function	-
R41	4p radial function	-
R32	3d radial function	-
R42	4d radial function	-
R43	4f radial function	-
X10	p (m=0) angular function	-
X11	p (m=1) angular function	-
X20	d (m=0) angular function	-
X21	d (m=1) angular function	-
X22	d (m=2) angular function	-
X30	f (m=0) angular function	-
X31	f (m=1) angular function	-
X32	f (m=2) angular function	-
X33	f (m=3) angular function	-
Θ	azimuthal angle	0
ao	Bohr radius*	m

Bohr radius is defined as 5.2917706E-11_m and is not entered by the user.

Example: At what distance from the hydrogen atom (Z=1) is the first node in the 3s radial function? There are two nodes in the 3s radial function.

The easiest way to solve this problem is to plot the 3s function versus ρ , find ρ at the first node, then solve for r.



After entering Z=1, plot the R30 function (in s orbitals) from $\rho=0$ to $\rho=10$, as shown below (autoscale y):

x1 = 0x2 = 10 autoscale y

te first node to display the

RED (NO UNITS)

Move the cursor to the first node and press **COORD** to display the

(x,y) coordinates of the node. This yields:

The first node occurs at $\rho = 1.23$. Pressing \overline{ON} key returns to the EQNS screen. Press **SOLVE** to go to the solver screen. Enter $\rho = 1.23$ and press **CALC**. The result of the calculation is r = 0.033 nm.

Diatomic Moment

The first equation in this subtopic relates the moment of inertia of a diatomic molecule to its molecular geometry. The second equation relates the rotational constant to the moment of inertia.



PRESS CENTERS TO RETURN TO LIST ...

1	$1 m1 \cdot m2_2$	h h
l	$=$ \cdots \cdot r^{-}	B =
	NA m1+m2	$8 \cdot \pi^2 \cdot I \cdot c$

Variable	Description	Units
1	moment of inertia	kg.cm ²
m1	mass of 1	kg/mol
m2	mass of 2	kg/mol
r	internuclear distance	m
В	rotational constant	1/cm

Example: What is the moment of inertia and rotational constant of HCl? Assume the interatomic distance between H and Cl to be 1.27460_Å, and get the gram molecular weight from the Periodic Table function.

Given	Result
m1 = 1.00797 g/mol	$I = 2.644E-40 \text{ kg.cm}^2$
m2 = 35.453 g/mol	B = 10.59_1/cm
r = 1.27460_Å	

Symmetrical Moment

These equations relate the moment of inertia of a bent symmetrical molecule to the internuclear geometry.



c o n s t a n t =
$$\frac{1}{2} \cdot \sqrt{3}$$

 $Iy = \left(\frac{2}{NA}\right) \cdot m1 \cdot r^2 \cdot SIN^2\left(\frac{\theta}{2}\right)$

Iz = Ix + Iy

Variable	Description	Units
ly	moment of inertia about y	kg. m ²
İx	moment of inertia about x	kg. m ²
lz	moment of inertia about z	kg. m ²
m1	mass of 1	Kg/mol
m2	mass of 2	kg/mol
r	internuclear distance	m
θ	bond angle	0

Example:	What is the moment of inertia of water?		
G	iven	Result	
r	= 0.96 Å	lx = 1.02E-40 g. m ²	
m	1 = 1.0079 g/mol	$ly = 1.94E-40 \text{ g}. \text{ m}^2$	
m	2 = 15.9994 g/mol	Iz = 2.96E-40 g. m ²	
θ	= 104.9 °	U	

Solids/Liquids

The following topics contain equations describing characteristics of solids and liquids.

Concentration
Raoult's Law
BP/FP (Colligative)
Molarity/Dilution
Clausius Clapeyron
Capillary Rise

Heat Capacity

The Einstein and Debye models of solids yield equations which predict heat capacity at different temperatures. These two equations are included here.

Einstein:

$$CvE = 3 \cdot R \cdot \left(\frac{\theta e}{T}\right)^2 \cdot \frac{e^{-\left(\frac{\theta e}{T}\right)}}{\left(1 - e^{-\left(\frac{\theta e}{T}\right)}\right)^2}$$
Debye:

$$CvD = 9 \cdot R \cdot \left(\frac{T}{\theta e}\right)^3 \cdot \int_{0}^{\frac{\theta d}{T}} \frac{x^4 \cdot e^x}{\left(e^x - 1\right)^2} \cdot dx$$

Variable	Description	Units
CvE	Einstein heat capacity	J/(mol.K)
CvD	Debye heat capacity	J/(mol.K)
θ e	Einstein characteristic temperature	ĸ
θd	Debye characteristic temperature	К
т	Temperature	K

* This equation can take several minutes to solve. Note that given a single heat capacity at a certain temperature, it is not possible to solve uniquely for Debye or Einstein temperatures. Both Debye and Einstein temperatures are defined by the equation $\theta = h.\upsilon_m/k$.

Example: The Debye characteristic temperature of Pb is $\theta d = 88K$. Estimate the heat capacity of Pb at 20K and 25°C. First enter θd and T=20_K, and solve for CvD. Next enter T=25_°C and solve again for CvD.

> Given Result $\theta d = 88_K$ CvD = 1.1_J/(mol•K) @ 20_K

$$T = 20_K$$
 $CvD = 24.8_J/(mol \cdot K) @ 25 °C$
 $T = 25 °C$

Blackbody Radiation

The equations which describe the emission at various frequencies and the total emission of an ideal blackbody are shown below:

$$E\gamma = \frac{8 \cdot \pi \cdot h \cdot \gamma^{3}}{c^{3} \left(e^{\frac{h \cdot \gamma}{k \cdot T}} - 1 \right)}$$

$$ET = \sigma \cdot T^4$$

Variable	Description	Units
Εγ	energy density	J∙s/m ³
ET	total energy density	J/m ³
т	absolute temperature	К
γ	frequency	Hz

Example: What is the total output of a radiating surface at 5000_K? At what frequency does emission fall to zero?

Given	Result
T = 5000 K	ET = 35439500_W/m ²

To solve the second part of the problem, set T=5000 K and plot $E\gamma$ versus over a wide range of frequencies (this example uses 1E12_Hz to 1 E15 Hz), as shown:



Move the cursor to the low frequency and high frequency intersection (where intensity is zero) and press **COORD**. This displays the approximate coordinates of the low frequency limit of $\sim 8.7E12$ _Hz and the high frequency limit of $\sim 1.2E15$ _Hz. Note that a more accurate determination of the intercept may be obtained by using a more expanded graph.

Equation of State

This equation is general to solids and relates volume, pressure and temperature.
$VTP = Vo \cdot (1 + \alpha s \cdot (t2 - 0_{\circ} C)) \cdot (1 - \rho s \cdot (p2 - 1_{atm}))$		
Variable	Description	Units
VTP	volume at any temperature & pressure	m ³
Vo	reference volume	m ³
αs	thermal expansion coefficient	1/K
t2	temperature	К
ρ s	compressibility coefficient	1/Pa
p2	pressure	Pa

Example: A 1.000_cm³ solid has a coefficient of expansion of α s=1.03E-4_1/K and a compressibility coefficient of ρ s=2.86E-6_1/atm. What is the volume at 360 °F and pressure of 1800_psi?

GivenResult $Vo = 1.000 \text{ cm}^3$ $VTP = 1.02 \text{ cm}^3$ $\alpha s = 1.03E-4 1/ °C$ $\rho s = 2.86E-6 1/atm$ t2 = 360 °F $\rho 2 = 1800 \text{ psi}$

Bragg Law

The Bragg diffraction law describes the diffraction that occurs when electromagnetic radiation impinges on planes of atoms separated by a distance d.

$$SIN(\theta) = \frac{n \cdot \lambda d}{2 \cdot d}$$

Variable	Description		Units
Θ	diffraction angle	0	
n	order		-
λd	wavelength		m
d	distance between planes		m

Example: At what angle does the (hkl=100) first-order diffraction occur when Cu α radiation ($\lambda d=1.44$ _Å) impinges on NaCl (d=5.627_Å)?

Given	Result	
d = 5.627_Å	Θ = 7.35_°	
n = 1		

 $\lambda d = 1.44$ Å

Born-Haber Cycle

Lattice energies in a salt are difficult to measure. However, they may be calculated from other thermodynamic quantities by means of the Born-Haber Cycle.

	Na + 1/2C12 AHFMX
PRESS	(ENTER) TO RETURN TO LIST

$$\Delta Hlmx = \Delta Hcry + \Delta Hfmg + \frac{1}{2} \cdot \Delta Hfx2g + \mathrm{Img} + Axg$$

Variable	Description	Units
∆Hfmx	heat of formation of mx	J/mol
∆Hcry	heat of crystalization of mx	J/mol
∆Hfmg	heat of formation of gaseous m	J/mol
∆Hfx2g	heat of formation of gaseous x2	J/mol
Img	ionization energy of m	J/mol
Axg	electron affinity of x	J/mol

Melting Point

This equation is the integrated form of the Clapyron equation and relates the melting point at any temperature to pressure.

$$P2 = P \cdot \left(\frac{\Delta H f us}{\Delta V f us}\right) \cdot LN\left(\frac{T2m}{T1m}\right)$$

Variable	Description	Units
P2	pressure	Pa
P1	reference pressure	Pa
∆Hfus	heat of fusion	J/mol
∆Vfus	volume change upon fusion	m ³ /mol
T1m	reference melting point	K
T2m	new melting point	K

Concentration

The concentration of a solute in a solution is often given in molarity (mol/l), molality (mol/kg), mole fraction (no units), and parts-per-million (no units). In the case of a solute "a" dissolved in a solvent "b", the

following equations relate these concentrations to various parameters of the solution.

gs = gs + gb	$ma = \frac{na}{gb}$
$na = \frac{ga}{MWTa}$	$xa = \frac{na}{na + nb}$
$ga = wa \cdot \frac{gs}{100}$	wa + wb = 100
$gb = wb \cdot \frac{gs}{100}$	$nb = \frac{gb}{MWTb}$
$gs = vs \cdot \rho s$	$ppma = \frac{ga \cdot 1E6}{gb}$
$Ma = \frac{na}{vs}$	$gb = vb \cdot \rho b$

Variable	Description	Units
ga	mass solute	kg
gb	mass solvent	kg
na	moles solute	mol
nb	moles solvent	mol
MWTa	molecular weight solute	kg/mol
MWTb	molecular weight solvent	1_kg/mol
wa	weight % solute	-
wb	weight % solvent	-
ρb	pure solvent density	kg/m ³
vb	volume of solvent	m ³
gs	mass solution	kg
VS	volume solution	m ³
ρ s	density solution	kg/m ³
Ma	molarity solution	mol/m ³
ma	molality solution	mol/kg
ха	mole fraction solution	-
ppma	solute concentration	-

Example 1: Calculate the molality of Br⁻ in a 1000_g solution containing 4600 ppm of the ion.

Given Result gb = 1000_g ma = 5.8E-2_mol/kg MWTa = 79.904_g/mol ppma = 4600

Example 2: Given that the density of a solution of 5.0_g of toluene and 225.0_g benzene is 0.876_g/mol, calculate the solution concentration in: a) molarity, b) mole fraction, and c) weight percentage.

 $\begin{array}{ll} Given & Result \\ ga = 5.0_g & Ma = 0.206_mol/l \\ gb = 225.0_g & xa = .0185 \\ MWTa = 92.1402_g/mol & wa = 2.17 \\ \rhos = 0.876_g/ml \\ MWTb = 78.1134_g/mol \end{array}$

Other variables solved for are:

na = 0.054 mol	gs = 0.23 kg
nb = 2.88 mol	$vs = 0.263_1$
wb = 97.8	ma = 0.24 mol/kg
ppma = 22222.2	

Raou'lts Law

When non-volatile solutes are added to a liquid solvent, the vapor pressure is lowered. The relationship which describes the vapor pressure lowering of a solvent, b, by the addition of a solute, a, is called Raoult's Law.

