

The PocketProfessional™

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 PocketProfessional™ 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.

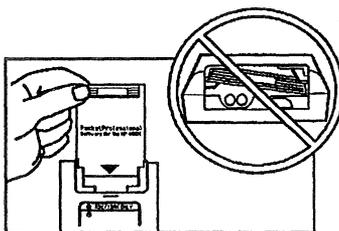
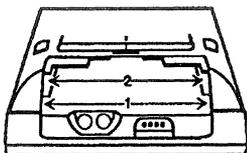
Installing, Removing the Pocket Professional

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

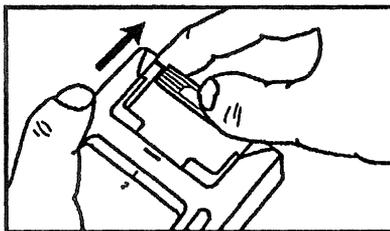
- Turn off the calculator. Do not press **[ON]** until you have completed the installation procedure.
- Remove the port cover. Press against the grip lines and push forward. Lift the cover to expose the two plug-in ports.
- Select either empty port for the Pocket Professional card.
- Position the card 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

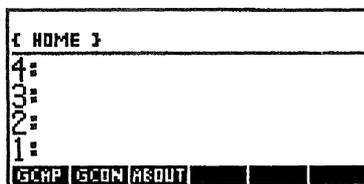
1. Turn the calculator off. Do not press **ON** until you have completed the procedure.
2. Remove the port cover. Press against the card's grip and slide the card out of the port.
3. Replace the port cover.



To Access the Chemistry Application Pac

After you turn your calculator **ON**, there are three ways to access the Chemistry Application Pac.

First Method: Press **LIBRARY** to display all libraries available to the HP 48GX. Press the **GCAP**, "softkey" to start the General Chemistry Application



Pac. Pressing the second softkey available at this level, **ABOUT**, displays the revision number of the software. Pressing the **CONT** keys exit the revision screen and returns you to the screen shown above.

Second Method: Type in the letters **GCAPP** and press **ENTER**.

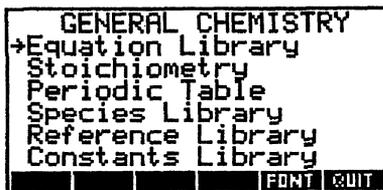
down if the pointer is already at the bottom of the screen. Pressing   moves to the top of the screen or pages up if the pointer is already at the top of the screen. Pressing   moves the pointer to the bottom of the list or   moves to the top of the list.

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 **VIEW** to display the rest of the text. To return the previous display, press **ON** key.

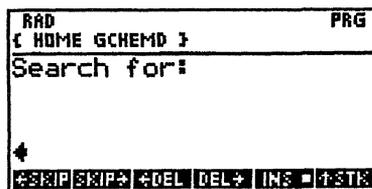
Changing the Font Size

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  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 entry mode overrides the function of the standard keyboard. This means that each key that has a white capital letter printed to its lower right loses 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 **ENTER**. The search function is case sensitive. To enter a lower case letter in the alpha entry mode press  key before typing the letter.



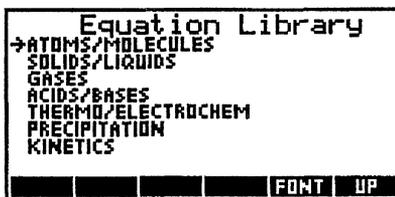
Editing Text Entries

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:

< - SKIP	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	Accesses a version of the interactive stack in which 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:

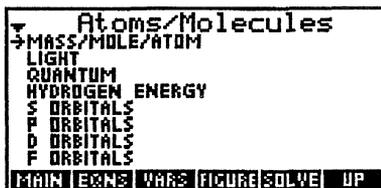


- Select the equation category and topic from the main menu.
- List all the equations in a topic.
- Solve a specific equation or a set of equations.
- View a description of the variables.
- View a figure that illustrates the problem.
- Plot the equation.