$P = xb \cdot Pin$	$\Delta P = -xa \cdot Pin$
$\Delta P = P - Pin$	$na = \frac{nb}{MWTa}$
$nb = \frac{gb}{MWTb}$	$xa = \frac{na}{na + nb}$
$xb = \frac{nb}{na+nb}$	xa = 1 - xb

Varial	ble Description	Units
Р	solvent partial pressure	1_Pa
xb	solvent mole fraction	1
Pin	solvent initial pressure (pure)	1_Pa
ΔΡ	pressure difference	1_Pa

xa	solute mole fraction	1
na	moles of solute	1_mol
ga	mass of solute	1_kg
MWTa	molecular weight of solute	1_kg/mol
MWTb	molecular weight of solvent	1_kg/mol
nb	moles of solvent	1_mol
gb	mass of solvent	1_kg

Example: Calculate the vapor pressure lowering caused by the addition of 100_g sucrose ($C_{12}H_{22}O_{11}$) to 1000_g of water if the initial vapor pressure of water at 25_°C is 23.8_torr.

Given	Result
$Pin = 23.8$ _torr	$P = -0.125$ _torr
$ga = 100_g$	$P = 23.68$ _torr
MWTa = 342.2992_g/mol	$xa = 5.24 \times 10^{-3}$
MWTb = 18.0152 g/mol	na = 0.292 mol
gb = 1000_g	xb = 0.995

BP/FP Colligative

When a non-volatile soluble material is added to a solvent, the freezing point of the solvent is lowered and the boiling point is raised. The following equations describe this behavior.

$\Delta Tb = Kb \cdot ma$	$ma = \frac{na}{gb}$
$nb = \frac{ga}{MWTa}$	$\Delta Tf = -Kf \cdot ma$

Variable	Description	Units
ΔTb	boiling point elevation	1_K
Kb	ebullioscopic constant	1_K·kg/mol
ma	solute concentration in molality	1_mol/kg
na	moles of solute	1_mol
gb	mass of solvent	1_kg
ga	mass of solute	1_kg
MWTa	molecular weight of solute	1_kg/mol
ΔTf	freezing point depression	1_K
Kf	cryoscopic constant	1_K·kg/mol

Note that once calculated, the values of ΔTb and ΔTf may not be converted into other temperature values. When entering a value for ΔTf , it <u>must</u> be negative.

Example: What is the freezing point depression and boiling point elevation of a solution composed of 100_g ethylene glycol ($C_2H_6O_2$) in 900_g water?

Given	Result
$Kb = 0.52 K \cdot kg/mol$	$\Delta Tb = 0.932$ °C
$gb = 900_g$	ma = 1.79 mol/kg
ga = 100_g	na = 1.61_mol
MWTa = 62_g/mol	$\Delta Tf = -3.33$ _°C
$Kf = 1.86 K \cdot kg/mol$	

Molarity/Dilution

The following equations relate the final concentration of solute to the initial concentration after dilution.

$M_i - \frac{na}{n}$	$na = \frac{ga}{ga}$
V	MWTa
$Vf \cdot Mf = Vi \cdot Mi$	

Variable	Description	Units
Mi	initial concentration, Molarity	1_mol/m^3
na	moles of solute	1_mol
Vi	initial volume	1_m^3
ga	mass of solute	1_kg
MWTa	molecular weight of solute	1_kg/mol
Vf	final volume	1_m^3
Mf	final concentration	1_mol/m^3
V	solution volume	1_m^3

Example: 4.5060_g of NaOH is added to a 250.00_ml volumetric flask. 10.00_ml of this solution is then diluted to 500.00_ml in a second volumetric flask. What is the final concentration?

Given	Result
ga = 4.5060_g	Mi = 0.4506 mol/l
MWTa = 39.99707 g/mol	$Mf = 9.013 \times 10^{-3} \text{mol/l}$
$V = 250.00$ _ml	$na = 0.1127$ _mol
$Vi = 10.00$ _ml	

 $Vf = 500_ml$

Clausius Clapyron

The Clausiu Clapyron equation relates the vapor pressure of a liquid to temperature.

$$LN\left(\frac{P}{Po}\right) = \frac{RH\nu}{V} \cdot \left(\frac{1}{To} - \frac{1}{T}\right)$$

Variable	Description	Units
Р	vapor pressure	1_Pa
ΔHv	heat of vaporization	1_J/mol
То	reference temperature	1_K
Т	temperature	1_K
Ро	reference vapor pressure	1_Pa

Example: The vapor pressure of white phosphorus has the values: P at $(76.6\°C) = 1.0\mmodel{mmHg}$, P at $(197.3\°C) = 100.0\mmodel{mmHg}$. Calculate the heat of vaporization of liquid phosphorus.

Given

 $Po = 1.0_mmHg$ To = 76.6_°C P = 100.0_mmHg T = 197.3_°C **Result** $\Delta Hv = 12.47 \text{ kcal/mol}$

Capillary Rise

These equations describe the capillary rise phenomenon observed with fluids. The first equation is an approximate PRESS CENTERT TO RETURN TO LIST ...

equation, assuming no interaction between the capillary surface and the liquid ($\theta=0_{\circ}$), and no edge effects. The second equation includes these contributions.

$$h = \frac{2 \cdot \gamma l}{\rho l \cdot g \cdot r} \qquad hex = \frac{2 \cdot \gamma l \cdot COS(\theta)}{(\rho l - \rho v) \cdot g \cdot r} - \frac{r}{3}$$

Variable	Description	Units
h	capillary rise	1_m

γl	surface tension	1_N/m
ρl	liquid density	1_kg/m^3
r	capillary radius	1_m
θ	meniscus angle	1_°
ρv	vapor density	1_kg/m^3
hex	capillary rise (exact)	1_m

Example: A capillary (r=0.100_mm) is inserted into a fluid $\gamma l= 46.0$ _dyn/cm) with a density of 1.06_g/cm^3. The contact angle is measured to be 76_° and the vapor has a density of 1.0_g/l. What is the predicted capillary rise using the simple and exact expressions?

 Given
 Result

 $\gamma l = 46.0_dyn/cm$ $h = 88.5_mm$
 $\rho l = 1.06_g/cm^3$ $hex = 21.4_mm$
 $r = 0.10_mm$ $\theta = 76_^\circ$
 $\rho v = 1.0_g/l$ $\rho l = 1.0_g/l$

Gases

The equations in this topic describe the pressure, temperature, and volume relationships of ideal and non-ideal gases as well as kinetic and collision theory.

- Ideal Gas
- Van der Waals Gas
- State Changes
- Kinetic Theory

- Gas Over Water
- Graham's Law
- Barometric Equation
- Collision Theory

Ideal Gas

An "ideal" gas behaves according to the equations below.

$$P = \frac{n \cdot R \cdot T}{V} \qquad \qquad n = \frac{mg}{MWT} \qquad \rho = \frac{mg}{V}$$

Variable	Description	Units
Р	pressure	1_Pa
n	moles of gas	1_mol
Т	temperature	1_K

V	volume	1_m^3
mg	mass of gas	1_kg
MWT	molecular weight	1_kg/mol
ρ	density	1_kg/m^3

Example: A 2.889_g sample of gas with unknown molecular weight expands to 933_ml at a pressure of 735_mmHg and at a temperature of 31_°C. Assuming ideal gas behavior, what is its molecular weight?

Given	Result
$P = 735 \text{_mmHg}$	$n = 3.62 \times 10^{-2} \text{-mol}$
V = 933 ml	$\rho = 3.09 \text{ x} \ 10^{-2} \text{ g/cm}^3$
T = 31°C	MWT = 79.9 g/mol
$mg = 2.889_g$	

State Changes

For an ideal gas undergoing a change in pressure, temperature, volume, or mass (a state change), the following equations apply. (complete state change)

$\frac{P1 \cdot V1}{n1 \cdot T1} = \frac{P2 \cdot V2}{n2 \cdot T2}$	
$\frac{P1 \cdot V1}{T1} = \frac{P2 \cdot V2}{T2}$	(n, constant)
$P1 \cdot V1 = P2 \cdot V2$	(n, T constant)
$\frac{P1}{T1} = \frac{P2}{T2}$	(n,V constant)
$\frac{V1}{T1} = \frac{V2}{T2}$	(P, n constant)
$P1 \cdot V1 = n1 \cdot R \cdot T1$	
$P2 \cdot V2 = n2 \cdot R \cdot T2$	

Note: The first five equations are not independent relations. To solve a problem using this equation set, first select the appropriate equations (n constant, P and V constant, etc..).

Variable	Description	Units
P1	initial pressure	1_Pa
V1	initial volume	1_m^3
n1	initial moles	1_mol
T1	initial temperature	1_K
P2	final pressure	1_Pa
V2	final volume	1_m^3
n2	final moles	1_mol
T2	final temperature	1_K

Example: A 45.0_ml sample of gas at 246_°C and 1.68_mmHg is compressed and cooled to 36.0_ml and 25_°C. What is the final pressure?

Result

P2 = 1.21 mmHg

To solve this problem, select the second equation and press **SOLVE** (since moles remain constant in this problem). Then:

Given P1 = 1.68_mmHg V1 = 45_ml T1 = 246_°C V2 = 36_ml T2 = 25_°C

Gas Over Water



Consider the general chemical reaction:

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$aA + Reactants \rightarrow bB_{(g)} + Products$

Often, the gaseous product is collected by displacing liquid from a graduated cylinder filled with water. The following equations relate the volume, temperature, pressure, and number of moles of gas to the quantity of reactant consumed in the reaction. Note that the vapor pressure of water at the temperature of collection, Pw, must be included to account for the partial pressure of water vapor in the graduated cylinder.

Variable	Description	Units
na	moles a	1_mol
a	a coefficient, reactant	1
b	b coefficient, gaseous product	1
nb	moles b	1_mol

mass b molecular weight b	1_kg 1_kg/mol
mass a	1_kg
molecular weight a	1_{m^2}
temperature	1_m 5 1 K
total moles collected	1_mol
moles of water collected	1_mol
total pressure	1_Pa
water partial pressure	1_Pa
	mass b molecular weight b mass a molecular weight a collected gas volume temperature total moles collected moles of water collected total pressure water partial pressure

Example: Consider the decomposition of CaCO₃ according to the reaction:

$$CaCO_3 \rightarrow CaO + CO_2$$
 (g)

When 4.6_g of CaCO₃ decomposes, what volume of gas is collected at 1.0_atm and 26_°C? Note that the partial pressure of water at 26_°C is 25.0_torr. Use all seven equations.

Given Result $V = 1.17 \ 1$ a = b = 1 $nb = 4.60 \text{ x } 10^{-2} \text{ mol}$ $MWTb = 44.0098 \text{ g/mol}(CO_2)$ $gb = 2.02 \times 10^{-3}$ kg $MWTa = 100.0892 \text{ g/mol}(CaCO_3)$ Pb = 0.967_atm ga = 4.6 g $na = 4.60 \times 10^{-2} \text{mol}$ T = 26 °C $nt = 4.75 \times 10^{-2} mol$ Pt = 1.0 atm $nw = 1.56 \times 10^{-3} mol$ Pw = 25.00 torr

Barometric Equation

The barometric equation describes the variation in pressure and concentration of a gas above sea level.

$$P = Po \cdot EXP\left(\frac{-MWT \cdot g \cdot h}{R \cdot T}\right)$$
$$Co = \frac{Po}{R \cdot T} \qquad C = \frac{P}{R \cdot T}$$

Variable	Description	Units
Р	pressure at height, h	1_Pa

Ро	reference pressure	1_Pa
MWT	molecular weight of gas	1_kg/mol
h	height above sea level	1_m
Т	temperature	1_K
Со	reference concentration	1_mol/m^3
С	concentration at height, h	1_mol/m^3

Example: What is the pressure and concentration of air (average molecular weight = $29_g/mol$) at a height of 1.0 km above sea level? Plot the pressure of air versus height above sea level (Assume T is $75_{\circ}F$).

Given	Result
Po = 1.0 atm	P = 0.89 atm
MWT = 29 g/mol	Co = 4.1 E-2 mol/l
h = 1 km	C = 3.6 E-2 mol/l
$T = 75_{\circ}F$	P (ATM) P=PDXEXP(-MWTXGXHBA/(R
Plotting the barometric	equation yields:
x1 = 0 km	autoscale y

Van der Waal Gases

x2 = 50 km

The Van der Waals equation is a semi-empirical equation of state for a non-ideal gas:

┢

HBA (KM)

Eù

$$p = \frac{n \cdot R \cdot T}{V - n \cdot b} - \frac{n^2 \cdot a}{V^2}$$

$$Z = P \cdot \frac{V}{n \cdot R \cdot T}$$

$$Vc = 3 \cdot n \cdot b$$

$$Pc = \frac{a}{27 \cdot b^2}$$

$$n = \frac{ga}{MWT}$$

Variable	Description	Units
р	pressure of gas	1_Pa
n	moles of gas	1_mol
V	volume of gas	1_m^3
Т	absolute temperature	1_K
a	Van der Waal's constant (attractive)	1_m^6.Pa/mol^2
b .	Van der Waal's constant	1_m^3/mol

	(repulsive)		
Ζ	compressibility factor	1	
Tc	critical temperature	1_K	
Vc	critical volume	1_m^3	
Pc	critical pressure	1_Pa	
ga	mass of gas	1_kg	
MWT	molecular weight of gas	1_kg/mol	
	1 0 0 0 0 1 0 1 0	τ 、 ·	 1.

Example: A 8000_g sample of nitrogen (N₂) is compressed in a vessel to 100_1 at 300_°C. What is the pressure?

Given
UIIVUI

Result

T = 300 °C	p = 139.9_atm
$V = 100_1$	n = 285.7 mol
$b = 0.03913$ _l/mol	Z = 1.04
$a = 1.390 l^2 \cdot atm/mol^2$	Tc = 128.3 K
ga = 8000_g	$Vc = 33.54_{1}$
MWT = 28.0134_g/mol	$Pc = 33.6$ _atm

Kinetic Theory

The velocity distribution of gas molecules is expressed by Maxwell-Boltzman statistics. Equation 1 provides the probability that velocity is in the range of C to C + dC. The next three equations give net results of Maxwell-Boltzmann distribution function for all velocities: the most probable velocity (cmp), the average velocity (cavg) and the rms velocity (crms).

$$fC = 4 \cdot \pi \left(\frac{MWT}{2 \cdot \pi \cdot R \cdot T}\right)^{\frac{3}{2}} \cdot C^{2} \cdot EXP\left(\frac{-MWT \cdot C^{2}}{2 \cdot R \cdot T}\right)$$
$$cmp = \left(\frac{2 \cdot R \cdot T}{MWT}\right)^{\frac{1}{2}}$$
$$cavg = \left(\frac{8 \cdot R \cdot T}{\pi \cdot MWT}\right)^{\frac{1}{2}}$$
$$crms = \left(\frac{3 \cdot R \cdot T}{MWT}\right)^{\frac{1}{2}}$$

Variable

Description

Units

fC	probability that velocity is within dC	1
MWT	molecular weight of gas	1_kg/mol
Т	absolute temperature	1_K
С	velocity of molecules	1_m/s
dC	velocity range	1_m/s
cmp	most probable velocity	1_m/s
cavg	average velocity	1_m/s
crms	root mean-square velocity	1_m/s

Example: What is the average velocity of an oxygen molecule at 300_K? Use equation 3.

Given Result MWT = 31.9988_g/mol cavg = 395_m/s T = 300_K

For an oxygen molecule, plot the velocity distribution at T = 300 K and T = 1000 K (assume dC = 1_m/s). This yields: x1 = 0x2 = 2000y1 = 6.0 E-4y2 = 3 E-3



Note that the maximum shifts from C=400_m/s to C=707_m/s with the increase in temperature.

Graham's Law

Thomas Graham discovered (in 1830) that the effusion rate of gases was inversely proportional to the square root of the masses.

$f = \left(\frac{MWT2}{MWT2}\right)^{\frac{1}{2}}$	$\frac{1}{2}$ f	=	$\frac{r1}{2}$
$\int (MWT1)$	J		r2

Variable	Description	Units
f	enrichment factor	1
MWT2	molecular weight of gas 2	1_kg/mol
MWT1	molecular weight of gas 1	1_kg/mol
r1	rate of effusion of gas 1	1_m^3/s

Example: What is the enrichment factor of nitrogen compared to oxygen?GivenResultMWT2 = 28.0134_g/molf = 0.9357MWT1 = 31.9988 g/mol

Collision Theory

The Maxwell Boltzman distribution function leads to the following collision and transport parameters (see Adamson, 1979 for a detailed description).

$cavg = \sqrt{\left(\frac{8 \cdot R \cdot T}{\pi \cdot MWT}\right)}$	
$n = \frac{NA \cdot P}{R \cdot T}$	$Z = \frac{1}{4 \cdot NA} \cdot n \cdot cavg$
$Z1 = \frac{2 \cdot d \cdot \sqrt{\left(\frac{\pi \cdot R \cdot T}{MWT}\right)}}{NA}$	$\frac{1}{2} \cdot n^2$
$\lambda mfp = \frac{1}{\sqrt{2} \cdot \pi \cdot d^2 \cdot n}$	
$D = \frac{1}{2} \cdot cavg \cdot \lambda mfp$	
$\rho = \frac{MWT \cdot p}{R \cdot T}$	$\eta = \frac{1}{2} \cdot \rho \cdot cavg \cdot \lambda mfp$
$n = \frac{\rho \cdot NA}{MWT}$	

Variable	Description	Units
cavg	average velocity	1_m/s
Т	absolute temperature	1 K
MWT	molecular weight	1_kg/mol
n	particle density	1_1/m^3
Р	pressure	1_Pa
Z	surface collision frequency	$1 \mod (m^2 \cdot s)$
Z1	bimolecular collision frequency	$1_mol/(m^3 \cdot s)$
P Z Z1	pressure surface collision frequency bimolecular collision frequency	1_Pa 1_mol/(m^2·s) 1_mol/(m^3·s)

d	collision diameter	1_m
λmfp	mean free path	1_m
D	self diffusion coefficient	1_m^2/s
ρ	density of gas	1_kg/m^3
η	viscosity coefficient	$1_kg/(m \cdot s)$

Example: Calculate the surface collision frequency, bimolecular collision frequency, mean free path, and viscosity coefficient of O_2 (Molecular weight = 31.9988_g/mol) at 25_°C.

Given	Result
$P = 1.0_{atm}$	$cavg = 444_m/s$
T = 25_<198>C	$n = 2.46 E19_1/cm^3$
MWT = 31.9988_g/mol	$Z = 0.454 \text{_mol/(cm^2 \cdot s)}$
d = 3.61 Å	$Z1 = 1.29 \text{ E5}_mol/(cm^3 \cdot s)$
	$\lambda m f p = 701 \AA$
2	$D = 0.156 cm^{2/s}$
	$\rho = 1.31 \text{ E-3_g/cm^3}$
	η= 2.04 E-4_g(cm·s)

Acids/Bases

In this category, the pH of solutions of strong acids and bases, weak acids and bases, and titration curves are included.

pH Function	Titration (SA/SB)
Strong Acids	Titration (SB/SA)
Strong Bases	Titration (WA/SB)
Weak Acids/Bases	Titration (WB/SA)
Henderson-Hasselbach	

Note that in the equation library, SA indicates a strong acid, SB a strong base, WB a weak base, and WA a weak acid. Although it is common to denote concentrations of ions in solution with brackets,

i.e $[H^{+}]$, this notation is not supported by the HP 48SX. Therefore, all concentrations are enclosed by parenthesis.

pH Function

The following equations define pH, pOH, pKb, pKa and pKw for aqueous systems. Note that in all cases, concentrations used in the "p" function must be in moles/liter. Concentrations in SI or other units

are converted to moles/liter prior to the calculation.

pH = -LOG(H)	pOH = -LOG(OH)
pKw = -LOG(Kw)	pKa = -LOG(Ka)
pKb = -LOG(Kb)	$Kw = Ka \cdot Kb$
$Kw = H \cdot OH$	

ol/m^3
ol/m^3
ol^2/m^6
ol/m^3
ol/m^3

Example: The hydrogen ion concentration in a sample $(H^+) = 0.01 \text{ mol/l}$ at 25_°C. What is pH, pOH and OH? Use equations 1,2, 3 and 7.

Given H = 0.01_mol/l Kw = 1.01 E-14_mol^2/l^2 pOH = 12.0 pKw = 14.0 **Result** pH = 2 OH = 1.01 x 10^-12 mol/l

Strong Acids

This set of equations defines the concentration of hydrogen ion and the resulting pH made by dissolving a strong acid in water.

$H - n = \frac{ga}{ga}$	nHIOG(H)
$MWTa \cdot V$	pm = Loo(m)

Variable	Description	Units
Н	hydrogen ion concentration	1_mol/m^3
ga	mass of acid	1_kg
MWTa	molecular weight of acid	1_kg/mol
V	volume of solution	1_m^3

pH	pH function	1
n	Number of hydrogen ions per molecule	1

Example: 0.50_g of a diprotic acid (MWT=98.0734_g/mol) is dissolved in 100_ml of water. What is the pH?

 Given
 Result

 ga = 0.50 g H = 0.101 mol/l

 V = 100 ml pH = 0.991

 MWTa = 98.0734 g/mol
 n = 2

Strong Bases

This set of equations defines the concentration of hydroxide ion and the resulting pH made by dissolving a strong base in water.

$$OH = n \cdot \frac{gb}{MWT \cdot V}$$
$$H = \frac{Kw}{OH} \qquad pH = -LOG(H)$$

Variable Description Un	its
OH hydroxide ion concentration 1 r	nol/m^3
H hydrogen ion concentration 1 r	nol/m^3
gb mass of base 1	cg
MWTb molecular weight of base 1	g/mol
V volume of solution 1 r	n^3
pH pH function 1	
Kw water dissociation constant 1 r	nol^2/m^6
n No. of hydroxide ions/ molecule 1	

Example: 4.5617_g of primary standard NaOH (MWT = 39.99707_g/mol) is dissolved in a 500_ml volumetric flask. What is the pH?

Given	Result
gb = 4.5617_g	pH = 13.35
MWTb = 39.99707 g/mol	$H = 4.43 \times 1E-14 \mod/1$
V = 500 ml	OH = 0.228 mol/l
$Kw = 1.01 X 1E-14 mol^{2}/l^{2}$	
n = 1	

Weak Acids/Bases

These six equations allow calculation of pH for a solution composed of a weak acid or a weak base.

$$H^{3} + Ka \cdot H^{2} - (Ca \cdot Ka + Kw) \cdot H - Ka \cdot Kw = 0$$

$$OH^{3} + Kb \cdot OH^{2} - (Cb \cdot Kb + Kw) \cdot OH - Kb \cdot Kw = 0$$

$$Kw = H \cdot OH \qquad pH = -LOG(H)$$

$$Ca = \frac{ga}{MWT \cdot V} \qquad Cb = \frac{gb}{MWT \cdot V}$$

Variable	Description	Units
Ca	acid concentration	1 mol/m^3
Cb	base concentration	1 mol/m^3
Ka	acid dissociation constant	1 mol/m^3
Kb	base dissociation constant	1 mol/m^3
Kw	water dissociation constant	1 mol^2/l^2
Н	hydrogen concentration	1 mol/m^3
OH	hydroxide concentration	1 mol/m^3
pH	pH value	1
ga	mass of acid	1_kg
gb	mass of base	1_{kg}
MWT	molecular weight	1_kg/mol
V	primary standard volume	11

Example: 0.3862 grams of iodic acid, HIO3 (Ka = 0.162), is dissolved in 1.0 liter of water. What is the pH? Use equations 3-5.

Given	Result
ga = 0.3862 g	$Ca = 2.20 \times 10E-3 mol/l$
Ka = 0.162 mol/l	$H = 2.17 \times 10E-3 \text{ mol/l}$
$V = 1.0 \ 1$	pH = 2.66
MWT = 175.9106 g/mol	-
$Kw = 1.01 X 10-14 mol^{2}$	2/1^2

Note that when solving for the hydrogen ion concentration, it is important to seed the solver properly to ensure that the positive root is found.