Solving a Single Equation

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

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 **ENTER**. 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:

```
GENERAL CHEMISTRY
→EQUATION LIBRARY
STOICHIOMETRY
PERIODIC TABLE
SPECIES LIBRARY
REFERENCE LIBRARY
CONSTANTS LIBRARY
FONT QUIT
```

Selecting and Displaying Equations

Move the pointer to the topic "MASS/MOLE/ATOM" and press **ENTER**, or press the **EQNS** soft key, to display the equation set for mass-to-mole 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

```
Mass/Mole/Atom
→n=ga/MWT
MATOMS=MAXN
MAIN SELECT WARS PLOT SOLVE UP
```

```
HP 485X EQUATION WRITER
n =  $\frac{ga}{MWT}$ 
PRESS [ENTER] TO RETURN TO LIST ...
```

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 **▶** or **◀** scrolls the screen to the left or to the right to display the entire equation. Press **ENTER** or **◀** 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:

```
Mass/Mole/Atom
→N: (MOL) MOLES
GA: (KG) MASS
MWT: (KG/MOL) MWT

MAIN EQNS VARS FIGURE SOLVE UP
```

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 **ENTER**. This displays the following screen:

```
Mass/Mole/Atom
→ N: '0_MOL'
GA: '0_KG'
MWT: '0_KG/MOL'

CALC EQNS VARS UNIT SETS UP
```

```
PRG
[ HOME GCHEMD ]
Set ga, Mass:

←
_KG _G _MG _U _LB _T
```

Enter the mass of iron at the prompt.

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

```

RAD                               PRG
┌ HOME GCHEMD ┤
│ Set ga, Mass:                    │
│                                  │
│ 1.5                              │
│ ─KG  _G  _MG  _U  _LE  _T      │
└──────────────────────────────────┘
    
```

```

RAD                               PRG
┌ HOME GCHEMD ┤
│ Set ga, Mass:                    │
│                                  │
│ 1.5_t                            │
│ ─KG  _G  _MG  _U  _LE  _T      │
└──────────────────────────────────┘
    
```

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

In this example, press **-T** 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**:

```

Mass/Mole/Atom
N: '0_MOL'
└GA: '1.5_T'
└MWT: '0_KG/MOL'
┌CALC┐┌EQNS┐┌VARS┐┌UNIT┐└STK┐└UP┐
    
```

```

Mass/Mole/Atom
→N: '0_MOL'
└GA: '1.5_T'
└MWT: '55.847_G/MOL'
┌CALC┐┌EQNS┐┌VARS┐┌UNIT┐└STK┐└UP┐
    
```

The triangular tag indicates that **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:

```

Mass/Mole/Atom
→*N: '26859.0971762_MOL'
└GA: '1.5_T'
└MWT: '55.847_G/MOL'
┌CALC┐┌EQNS┐┌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

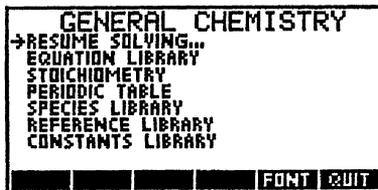
Suppose you want to convert the mass

```

Mass/Mole/Atom
→*N: '26859.0971762_MOL'
└GA: '1.5_T'
└MWT: '55.847_G/MOL'
┌KNOW┐┌WANT┐┌CLEAR┐┌PURGE┐┌CONV┐└UP┐
    
```


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:



$$gs = ga + gb$$

$$ma = \frac{na}{gb}$$

$$na = \frac{ga}{MWTa}$$

$$xa = \frac{na}{na + nb}$$

$$ga = ga \cdot \frac{gs}{100}$$

$$wa + wb = 100$$

$$gb = wb \cdot \frac{gs}{100}$$

$$nb = \frac{gb}{MWTb}$$

$$gs = vs \cdot ps$$

$$ppma = \frac{ga \cdot 1E6}{gb}$$

$$Ma = \frac{na}{vs}$$

$$gb = vb \cdot pb$$

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

To view the variables for this equation set, press **VAR_S**. 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	-
pb	pure solvent density	kg/m ³
vb	volume of solvent	m ³
gs	mass solution	kg
vs	volume solution	m ³
ps	density solution	kg/m ³
Ma	molarity solution	mol/m ³
ma	molality solution	mol/kg
xa	mole fraction solution	-
ppma	solute concentration	-

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, 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.

Concentration	
*GA:	'0.0004224_T'
*GB:	'7.61600000002E-2_KG'
*NA:	'1.17495722201_MOL'
*NB:	'4.22754118745_MOL'
*MWTa:	'36.4609_G/MOL'
*MWTb:	'18.0152_G/MOL'
*WA:	36
*WB:	64.0000000002
CALC EQNS VAR_S UNIT STK UP	

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:

Given	Result
MWta =	36.4609_g/mol (HCl)
Ma =	11.7_mol/l
MWtb =	18.0152_g/mol (H ₂ O)
wa =	36.0
vs =	100_ml
ps =	1.19_g/ml