Henderson-Hasselbach

Henderson-Hasselbach is an approximate expression relating the observed pH of a solution composed of a weak acid and its conjugate base.

$Ca = \frac{ga}{MWTa \cdot V}$	$Ccb = \frac{gb}{MWTb \cdot V}$
pKa = -LOG(Ka)	$pH = pKa - LOG\left(\frac{Ca}{Ccb}\right)$

Variable	Description	Units
Ca	acid concentration	1_mol/m^3
ga	mass acid	1_kg
MWTa	acid molecular weight	1 kg/mol
v	volume	$1 kg/m^3$
Ccb	base concentration	1_mol/m^3
gb	mass base	1_kg
MWTb	pKa function	1
Ka	acid dissociation constant	1_mol/m^3
pH	pH value	1

Example: 0.45 grams of NaCH3COCOO is placed in a beaker known to contain 100_ml of 0.01_mol/l acetic acid. What is the resulting pH? (The Ka of acetic acid is 1.78 x 1E-5_mol/l).

Given	Result
gb = 0.45 g	pKa = 4.75
MWTb = 110.04467 g/mol	$Ccb = 4.09 \times 1E-2 mol/l$
$V = 100$ _ml	pH = 5.36
Ca = 0.01 mol/l	
$Ka = 1.78 \times 1E-5 mol/l$	

Note that the Henderson-Hasselbach equation is valid when the acid to base concentration is $10 \ll acid/base \ll 0.1$.

Titration (SA/SB)

The following equations describe the pH of a solution obtained when a sample of strong monoprotic acid is titrated with a monoprotic strong base.

$$Ve = \frac{Ca}{Cb} \cdot Va$$
$$pH = -LOG\left(\frac{-(Vb \cdot Cb - Va \cdot Ca)}{2(Va + Vb)} + \frac{1}{2} \cdot \left(\left(\frac{Vb \cdot Cb - Va \cdot Ca}{Va + Vb}\right)^2 + 4 \cdot Kw\right)$$

pH = -LOG(H)

$$Cb = \frac{gb}{MWT \cdot V}$$

Description	Units
acid concentration	1_mol/m^3
base (titrant) concentration	1_mol/m^3
equilibrium volume	1_m^3
volume of acid solution	1_m^3
volume of base titrant	1_m^3
water dissociation constant	1_mol^2/m^6
hydrogen ion concentration	1 mol/m^3
pH value	1
mass of base primary standard	1_Kg
molecular weight of base	1_kg/mol
primary standard volume	1_m^3
	Description acid concentration base (titrant) concentration equilibrium volume volume of acid solution volume of base titrant water dissociation constant hydrogen ion concentration pH value mass of base primary standard molecular weight of base primary standard volume

Example: A primary standard solution was made by adding 0.3986_g of NaOH (MWT = 39.99707_g/mol) to 1.000_1 of water. A 100 ml acid sample of



unknown concentration was titrated to an equivalent point of 49.68_ml at 25_°C. What is the concentration of acid and predict the pH curve expected for such a titration.

Given gb = 0.3986_g MWT = 39.99707_g/mol V = 1.000_1 Kw = 1.01 x 1E-14_mol^2/l^2 Ve = 49.68_ml Va = 100_ml Result Ca = 4.951 x E-3_mol/l Cb = 9.966 x 1E-3_mol/l

With Ca and Cb calculated and tagged as knowns, you may plot pH versus the volume of added base, Vb, as shown (after changing Vb to ml):

x1 = 0 ml	$x^{2} = 100$ _ml
$y_1 = -3$	$y^2 = 16$

Titration (SB/SA)

The following equations describe the pH of a solution obtained when a sample of strong monoprotic base is titrated with a monoprotic strong

Chemistry	Application	51
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acid.

$$Ve = \frac{Cb}{Ca} \cdot Vb$$

$$pH = -LOG(Kw) + LOG\left(\frac{-(Va \cdot Ca - Vb \cdot Cb)}{2 \cdot (Va + Vb)} + \frac{1}{2} \cdot \left(\frac{Va \cdot Ca - Vb \cdot Cb}{Va + Vb}\right)$$

$$pH = -LOG(H)$$
$$Ca = \frac{ga}{MWT \cdot V}$$

Variable	Description	Units
Ca	concentration of acid titrant	1_mol/m^3
Cb	concentration of base	1_mol/m^3
Ve	equilibrium volume	1_m^3
Va	volume of acid solution	1_m^3
Vb	volume of base titrant	1 m^3
Kw	dissociation constant of water	1 mol^2/l^2
H	hydrogen concentration	1 mol/m^3
pН	pH value	1
ga	mass primary standard	1 kg
MWT	molecular weight	1 kg/mol
V	primary standard volume	1_m^3
Frampla	Plot the family of PH (ND UNITS)	TITRATION (SB/SA) PH=-LOG(KW)+LOG(-+

Example: Plot the family of titration curves, starting with 25_ml of 0.1, 0.001, and .00001_mol/l of base, with identical concentrations of acid.



Titration (WA/SB)

The following equations describe the concentration of H^+ in a solution made from a titration of a weak acid with volume of strong base.

$$H^{3} + \left(\frac{Cb \cdot Vb}{Va + Vb} + Ka\right) \cdot H^{2} - \left(\frac{Ca \cdot Va - Cb \cdot Vb}{Va + Vb} \cdot Ka + Kw\right) \cdot H - Ka$$

$$Vb = Va \cdot \frac{\frac{Ca \cdot Ka}{Ka + H} - H + \frac{Kw}{H}}{Cb + H - \frac{Kw}{H}}$$
$$pH = -LOG(H)$$

Note that the first two equations are equivalent. When solving for the hydrogen ion concentration, it is important to seed the solver properly to ensure that the positive root is found

Variable	Description	Units
Ca	acid concentration	1_mol/m^3
Cb	base (titrant) concentration	1_mol/m^3
Ka	acid dissociation constant	1_mol/m^3
Kw	water dissociation constant	1_mol^2/l^2
Va	volume acid solution	1_m^3
Vb	volume base titrant	1_m^3
Н	hydrogen concentration	1_mol/m^3
pH	pH value	1

Example: What will be the pH of a 25_°C solution made by mixing 25.0_ml of 0.1_mol/l HAc(Ka=1.78 x 1E-5_mol/l) with 10.00_ml of 0.10_mol/l NaOH? How much does the pH change if 2.50_ml of additional NaOH are added? 2.50 ml more?

Given	Result
Ca = 0.1 mol/l	10.0_ml
Cb = 0.1 mol/l	$H = 2.67 \times 1E_{-5} \text{mol/l}$
Kw = 1.01 1E-14 mol ² /l ²	pH = 4.57
Ka = 1.78 E-5 mol/l	12.50_ml
$Va = 25.0 \text{ ml}^{-1}$	$H = 1.78 \times 1E_{5} mol/l$
Vb = 10.0 ml	pH = 4.75
_	15.0_ml
	$H = 1.19 \times 1E_{-5} mol/l$
	pH = 4.92

Titration (WB/SA)

The following equations describe the concentration of H^+ in a solution of a weak base titrated with a weak acid.

$$OH^{3} + \left(\frac{Ca \cdot Va}{Va + Vb} + Kb\right) \cdot OH^{2} - \left(\frac{Cb \cdot Vb - Ca \cdot Va}{Va + Vb} \cdot Kb + Kw\right) \cdot OH$$
$$-Kb \cdot Kw = 0$$

$$Vb = Va \cdot \frac{\frac{Cb \cdot Kb}{Kb + OH} - OH + \frac{Kw}{OH}}{Ca + OH - \frac{Kw}{OH}}$$

 $Kw = H \cdot OH$ pH = -LOG(H)

Note: Equations 1 and 2 are equivalent. When solving for the hydrogen ion concentration, it is important to seed the solver properly to ensure that the positive root is found.

Variable	Description	Units
Ca	concentration of acid titrant	1_mol/m^3
СЪ	concentration of base (titrant)	1 mol/m^3
Kb	dissociation constant of base	1_mol/m^3
Kw	water dissociation constant	$1_{mol^{2}/l^{2}}$
Va	volume of added titrant	1_m^3
Vb	volume of base solution	1_m^3
Н	hydrogen concentration	1 mol/m^3
OH	hydroxide concentration	1_mol/m^3
pH	pH value	1

Example: 10.0_ml of 0.1_mol/l HCl is added to 30.0_ml of 0.1_mol/l NH4OH (Kb=1.80 x 1E-5 mol/l). What is the pH?

GivenResult $Ca = 0.100 \text{_mol/l}$ $H = 2.81 \text{ x } 1E-10 \text{_mol/l}$ $Cb = 0.100 \text{_mol/l}$ $OH = 3.59 \text{ x } 1E-5 \text{_mol/l}$ $Kb = 1.80 \text{ x } 1E-5 \text{_mol/l}$ pH = 9.55 $Kw = 1.01 1E-14 \text{_mol}^2/1^2$ Va = 10.0 ml

Thermo/Electrochemistry

Seven topics in this category focus on thermal and thermodynamic properties, and electrochemical reactions.

Heat Transfer Heat Capacity Heat Engines Nernst Law Free Energy Reduction Thermodynamics

Heat Transfer

The following relations describe the heat flow equations which govern the flow of heat between two bodies of different temperatures with no phase change.



$$qa = ma \cdot cpa \cdot (Tf - Ta)$$

$$qa = -qb$$

$$Tf = \frac{mb \cdot cpb \cdot Tb + ma \cdot cpa \cdot Ta}{ma \cdot cpa + mb \cdot cpb}$$

сра	=	Сра
		MWTa

$$cpb = \frac{Cpb}{MWTb}$$

Variable	Description	Units
qa	heat flow in or out of material a	1_J
qb	heat flow in or out of material b	1_J
ma	mass of a	1_kg
mb	mass of b	1_kg
сра	specific heat of a	1_J/(kg·K)
cpb	specific heat of b	1_J/(kg·K)
Сра	molar heat capacity of a	$1_J/(mol \cdot K)$
Cpb	molar heat capacity of b	1_J/(mol·K)
TĪ	final temperature	1_K
Ta	temperature of a	1_K
ТЬ	temperature of b	1_K
MWTa	molecular weight of a	1_kg/mol

molecular weight of b

1 kg/mol

Example: Suppose a 20_g block of copper at 90_°C is placed in 100_g of water at 25.0_°C. What is the final temperature?

 Given
 Result

 $cpa (copper) = 0.385 J/(g\cdot K)$ qa = -491 J

 ma = 20 g qb = 491 J

 Ta = 90 °C Tf = 26 °C

 $cpb (water) = 4.184 J/(g\cdot K)$ mb = 100 g

 Tb = 25 °C Tb = 25 °C

Cannot solve for MWTa, MWTb, Cpa, and Cpb.

Heat Engines

The thermal efficiency and coefficient of performance for a hermodynamic heat engine are given by the equations below.

$$\eta = 1 - \frac{Tc}{Th} \qquad \qquad Cop = \frac{Tc}{Th - Tc}$$

Variable	Description	Units
η	thermal efficiency	1
Cop	coefficient of performance	1
Tc	temperature of cold reservoir	1 K
Th	temperature of hot reservoir	1_K

Example: What is the operating efficiency and coefficient of performance of an engine operating between a temperature of 459_°F and 25_°C?

Given	Result
Th = 459_°F	$\eta = 0.42$
$Tc = 25_{C}$	Cop = 1.4

Free Energy

The following equations define free energy.

 $\Delta G = \Delta H - T \cdot \Delta S \qquad \Delta G = -R \cdot T \cdot LN(Keq)$

Variable	Description	Units
ΔG	free energy change	1_J/mol
ΔH	enthalpy change	1_J/mol
Т	temperature	1_K
ΔS	entropy change	$1_J/(mol \cdot K)$
Keq	equilibrium constant	1

Example: The reaction below has a ΔH and a ΔS of +37.6_kJ/mol and 58.5 J/mol·K at 25 °C.

$$NOCl(s) \longrightarrow NO(g) + \frac{1}{2} \cdot Cl_2$$

Is this a spontaneous reaction? If not, at what temperature is it spontaneous?