```

Concentration
→*GA: '0.576_KG'
*GB: '1.024_KG'
*MA: '1.57808219178_MOL'
*MB: '5.67313019391_MOL'
*PMTA: '36.5_G/MOL'
*PMTB: '18.05_G/MOL'
*WA: 36
*WB: 64.0000000001
*PS: '0_KG/M^3'
*VS: '0_M^3'
*GS: '16_KG'
*VS: '100_ML'
*PS: '1.6_G/CM^3'
*MA: '1.57808219178_MOL/M^3'
*MB: '15.4109589041_MOL/KG'
*MA: 217690115882
*PMTA: 562500
VALUE ERRS VARS UNIT CALC UP
  
```

With the information given, the solver found all variables but two, **pb** and **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.

```

Concentration
VB: '0_M^3'
GS: '0_KG'
*VS: '100_ML'
*PS: '1.19_G/ML'
?MA: '0_MOL/M^3'
MA: '0_MOL/KG'
*MB: 0
→ PPMa: 0
CALC ERRS VARS UNIT ?*TE UP
  
```

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:

```

Titration (SA/SB)
→VE=CA/CEXVA
PH=-LOG(-(VB*CB-VA*CA)/(CEXVA+V...
PH=-LOG(H)
CE=GB/(M+WT*V)