Given	Result
$\Delta H = 37.6 kJ/mol$	$\Delta G = 20.2 kJ/mol$
$\Delta S = 58.5 J/(mol \cdot K)$	Keq = 2.94042E-4
$T = 25_{C}$	(Ln Keq = -8.13)

The reaction is non-spontaneous at 25_°C, solving for the equilibrium temperature where $\Delta G=0$.

Given	Result
$\Delta G = 0$	T = 369_°C
$\Delta H = 37.6 kJ/mol$	Keq = 1
$\Delta S = 58.5 J/(mol \cdot K)$	(Ln Keq = 0)

Note: To solve this problem the temperature "T" must be "Unknown" ΔG vs. T is plotted below (Note: Temperature variable T must be converted to _K before this plot is generated): x1 = 200 x2 = 800y = autoscale

Thermodynamics

Empirical heat capacities are usually of the form given in the first equation. Enthalpy and entropies are obtained by simple integration over temperature.

$$Cp = A + B \cdot T + C \cdot T^{2} + \frac{D}{T^{2}}$$

$$\Delta H = A \cdot T + \frac{B}{2} \cdot T^{2} + \frac{C}{3} \cdot T^{3} - \frac{D}{T} - H_{298}$$

$$\Delta S = 2.303 \cdot A \cdot LOG(T) + B \cdot T + \frac{C}{2} \cdot T^{2} - \frac{1}{2} \cdot \frac{D}{T^{2}} - S_{298}$$

Variable	Description	Units
Ср	heat capacity	1_J/(mol·K)
ΔH	enthalpy at T	1_J/mol
ΔS	entropy at T	1 J/(mol·K)
Α	empirical constant	1_J/(mol·K)
В	empirical constant	$1 J/(mol \cdot K^2)$
C .	empirical constant	$1 J/(mol \cdot K^3)$
D	empirical constant	1_J*K/mol
Т	absolute temperature	1_K
H298	enthalpy at 298 K	1_J/mol
S298	entropy at 298_K	1_J/(mol·K)

Example: What is the heat capacity, enthalpy and entropy of Al2O3(s) at 600_K? The appropriate constants are given below:

Heat Capacity

For any material, the following equations relate the difference in heat capacity at constant volume and pressure to fundamental parameters of the material.

$$\Delta C = \frac{\alpha^2 \cdot V \cdot T}{\varepsilon} \qquad \Delta C = Cp - Cv$$

Variable Description

Units

ΔC	heat capacity difference	1_J/(mol·K)
α	expansion coefficient	1_1/K
V	molar volume	1_m^3/mo1
Т	temperature	1_K
3	compressibility coefficient	1_1/Pa
Ср	heat capacity (constant pressure)	1_J/(mol·K)
Cv	heat capacity (constant volume)	1_J/(mol·K)

Example: What is the difference in the heat capacities at constant volume and pressure for water at $25_{\circ}C$?

Given $\alpha = 2.07 \times 1E-4_1/K$ $V = 18.087_cm^3/mol$ $T = 25_°C$ $\epsilon = 45.3 \times 1E-6_1/atm$ **Result** $\Delta C = .517 \text{ x } 1\text{E}-3 J/(\text{mol}\cdot\text{K})$

Nernst Law

The Nernst Law relates the electrode potential to the concentrations of materials in a reaction of the form: $aA + bB \rightarrow cC + dD$.

$$E = Eo - 2.303 \cdot \frac{R \cdot T}{n \cdot F} \cdot LOG(Q) \qquad Q = \frac{(C)^{c} \cdot (D)^{d}}{(A)^{a} \cdot (B)^{b}}$$
$$Eo = 2.303 \cdot \frac{R \cdot T}{n \cdot F} \cdot LOG(K) \qquad \Delta G = -n \cdot F \cdot E$$

 $\Delta Go = -n \cdot F \cdot Eo$

Variable	Description	Units
E	cell potential	1 V
Eo	standard cell potential	1_V
Т	temperature	1_K
n	moles electrons	1
Q	reaction quotient	1
a,b,c,d	product/reactant coefficients	1
A,B,C,D	product/reactant concentrations	1_mol/m^3
ΔG	free energy change	1 J/mol
ΔGo	standard free energy change	1 J/mol
K	equilibrium constant	1

Example: Calculate the half-potential, measured at 49_°C, for the reaction

$$Cu^{+2}(aq) + 2e^{-} \longrightarrow Cu(s)$$

GivenResult $Eo = 0.34 \ V$ $E = 0.36 \ V$ $T = 49 \ <198 > C$ Q = 0.2n = 2 $\Delta G = -16.7 \ kcal/mol$ A = 5 $\Delta Go = -15.7 \ kcal/mol$ a = 1 $K = 4.3x \ 1E10$ B = C = D = 1b = c = d = 0

Reduction

The following equations describe the quantity of **a** produced by electrolytic reduction for time **t** by the chemical equation:

Reactant	$+ n e^- \rightarrow aA.$	
$Q = A \cdot t$	$ne = \frac{Q}{F}$	
$na = \left(\frac{a}{n}\right) \cdot ne$	$ma = MWTa \cdot na$	
Variable	Description	Units
Q	charge	1_C
A	current	1_A
t	time	1_s
ne	moles of electrons	1_mol
na	moles of a produced	1_mol
а	coefficient of a	1
n	coefficient of n	1
ma	mass of a produced	1_kg
MWTa	molecular weight of a	1 kg/mol

Example: An electrolytic cell is constructed in which silver chloride is reduced to silver metal and chloride ion according to the reaction

$AgCl(s) + e^{-} \rightarrow Ag(s) + Cl^{-}$

A current of 50_mA is passed through the cell for 4.5_h. What is the mass of silver deposited?

Given	Result
$t = 4.5_h$	Q = 810 C
A = 50.0 mA	$ne = 8.40 \times 1E-3 mol$
a = n = 1	$na = 8.40 \times 1E-3$ _mol
MWTa = 107.87_g/mol	ma = 0.906_g

Precipitation

The condition for precipitation of a salt in water defines the solubility product Ksp. For a salt of the solubility of the form AaBb, the solubility product is defined as $Ksp=[A]^{a}[B]^{b}$.

The following equations relate the solubility product to the overall solubility of the salt.

$$Ksp = fa \cdot fb \cdot s^2$$
 AB

$$Ksp = 4 \cdot fa^2 \cdot fb \cdot s^3 \qquad A2B$$

$$Ksp = 4 \cdot fa \cdot fb^2 \cdot s^3 \qquad AB2$$

$$Ksp = 27 \cdot fa^3 \cdot fb \cdot s^4$$
 A3B

$$Ksp = 27 \cdot fa \cdot fb^3 \cdot s^4$$
 AB3

$$Ksp = 108 \cdot fa^2 \cdot fb^3 \cdot s^5 \qquad A2B3$$

$$Ksp = 108 \cdot fa^3 \cdot fb^2 \cdot s^5 \qquad A3B2$$

$$s = \frac{ga}{MWT \cdot V}$$

Variable	Description	Units
Ksp	solubility product	*
fa	activity coefficient of a	**

fb	activity coefficient of b	1
s	solubility	1_mol/m^3
ga	mass of a	1_kg
MWT	molecular weight of a	1_kg/mol
v	volume	1_m^3

* Units of Ksp depend on the stoichiometric ratios within the dissolving species.

**Activity coefficients are equal to 1 if ideal.

Example: What is the solubility of BiI3(s) (AB3, Ksp=8.1x1E-19 in a solution such that, at equilibrium, fBi⁺3=0.110 and fI⁻=0.200. How many grams of BiI3 are dissolved in 100_ml at equilibrium? Compare your results assuming ideality and non-ideality.

Case 1: Non-Ideal	
Given	Result
fb = 0.200	$s = 7.6 \times 1E-5 mol/l$
fa = 0.110	ga = 4.5 mg
$Ksp = 8.1 \times 1E-19 \mod \frac{4}{l^{-1}}$	
V = 100 ml	
MWT = 589.6939 g/mol	
Case 2: Ideal	
Given	Result
fb = 1	$s = 1.3 \times 10 < M^{>-5} < D^{mol/l}$
fa = 1	ga = 0.776 mg
$K_{sp} = 8.14 \text{ x } 1E-19 \text{ mol}^4/l^4$	

Kinetics

V = 100 ml

MWT = 589.6939 g/mol

Chemical kinetics is the study of the time dependence of chemical reactions. The following topics represent common kinetic studies.

First Order Second Order (II) Parallel First Order Arhenius Law First Order Consecutive Fractional Life Second Order(I)

First Order

A reaction: $A \rightarrow^{k1st}$ Products, which proceeds in first order, behaves according to the following equations.

$$Rate = k1st \cdot Ca$$
$$Ca = Cao \cdot e^{-k1st \cdot t}$$
$$thalf = \frac{LN(2)}{k1st}$$

Variable	Description	Units
Rate	rate of reaction	$1_mol/(m^3 \cdot s)$
klst	rate constant	1_1/s
Ca	concentration A (t)	1_mol/m^3
Cao	concentration A (t=0)	1_mol/m^3
t	time	1_s
thalf	half life	1_s

Example: At 25_°C, a first order reaction takes 15.0 minutes to reach the point where half the initial concentration of the reactant has been consumed (half life). How long before less than 1% is left over?



Given	Result
Ca = 1.0 mol/l (assumed)	$k1st = 7.7 \times 1E-4_1/s$
Cao = 0.01 mol/l (assumed)	$t = 5979$ _s
$thalf = 15_{min}$	Rate = $7.7 \times 1E-6 \mod (m^3*s)$

If the reaction is heated to 125_°C, the reaction has a half life of only 1.0_min. Under these conditions, how long does it take to reach 1.0% of initial concentration: Plot the reactant concentration vs. time for these two cases.

 $x1 = 0_s$ $x2 = 6000_s$ autoscale yResult

thalf = 1.0 min

 $k1st = 1.16 \times 1E-2_{1/s}$

Cao = 1.0 mol/lCa = 0.01 mol/l t = 398 s

Parallel First Order

The following reactions describe concentrations of reactants for first order, irreversible, parallel reactions of the form:

$$A = Ao \cdot e^{-(kb+kc)\cdot t}$$
$$B = Bo + \frac{kb \cdot Ao}{kb + kc} \left(1 - e^{-(kb+kc)\cdot t}\right)$$
$$C = Co + \frac{kc \cdot Ao}{kb + kc} \cdot \left(1 - e^{-(kb+kc)\cdot t}\right)$$

 $-(kb+kc)\cdot t$

Variable	Description	Units
В	concentration B (t)	1_mol/m^3
Bo	concentration B (t=0)	1_mol/m^3
kb	rate constant for reaction B	1_1/s
Ao	concentration A (t=0)	1_mol/m^3
kc	rate constant for reaction C	1_1/s
t	time	1_s
С	concentration C (t)	1_mol/m^3
Со	concentration C (t=0)	1_mol/m^3
Α	concentration A (t)	1_mol/m^3

Example: A parallel reaction can produce two products with rate constants of 1.0 1/s and 0.5 1/s. Starting with 1 mol/l of initial reactant, plot the concentration profiles of A, B and C vs. time.



Given

Bo = 0 mol/lkb = 1.0 1/s Ao = 1.0 mol/l

and

x1 = 0	$x2 = 5_s$
y1 = -0.1363	$y^2 = 1.0$

$kc = 0.5 \ 1/s$ Co = 0 mol/l

First Order Consecutive

The simplest form of consecutive reactions is a series of first order reactions of the form:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$

These four equations describe the kinetics of such a system.

$$A = Ao \cdot e^{-k \cdot t}$$

$$B = Bo \cdot e^{-k2 \cdot t} + \frac{k1 \cdot Ao}{k2 - k1} \cdot \left(e^{-k1t} - e^{-k2 \cdot t}\right)$$

$$C = Co \cdot e^{-k3 \cdot t} + Bo \cdot \left(\frac{k2 \cdot e^{-k2 \cdot t}}{k3 - k2} - \frac{k2 \cdot e^{-k3t}}{k3 - k2}\right)$$

$$+ Ao \cdot \left(\frac{k1 \cdot k2 \cdot e^{-k1t}}{(k3 - k1) \cdot (k2 - k1)} - \frac{k1 \cdot k2 \cdot e^{-k2 \cdot t}}{(k3 - k2)(k2 - k1)} + \frac{k1 \cdot k2 \cdot e^{-k3 \cdot t}}{(k3 - k2)(k3 - k2)(k3 - k2)}\right)$$

Variable	Description	Units
Α	concentration A (t)	1_mol/m^3
Ao	concentration A (t=0)	1_mol/m^3
В	concentration B (t)	1_mol/m^3
Во	concentration B (t=0)	1_mol/m^3
С	concentration C (t)	1_mol/m^3
Со	concentration C (t=0)	1_mol/m^3
k1	rate constant for $A \rightarrow B$	1_1/s
k2	rate constant for $B \rightarrow C$	1_1/s
k3	rate constant for $C \rightarrow D$	1_1/s
t	time	1_s

Example: Irreversible successive first order reactions kinetics is often used to describe radioactive decay. Consider the progressive series of reactions:

 $A \xrightarrow{5_1/h} B \xrightarrow{2.5_1/h} C \xrightarrow{4.5_1/h} D$

where A(t=0) = 1.0 mol/l and Bo=Co=0 mol/l. Plot the concentration

of B and C vs. time, and determine the point where the maximum concentration of each material occurs.

x1 = 0_s x2 = 6000_s y1 = -0.1363 y2 = 1 A (maximum) = 0.00_s B (maximum) = 0.50_mol/l, ~969_s C (maximum) = 0.22 mol/l, ~1800 s



Second Order (I)

These three equations describe the concentration versus time for a second order reaction of the form: $aA \rightarrow products$.

$$Rate = k2nd \cdot Ca^{2}$$

$$Ca = \frac{Cao}{(1 + a \cdot k2nd \cdot t \cdot Cao)}$$

$$thalf = \frac{1}{a \cdot Cao \cdot k2nd}$$

Description	Units
rate of reaction	1_mol/(m^3·s)
rate constant	$1_m^3/(mol \cdot s)$
concentration A (t)	1_mol/m^3
concentration A (t=0)	1_mol/m^3
stoichiometric coefficient	1
time	1_s
half life	1_s
	Description rate of reaction rate constant concentration A (t) concentration A (t=0) stoichiometric coefficient time half life

Example: The thermal decomposition of HI (2HI \rightarrow H2 + I2) proceeds in second order in HI. In this reaction, a 0.10_mol/l of HI sample reacts for 10 minutes in a spectrophotometer. After 10 minutes the concentration is 0.08_mol/l. What is the rate constant and half life?

Given	Result
Cao = 0.10 mol/l	$k2nd = 2.08 \times 1E-3_l/(mol \cdot s)$
$Ca = 0.08 \text{_mol/l}$	$thalf = 40_{min}$
$t = 10.0_{min}$	

66
a = 2

Second Order (II)

The following equations describe concentrations versus time for a second order reaction of the form: $aA + bB \rightarrow products$.



 $Rate = k2nd \cdot Ca \cdot Cb$

$$f = \left(\frac{Cbo}{Cao}\right) \cdot \exp\left(\left(a \cdot Cbo - b \cdot Cao\right) \cdot k2nd \cdot t\right)$$
$$f = \frac{CB}{CA}$$

Variable	Description	Units
Rate	rate of reaction	1_mol/(m^3·s)
k2nd	rate constant	1_m^3/(mol·s)
Ca	concentration A (t)	1_mol/m^3
Cb	concentration B (t)	1_mol/m^3
f	reactant ratio	1
Cao	concentration A (t=0)	1_mol/m^3
Cbo	concentration B (t=0)	1_mol/m^3
а	stoichiometric coefficient of a	1
b	stoichiometric coefficient of b	1
t	time	1_s

Example: The reaction of ethylene bromide with potassium iodide in 99% methanol proceeds in second order according to the following reaction:

$$C_2H_ABr + 3Kl \xrightarrow{k^2nd} C_2H_A + 2KBr + Kl_3$$

At 59.72_°C, k2nd is reported to be 5.0 x 1E-3 _l/(mol·s) when the initial concentration of ethylene bromide and potassium iodide are 0.02864_mol/l and 0.1531_mol/l, respectively. Calculate the reactant ratio at 0.1_h , 0.5_h , 1.0_h and 10_hr .

Given	Result
Cao = 0.02864_mol/l	$f(0.1_h) = 6.03$

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Cbo = 0.1531 mol/lk2nd = $5.0 \times 1\text{E}-3 \text{ l/(mol \cdot s)}$ a = 1 b = 3 t = 0.5 hx1 = 0x2 = 10y = autoscale

Arrhenius Law

These equations describe the Arhenius Law, which relates the rate constant to the temperature and activation energy of the reaction.

$$k1 = A \cdot e^{-\left(\frac{Ea}{R \cdot T}\right)}$$
$$LN\left(\frac{k1}{k2}\right) = \left(\frac{-Ea}{R}\right) \cdot \left(\frac{1}{T1} - \frac{1}{T2}\right)$$

Variable	Description	Units
k1	rate constant at T1	1
k2	rate constant at T2	1
Α	pre-exponential	1
Ea	activation energy	1 J/mol
T1	temperature at k1	1 K
T2	temperature at k2	1_K

Example: The rate constants for the rearrangement of methyl isonitrile are $2.52 \times 1E-5_1/s$ and $3.16 \times 1E-3_1/s$ at 189.7_{C} and 251.2_{C} respectively. From this data, calculate the activation energy and pre-exponential for this reaction.

Given

k1 = 2.52 x 1E-5 k2 = 3.16 x 1E-3 T1 = 189.7_°C T2 = 251.2_°C **Result** Ea = 159_kJ/mol A = 1.96 x 1E13

Fractional Life

The time necessary for a given fraction of a reagent to react will depend on the initial concentrations of reactants and the rate expression for the

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reaction. The following equations calculate the time necessary for the reactant to reach to a fraction of its original concentration.

$$tfract = \frac{\left(\frac{1}{1-f}\right)^{no-1} - 1}{(no-1) \cdot a \cdot kgen \cdot Cao^{no-1}} \qquad \text{If no} \neq 0$$

$$tfract = \frac{-LN(1-f)}{kgen}$$
 If no = 1

Description	Units
fractional life	1_s
reaction order	1
general rate constant	1_1/s*
general concentration	1
stoichiometric coefficient	1
fractional order	1
	Description fractional life reaction order general rate constant general concentration stoichiometric coefficient fractional order

*The units of kgen will be in the units of $(time)^{-1}$, times the units of Cao to the (1-no) power.Note that only one equation is shown in the calculator.

Example: A second order reaction $(2A \rightarrow \text{products})$ proceeds with a rate constant of 1.03 x 1E-3_1/(h mol). If the initial concentration of A is 0.01_mol/l, how long will it take for 10% of A to react? How about 25%, 50%, or 75%?

Given	Result
no = 2	tfract = 1.94 E7_s 10%
kgen = $1.03 \times 1E-3_1/h$	$tfract = 5.82 E7_s 25\%$
Cao = 0.01	$tfract = 17.5 E7_s 50\%$
a = 2	tfract = 52.4 E7_s 75%
f = 0.10	

3 Periodic Table

In This Chapter

The Periodic Table function is a quick reference tool that provides basic information, such as mass number, electron configuration, oxidation state, and atomic weight, for each element.

Using the Periodic Table

The Periodic Table screen displays after selecting this topic at the main menu. The figure below illustrates the information given on the screen for each element:

In the Periodic Table display, each square represents one element. The square, black cursor marks the selected element. The element name, mass number, symbol, atomic number and molecular weight, are displayed.

Properties of Each Element

2 HYDROGEN 34567 1 3456789012 H 1 3456789012 1.0079 1.007



Press **PROPS** or ENTER to view a list

of properties for the current element: Use the cursor keys to scroll down the list to the desired property. Pressing me places the data on the calculator stack. The properties listed for each element (if available) are:

- Atomic Number (Table)
- Mass Number (Table)
- Atomic Weight (Table)
- Density
- Oxidation State
- Electron Configuration
- Physical State
- Electronegativity (Pauling's)
- Atomic Radii
- Covalent Radii
- First Ionization Potential

- Boiling Point
- Group and Family
- Melting Point

Moving Around the Periodic Table

Use the cursor keys (TFAA) to move the pointer to any element. Pressing the Fakey with a cursor key moves the cursor to the beginning

or end of the current row or column. Pressing **FAST** eliminates the element information from the screen and allows you to quickly move from element to element using the cursor keys. Press **FAST** again to retrieve the screen information.

35		2	Э	4	С 5	HI 6	.0 7	Ri Ø	N 9	E	1	2	3	4	5	F	7	-
C1 17				_														
35.45			Ž					P		F	F	B		H	B	H	H	
PROPS	F	E	U	I	ŧΤ	ŀ	÷		LĪ	5		F	Ĥ:	T		1	P	

Using Search and List Utilities

To search for a particular element press the **FIND** softkey. At the prompt, type in the symbol or atomic number of the element you want to search for, as shown: If you are entering an element's symbol, the second letter must be lower case. Lower case entries are made by pressing **F** before typing in the letter. Press **ME** to move to the Periodic Table screen containing the element you were searching for, in this case, chlorine:

List of Element Names and Symbols

Pressing **LIST** displays the names and symbols of all the elements in the Periodic Table, in alphabetical order:

Searching for a Property

To search for particular property, press $\textcircled{\mbox{\sc only}}$ at the list of properties screen. At the "search for" prompt, type in the desired variable, remembering that

searches are case sensitive. For example, to search for the covalent radii of chlorine, type in "Cov" at the prompt, as shown:

Then press **ENTER** to initiate the search.



- Ele	ments	
Actinium	<u> </u>	
Americium	ŚÃŵŚ	
Antimony	(SP)	
Argon Arsenic		
PROPS FIND ATLAS	THELE FONT	UP





The following screen displays: Press **EXIT** to return to the Periodic Table screen.

Editing Text Entries During a Search

The search mode softkeys (\leq -SKIP, \leq -DEL, INS) along the bottom of the search screen are command line editing keys. They are built into the HP 48GX and allow you to edit the search string. Their functions are summarized below:

< - SK P	Moves the cursor to the beginning of the current word.
SKIP->	Moves the cursor to the beginning of the next word.
< - DEL	Deletes all the characters in the current word to the left
	of the cursor.
DEL ->	Deletes all the characters from the cursor's current
	position to the first character of the next word.
INS	Toggles between insert and typeover modes.

Using the Print Function

You can send data from the Periodic Table directly to an infrared (IR) printer compatible with the HP 48GX via the infrared port. Follow the instructions in the printer manual regarding operating and positioning the printer relative to the HP 48GX.

When you press the **PRIME** softkey at the Periodic Table screen, the next screen asks you to select *all* or *field*. If you press **ALL**, all data for the current element is sent to the printer. Pressing **FIELD** prints only the data item currently selected by the pointer.

Summary of Softkeys

MAIN	Returns to the main menu.
->STK	Copies selected entry to calculator stack.
PRINT	Sends selected data to an IR printer.
UNITS	Toggles units on and off. When off, all variables are assumed to be SI.
UNIT -	Indicates that units are on.
DEF	Exits to the Periodic Table or list of elements
FONT	Toggles the display font between large and small.
TABLE	Returns to the Periodic Table display from the element list.
PROPS	Displays a list of various properties for each element.

FIND	Initiates a search for an element name, number, symbol
	or property.
LIST	Displays an alphabetical listing of elements and
	symbols.
FAST	Toggles fast display mode on and off.
FAST •	Indicates that fast mode is on.
DEF	Places the atomic weight of the current element on the
	stack as a tagged object.

4 Stoichiometry

In this Chapter

The stoichiometry function allows you to build new chemical reactions, and perform theoretical yield and limiting reagent calculations, for liquid, solid, gas and solution reactions. The Species Library, which stores the chemical species needed to form these chemical reactions, is also discussed.

- Using the Stoichiometry Function
- Using the Species Library
- Creating a Chemical Reaction
- Summary of Softkeys

Using the Stoichiometry Function

The stoichiometry function is designed for you to enter, name, and store your own chemical reactions in the calculator's memory. The software checks for mass and charge balance and allows you to easily calculate theoretical yields and limiting reagents. Two chemical reactions, methane combustion and permanganate reduction, are included in the software as examples to demonstrate the stoichiometry function.

When you select STOICHIOMETRY at the main menu for the first time, only the two sample chemical reactions appear on the screen. As you enter and name your own reactions, they are added to the list. The next three sections use the sample reactions to illustrate how to access reactions and calculate theoretical yields and limiting reagents. The remaining sections explain how to build, check, and edit your own chemical reactions.

Selecting and Displaying a Chemical Reaction

Select STOICHIOMETRY at the main menu screen and press ment to display the reactions currently available in the calculator's memory:

When you first use the General Chemistry Application Pac, only the two sample reactions are listed on the STOICHIOMETRY menu. Move the pointer to METHANE COMBUSTION and press the softkey for the Chemical Equation Writer, **CHEW**, to view the methane combustion reaction, shown below:

Press ENTER to return to the STOICHIOMETRY menu screen. For reactions that are too lengthy to fit on the screen, use the \blacksquare and \blacktriangleright keys to scroll



the display to the right or to the left. Press (IN) key to return to the STOICHIOMETRY menu screen.

CH₄₉+20₂₉
$$\rightleftharpoons$$
 2H₂0₁+CO₂₉

SPARCOM CHEMICAL EQUA 8H⁺¹+MnO_{4aq}+5Fe⁺² ≠ Mn 9RESS ◀ AND ► TO SCRC PRESS CATINO TO RETUR

Calculating Theoretical Yields

Suppose you want to calculate the mass of O2 required to react with 1_g of CH4 during combustion. Move the pointer to the METHANE COMBUSTION reaction and press **STOLE**. This displays all reactants (labeled P) in t



(labeled R) and products (labeled P) in the reaction, as shown:

At this point the reaction is checked for mass and charge balance. If it is not balanced, a warning message appears, giving you the option of continuing, despite the imbalance.

Entering a Quantity of a Reactant

To enter a quantity of a reactant (or product), move the pointer to that species and press **MR**. Enter 1, then press the appropriate unit softkey to append a unit to your entry, as shown:

Press ENTER to store 1_g as the quantity of CH4:

(HOME GCAPPD } Enter quantity of	PRG
1CH4[9];	
LG _KG _MOL _LB _L	_ML

METHANE COMBUSTION R: (1_G) 1CH4[G] PR: (0) 2D2[G] P: (0) 2H2D[L] P: (0) 1CD2[G]
CALC CONV CLEAR VIEW ASTR EXIT

All quantities are displayed in brackets. To perform a theoretical yield calculation, press **CALC**. The quantity of the single, specified reactant (or product) is used to calculate the theoretical yields of all the other components, in grams.



To convert the mass of oxygen (or any reactant or product) into units other than grams, move the pointer to the reactant or product you want to covert (in this case, O2) and press **CONV**. This displays a list of available units:



Move the cursor to pounds and press MER. This converts the mass of oxygen from grams to pounds:

To perform another theoretical yield calculation, first press **CLEAR** to reset all quantities to zero.

Limiting Reagents

Suppose a reaction vessel contains 1_g of CH4 and 1_g of O2. The reaction will proceed until all of one reactant is consumed, leaving other reactants. The reactant that is totally consumed is termed a limiting reagent. To solve such a problem, simply enter both quantities into the stoichiometry list, as shown:



Press **CALC** to start the calculation. The result is shown below: This shows that all the O2 is consumed in the reaction (it's the limiting reagent) whereas only 0.25_g of CH4 was consumed. Limiting reagent calculations may be performed with any number of reactants and products specified.

Stoichiometry with Solutions

In some cases, reactions are most convenient if they proceed with reactants and/or products in the form of solutions. For example, consider the reaction of 25_ml of 0.01_mol/l of potassium permanganate, according to the permanganate reaction. To calculate theoretical yields in this case, simply select the permanganate reactant and press ME. Type in 25_ml and press ME.





The next screen asks you to enter the molarity of the permanganate solution. Type in 0.01_mol/l at the prompt: Press me to place the volume and

concentration onto the stoichiometry list for permanganate, as shown: Press **CALC** to initiate the theoretical yield calculation for this reaction. The result is shown below:

Using the Species Library

The Species Library stores the chemical species, or "building blocks" used to form new chemical reactions. When you first use the General Chemistry Application Pac, the Species Library includes the following default species:

CH4(g)	CO2(g)
Fe+2(aq)	Fe+3(aq)
H2O(l)	H+1(aq)
MnO4-1(aq)	Mn+2(aq)
O2(g)	OH-1(aq)

To view these chemical species, select SPECIES LIBRARY at the main menu: All chemical species must be entered into the Species Library before they can be used to build a chemical reaction. To add a new species to the Species Library, press the **MDD** softkey. The prompt asks for the formula, and optional state and charge, of the new chemical species:

Suppose you want to add NaOH to the list. Type N 🔄 A O H, as shown:

Chemistry Application

Press ENTER to place NaOH into the Species Library:

	SPEC	IES	LIE	RARY	
HDD I	ittene	EDIT	ChEI4	MMT2	ЦP



The softkeys along the bottom of the Species Library screen allow you to add, edit, or delete species from the list, evaluate their molecular weight and percent element composition, and display each species on the screen. The softkeys function in the Sparcom Chemical Equation Writer format.



```
MnO4[aq]-1
118.9356_9/mol
0 53.8% MN 46.2%
PRESS [STD] TO SAVE TO STACK ...
PRESS [ENTER] TO RETURN TO LIST ...
```

 SPECIES FE(AQ)+3 H201L1 H1AQ1+1 MNUTAQ1+2 MNUAQ1+2 MAIA 	LIBRARY	
PRAUN DZCGJ DHCAQJ-1 ROOD (DELETTE EOLT	CHEM MMTX	Ű₽

To evaluate the molecular weight of any species in the list, for example MnO4-1(aq), simply move the pointer to that species and press MWT%. The molecular weight and the percent

composition are then displayed on the screen, as shown:

Press to store the molecular weight on the calculator stack. Pressing ENTER returns you to the Species Library. Press **CHEW** to display the species on the screen:

Creating a Chemical Reaction

To perform stoichiometric calculations you must enter your own chemical reactions. Each entry consists of a name, a list of reactants and products, and their corresponding stoichiometric coefficients. Reactants and products are selected from the Species Library.

Upon entering the STOICHIOMETRY function of the General Chemistry Application Pac, all stored reactions are listed on the screen, as shown:

Suppose you wish to add the chemical reaction for the dissociation of water, given by:

Chemistry Application

$\mathrm{H20}_{[1]} \rightarrow \mathrm{H^{+}[aq]} + \mathrm{OH^{-}[aq]}$

STOICHIOMETRY →METHANE COMBUSTION PERMANGANATE	(HOME GCAPPD) PRG Edit reaction name:
ADD DELETE EDIT (CHEW STOIC) UP	WATER DISSOCIATION

Press the **ADD** softkey. At the prompt, type in the name of the reaction: (in this case WATER DISSOCIATION) and press **ME**. To edit or delete a reaction, press **EDIM** or **DELETE**. You are then prompted to enter the reactions and products for the reaction:



The "PRESS ADD" prompt indicates that no reactants or products have been entered for this reaction. To enter a reactant, press **ADD R**. This places you in the SPECIES LIBRARY where you will select a reactant from the sprecies in the list. Scroll down the list until you find H2O[L] and press **ENER**.

PRG { Home gcappd }	
Enter coefficient:	
1 PSRIPISRIPA POPL DELA INS -	ASTR

WATER →R: 1H2OCLJ	DISS	DCIA	TIO	N
ADD R ADD P	DELETE	DIT ST	01C	IJ٩

The prompt then asks for the stoichiometric coefficient, which in this case is 1. Type 1 at the prompt and press $\boxed{\text{MER}}$. This places H2O on the reaction list, labeled R for reactant. The coefficient 1 preceeds the species entry on the list.



Press ADD P to add a product species. Once again, scroll down the list until you find OH[aq]-1 and press MER. Repeat this procedure to add H+ to the reaction list as a product (look for H[aq]+1). If you make a mistake, press

DELETE to delete a reactant. Pressing **EDIT** allows you to enter a replacement species and new stoichiometric coefficient. This results in the complete reaction listing for the WATER DISSOCIATION reaction, as shown:



SPARCOM CHEMICAL EQUATION WRITER -1 MnO₄aq PRESS CENTER3 TO RETURN TO LIST ...

Press **STOIC** to perform stoichiometric calculations on this reaction. You may press **UP** to return to the main menu with the pointer at the reaction that you just added, as shown:

Press **CHEW** to view the reaction on the screen:

Entering Molecular Formulas

Species formulas consist of a series of element symbols and chemical groups of element symbols in parenthesis. Optional trailing multipliers may be entered to indicate more than one of a given element or group. Fractional multipliers may be entered, in decimal format. You may optionally include a state and/or charge in the format given in the prompt. A shortcut for entering the state is unlocking alpha-entry mode (by pressing \square and pressing the appropriate softkey. Charges must be preceded by the sign (either + or -). Parentheses may be entered by either pressing \square or the two softkeys shown in the display. (Note that \square does not require unlocking alpha-entry mode. Some examples of acceptable chemical formulas are:

Compound	Input
HCl	HCGL
HNO3	HNO3
Ca(NO3)2	C¶A ¶; NO3 ⊠→ 2

After unlocking alpha-entry mode to enter parentheses or to move the cursor, it is necessary to press \square once or twice to relock alpha-entry mode for subsequent alphabetic entry. For more information, see the HP 48SX Owner's Manual.

In some cases, it may useful to abbreviate large entries in the Species Library or to define new symbols. For example, suppose you are interested in performing stoichiometric calculations on the esterification reaction of a carboxylic acid by an alcohol:

R-COOH + Rz-OH \rightarrow Products.

To enter this reaction, you must enter the species RCO2H, Rz-OH, and Pro into the Species Library. After these are entered, you will be prompted for the molecular weight (in -g/mol only) of the unknown symbols R, Rz, and Pro. Once defined, these symbols are accessible to all species in the Species Library.

You must enter these user-defined symbols as single uppercase letters, optionally followed by one or two lowercase letters. Once created, a user defined symbol can not be modified or deleted except by deleting the USRSYMBS and USRATWTS files in the GCHEMD directory.

Summary of Softkeys

The following table lists the softkeys and their respective functions for the Stoichiometry and Species Library in the General Chemistry Application Pac.

Stoichiometry Softkeys

 Adds a reactant from the Species Library and a stoichiometric coefficient to the selected chemical reaction. Adds a product from the Species Library and a stoichiometric coefficient to the selected chemical reaction. CALC Utilizes the current species quantities to perform theoretical yield or limiting reagent calculations. CHEW Displays a chemical reaction on the screen in the da Vinci's Chemical Equation Writer format. CLEAR Clears all quantities in the stoichiometry function. CONV Deletes a chemical reaction or a reactant or product from 	ADD	Adds a new chemical reaction to the list.
 Adds a product from the Species Library and a stoichiometric coefficient to the selected chemical reaction. CALC Utilizes the current species quantities to perform theoretical yield or limiting reagent calculations. CHEW Displays a chemical reaction on the screen in the da Vinci's Chemical Equation Writer format. CLEAR Clears all quantities in the stoichiometry function. CONV Converts a quantity to a different unit. Deletes a chemical reaction or a reactant or product from 		Adds a reactant from the Species Library and a stoichiometric coefficient to the selected chemical reaction.
 stoichiometric coefficient to the selected chemical reaction. CALC Utilizes the current species quantities to perform theoretical yield or limiting reagent calculations. CHEW Displays a chemical reaction on the screen in the da Vinci's Chemical Equation Writer format. CLEAR Clears all quantities in the stoichiometry function. CONV Converts a quantity to a different unit. Deletes a chemical reaction or a reactant or product from 	ADD P	Adds a product from the Species Library and a
CALCUtilizes the current species quantities to perform theoretical yield or limiting reagent calculations.CHEWDisplays a chemical reaction on the screen in the da Vinci's Chemical Equation Writer format.CLEARClears all quantities in the stoichiometry function. Converts a quantity to a different unit.DELETEDeletes a chemical reaction or a reactant or product from		stoichiometric coefficient to the selected chemical reaction.
 theoretical yield or limiting reagent calculations. Displays a chemical reaction on the screen in the da Vinci's Chemical Equation Writer format. CLEAR Clears all quantities in the stoichiometry function. Converts a quantity to a different unit. Deletes a chemical reaction or a reactant or product from 	CALC	Utilizes the current species quantities to perform
CHEWDisplays a chemical reaction on the screen in the da Vinci's Chemical Equation Writer format.CLEARClears all quantities in the stoichiometry function.CONVConverts a quantity to a different unit.DELETEDeletes a chemical reaction or a reactant or product from		theoretical yield or limiting reagent calculations.
da Vinci's Chemical Equation Writer format.CLEARClears all quantities in the stoichiometry function.CONVConverts a quantity to a different unit.DELETEDeletes a chemical reaction or a reactant or product from	CHEW	Displays a chemical reaction on the screen in the
CLEARClears all quantities in the stoichiometry function.CONVConverts a quantity to a different unit.DELETEDeletes a chemical reaction or a reactant or product from		da Vinci's Chemical Equation Writer format.
CONVConverts a quantity to a different unit.DELETEDeletes a chemical reaction or a reactant or product from	CLEAR	Clears all quantities in the stoichiometry function.
DELETE Deletes a chemical reaction or a reactant or product from	CONV	Converts a quantity to a different unit.
	DELETE	Deletes a chemical reaction or a reactant or product from

81

	a chemical reaction.
EDIT	Edits a chemical reaction or a reactant or a product.
ENTER	Allows you to specify the quantity of a reactant or
	oduct.
EXIT	Exits the Stoichiometry solving screen.
→STK	Copies selected entry to calculator stack.
STOIC	Enters the stoichiometry solving screen after the selected emical reaction is mass and charge balanced.
UP	Moves up one level in the menu structure.
VIEW	Displays entries too wide to fit on the screen. It is not nctional if the line does fit on the screen.

Species Library Softkeys

ADD	Adds a new chemical species to the Species Library.
CHEW	Displays a chemical species on the screen in the
	da Vinci's chemical Equation Writer format.
DELETE	Deletes a chemical species from the Species Library.
EDIT	Edits a chemical species.
MWT%	Displays the molecular weight and percent composition
	of the selected species.
UP	Returns to the main menu.

5 Constants Library

In This Chapter

The Constants Library is a collection of useful constants commonly used in general chemistry.

- Using the Constants Library
- Constants Library Softkeys

Using the Constants Library

Select the Constants Library from the main menu screen: The Constants Library menu lists 29 constants and their symbols, listed below:

🗧 Constants Library
G : ACCEL OF GRAVITY
R2: GAS CONSTANT Wa: GAS CONSTANT
C : VEL DF LIGHT H : PLANCK'S CONST
K : BOLTZMANN'S CONST
VALUE #STK FONT UP

π
Acceleration of gravity
Universal gas constant - J/(mol*K)
Gas constant - atm/(mol*K)
Avogadro's number
Velocity of light
Planck's constant
Boltzmann's constant
Dirac's constant
Electron charge
Permittivity of vacuum
Electron mass
Classical electron radius
Proton rest mass
Rydberg's constant
Fine structure constant
Bohr radius
Bohr magneton
Wavelength for 1eV
Compton's wavelength
Stefan-Boltzmann
First radiation constant
Second radiation constant
Thermal voltage at 300_K
Permeability of free space

φo	Magnetic flux quantum
F	Faraday constant
μе	Electron magnetic moment
μр	Proton magnetic moment

Using the GCON Function

You can extract the value of any constant without entering the General Chemistry Application Pac with the GCON() function. In all cases, the constant name must be prefixed with a "\$" symbol, accessed by Africa. For example, suppose you want to retrieve the speed of light:

User Program Method

Inside a user program, use the commands '\$c' GCON or 'GCON(\$c)' we to call for the speed of light.

Stack Method

Type '\$c' into level 1 of the stack and press the **GCON** softkey or type the letters GCON and press **ETE**.

The constant value will have SI units if units are selected (i.e., if flag 61 is clear); otherwise, the value will have no units.

VALUE	Displays the value of the constant with units on the screen. Press EVER to return to the constants list.
•>STK	Places a copy of the selected constant on the calculator stack. Whether or not the value has units appended is controlled by the units key setting, which can be toggled at the Equation Library screen.
FONT	Toggles between large and small display font.
UP	Exits to the main menu.
MAIN	Exits to the main menu.

Constants Library Softkeys

6 Reference Library

In This Chapter

The Reference Library is a collection of useful data commonly used in general chemistry.

- Using the Reference Library
- Summary of Softkeys

Using the Reference Library

When you select the Reference Library from the main menu, the following screen appears: The Reference Library application, accessed from the main menu, consists of 10 topics. To access a given topic, move the pointer to the desired topic and press ENER. The 10 Reference Library topics are described below:

PKas	The dissociation constants of selected weak acids.
Common anions	Names and formulas of common anions.
Air composition	Percent composition (by mass) of air at sea level
Vapor pressure - H ₂ O	Vapor pressure of pure water at selected temperatures.
Water Kw vs. T	Dissociation constant of water at selected temperatures.
Van der Waals	Van der Waals constants for selected gases
Colligative	Normal boiling point,, freezing point, ebullioscopic constant and cryoscopic constant for common solvents.
Expansinon/Compr essibility	Coefficient of expansion and coefficient of compressibility of four common materials.
PKsps	Solubility product constants (at 25 °C for common precipitates.
Bond Energy/distance	Energies and distances of common bonds

Example Using the Reference Library

Suppose you need the vapor pressure of water at 25 °C for a gas law calculation you're working on in the calculator stack. Use the cursor keys to move the pointer to the VAPOR PRESSURE - H2O menu item. Press Enter to display the following screen: Move the pointer to 25 C and press Enter. This copies the value 23.8_torr onto the calculator stack. You need to exit the Pac to continue your calculation on the stack.

_	_
FONT	Toggles the dsplay font between condensed and
	large sizes.
UP	Moves up one level in the menu structure.
MAIN	Exits to the main menu.
->STK	Copies selected entry to calculator stack.
PRINT	Allows you to print a data field or the entire list of
	data to an IR printer.
ALL	Sends all the data in a list to an IR printer.
ONE	Sends the data in the field selected by the pointer to
	an IR printer
UNITS	Toggles key. Indicates units are off. When off, all
	variables are assumed to be SI.
UNIT	Toggle key. Indicates that units are on.

Summary of Softkeys

Appendix **A**

Warranty and Service

PocketProfessional Support

If you don't find the information in this manual or in the HP 48GX owner's manual, contact us in writing at:

da Vinci Technologies Group, Inc. 1600 SW Western Blvd, Sute 250 Corvallis, OR 97333 Tel: (541) 757-8416 Fax: (541) 753-7821 e-mail: support@dvtg.com Website URL http://www.dvtg.com

What is covered - The PocketProfessional is warranted by da Vinci Technologies Group, Inc. ("da Vinci")against defects in material and workmanship for one year from the date of original purchase. If you sell your card or give as a gift, the warranty is automatically transferred to the new owner and remains in effect for the original one-year period. During the warranty period, we will repair or replace (at no charge) a product that proves to be defective, provided you return the product and proof of purchase, shipping prepaid to da Vinci.

What is not Covered - No other warranty is given. The repair or replacement of a product is your exclusive remedy. Any other implied warranty of merchantability or fitness is limited to the one-year duration of this written warranty. In no event shall da Vinci be liable for consequential damages. Products are sold on the basis of specifications applicable at the time of manufacture. Da Vinci has no obligation to modify or update products, once sold.

If the Card Requires Service

Da Vinci will repair a card, or replace it with the same model or one of equal or better functionality, whether it is under warranty or not. **Service Charge** - There is a fixed charge for standard out-of-warranty repairs. This charge is subject to the customer's local sales or value-added

tax, wherever applicable. Cards damaged by accident or misuse are not covered by fixed charges. These charges are individually determined.

Shipping Instructions - If your card requires service, follow this procedure:

- 1. Call da Vinci (541) 757-8416 and obtain an approval by obtaining a RMA (Return Merchandise Authorization) number.
- 2. Ship the card back to da Vinci in the following manner:
 - Include your return address, phone number and a brief description of the nature of the problem.
 - Include the RMA number with the returned merchandise outside the package; otherwise the package will be returned unopened.
 - If the card is still under warranty, include proof of purchase.
 - Include a check, purchase order, or a credit card number (only VISA, MASTER CARD, AMERICAN EXPRESS and DISCOVER cards are honored) and the expiration date to cover the estimated charges. If there are extra charges for repair, Da Vinci Technologies will notify you and get your approval.
 - Ship the card, postage prepaid, in protective packing adequate to prevent damage. We strongly recommend that you insure your package. Ship the package to

Da Vinci Technologies Group, Inc. RMA #:_____ Technical Support 1600 SW Western Blvd, Suite 250 Corvallis, OR 97333 USA

Cards are serviced and reshipped in five business days.

Environmental Limits

Safe temperature and humidity range for PocketProfessional cards is:

- Operating temperature: 0 to 45°C (32 to 113°F)
- Storage temperature: -20 to 60°C (-4 to 140°F)
- Operating and storage humidity: 90% RH at 40°C(104°F)

Appendix **B**

Questions and Answers

Questions Commonly Asked

Q. I can't find the **COAP** subdirectory in the Library menu. How can I verify that the card and the calculator are functioning properly?

A. There are several possibilities:

- Check to make sure that the card is properly seated in the calculator port.
- Turn the calculator off and on.
- The calculator checks the application card when it turns on. If an "Invalid Card Data" or a "Port Not Available" message is displayed, the card may require service.

Q. I'm using the Equation Library to solve a problem. After selecting the equations and entering values for the variables, the calculator displays "Too many unknowns" What's wrong?

A. Not enough variables were specified to completely solve the problem. You will have to specify more values and solve again.

Q. I'm using the Equation Library to solve a problem. After selecting the equations, I'm ready to enter values for my variables. I find that some of the variables have values already displayed. What's wrong?

A. The variables with values displayed indicate that these variable names have been used in solving another equation. To start with a clean slate of values, use **CLEAR** to reset the values of all variables to 0.

Q. While using the Equation Library, I turned units off and all the numbers changed. What's wrong?

A. In no-units mode, the Equation Library assumes that all values are SI in order for the equations to solve correctly. Therefore, when units are turned off, all values are first converted to SI units, then the unit tags are eliminated.

Q. While using the Equation Library to solve an equation set, intermediate answers are given. Why?

A. The da Vinci's equation solver engine has the ability to solve a set of equations in a systematic fashion. The result of computation from each equation is reported, to keep you informed of the solver's progress.

Q. The calculator displays "Bad Guess(es)" while running the Equation Library. What's wrong?

A. The HP 48SX root finder encountered variable values or units that prevented a solution. You may need to start the root finding process by providing a proper "seed" value. See Chapter 1 for details.

Q. While solving for an angle, I got an answer that was too large: For example, 8752 instead of the expected answer of 112.

A. The calculated result may be offset by integer multiples of 360° . By seeding the variable properly, or by solving in no-units mode, you should be able to avoid this problem.

Q. I solved a problem some time ago, and I'm trying to recall those calculated values for a problem I'm working on now. The values from the past calculation have changed. What's wrong?

A. Most likely, the same variable name was used in solving another equation, so you will not be able to recall the old values.

Q. While searching a list of information, I used the alpha key, but the search function didn't work. Why?

A. Since the search function is case-sensitive, you most likely entered the letters in the incorrect case.

Appendix C

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