MAIN SELECT VARS PLOT SOLVE UP
    
```

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

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

where

Ca	acid concentration	mol/m ³
Cb	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
pH	pH value	-

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:

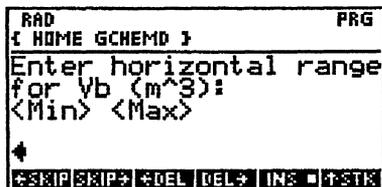
Ca = 0.1 mol/l
Cb = 0.1 mol/l
Va = 25 ml
Kw = 1.01 x 10⁻¹⁴ mol²/l²

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

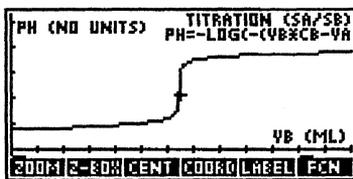
With these four variables entered, return to the equations screen by pressing **EQNS**. Move the pointer to the second equation and press **PLOT**. Since this equation is of the proper form, and all but V_b has been specified on the right hand side, it may be plotted.

Entering the X and Y Coordinates

The first prompt asks whether you want to erase the previous plot and reset the axes, **YES**, 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 **YES** 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 x_1 x_2 . Type the coordinates for the plot on the same line, separated by a space (use the **SC** 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 **ENTER** without typing in the y axis limits, the calculator autoscales the plot. Once the x and y axes limits are entered, press **ENTER**. 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 **UNIT** 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.

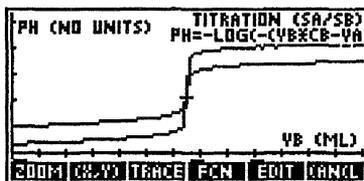
Softkeys for the Plot Function

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 **F** keys, inside the HP 48 **FCN** 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 **NXT** **NXT** and **KEYS**. Press **QWERT** 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 **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



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 equation(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 root-finder 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 **GCAP**, 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 **ENTER**. A prompt message asks you to enter the value. Press **☐/☐** to reveal the command line editing keys. Pressing **↑STK** displays the value in a limited version of the HP 48GX's interactive stack. Press **ECHO** then **ENTER**. This takes you back to the "enter value" prompt message. Press **ENTER** 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 ☐/☐ 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 libraries
USRSYMBMS	Contains user-defined chemical symbols
USRATWTS	Contains user-defined atomic weights

Summary of Softkeys

CALC	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 “*”.
CLEAR	Resets the values of the current variable set to zero.
EQNS	Enters the equation level of the current topic.
FIGURE	Displays a figure for the currently selected topic or displays “No figure”.
FONT	Toggles between small and medium display fonts of the HP 48GX.
KNOW	Toggles the currently selected variable between known and unknown, adding or removing the triangular tag.
MAIN	Returns to the main menu.
PLOT	Prompts the user for x-axis and y-axis values (with option for autoscale y). This feature only works for equations of the form $y=f(a,b, \dots)$ where y and one variable on the right are unknown.
PURGE	Purges the global copies (in the GCHEMD directory) of the current variable set displayed in the solver level.
QUIT	Exits the Chemistry Application Pac.
SELECT	Marks or unmarks the currently selected equation with the triangular tag. Only variables in the marked 7 equations will appear in the solver and variable levels. If no equations are selected, all will be used.
SOLVE	Enters the solver level of the current topic.
↑STK	Copies selected entry to calculator stack.
UNIT	Toggle key. Indicates that units are on.
UNITS	Toggle key. Indicates units are off. When off, all variables are assumed to be SI if entered with no units or are converted to SI units.
UP	Moves up one level in the software menu structure.
VARS	Enters the variable level for the current topic.
VIEW	Displays the full text entry for a variable description or value if the description is too wide to fit on the screen.
WANT	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

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 **ENTER** clears the command line, or returns you to the variables screen if the command line is already empty.

EXIT

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
- Precipitation
- Gases
- Kinetics
- Acids/Bases

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

π	π
g	Acceleration due to gravity
R	Universal gas constant
NA	Avogadro's number
c	Velocity of light
h	Planck's constant
k	Boltzmann's constant
q	Electron charge
R_{∞}	Rydberg's constant
a_0	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:

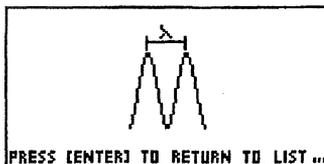
- Mass/Mole/Atom
- p, d and f Orbitals
- Light
- Diatomic Moment
- Quantum
- Symmetrical Moment
- Hydrogen Energy

Mass/Mole/Atom

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

$$\text{number of moles } n = \frac{ga}{MWT}$$

$$\text{Natoms} = NA \cdot n$$



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.

$$\lambda = \frac{c}{\gamma} \quad E = h \cdot \gamma \quad \text{nubar} = \frac{1}{\gamma}$$

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.

$$\lambda l = \frac{h}{m \cdot v}$$

$$E = m \cdot c^2$$

Variable	Description	Units
λl	de Broglie wavelength	m
m	mass	kg
v	velocity	m/s
E	energy	J
h	Plank's constant	J.s
c	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

$$m = 1.0_oz$$

$$v = 600_ft/s$$

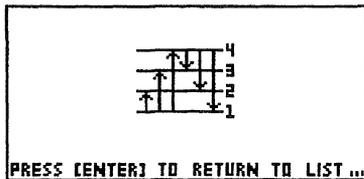
Result

$$\lambda l = 1.28 \text{ E-25_nm}$$

$$E = 2.55 \text{ E15_J}$$

Hydrogen Energy

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



$$E = \frac{-R\infty \cdot Z^2}{n^2}$$

$$\Delta E = -R\infty \cdot Z^2 \cdot \left(\frac{1}{n_l^2} - \frac{1}{n_i^2} \right)$$

$$\gamma = \frac{\Delta E}{h}$$

$$\lambda l = \frac{c}{\gamma}$$

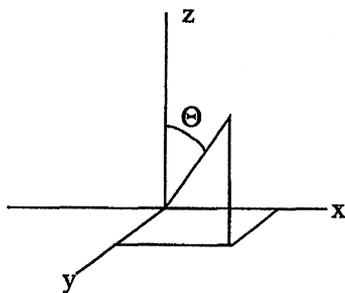
Variable	Description	Units
E	energy	J
Z	nuclear charge	-
n_i	initial quantum number	-

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

s, p, d and f Orbitals

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

$$\phi_{nlm} = R_{nl} \cdot X_{lm}$$



The normalization constant given below is provided for reference only and guarantees that the integrated probability over all space is unity.

$$\rho = \frac{2 \cdot Z \cdot r}{a_0}$$

Radial Functions:

$$(1s) \quad R_{n1} = R_{10} = Z^{\frac{3}{2}} \cdot e^{-\frac{\rho}{2}}$$

$$\text{constant} = \frac{2}{a_0^{\frac{3}{2}}}$$

$$(2s) \quad R_{20} = Z^{\frac{3}{2}} \cdot (2 - \rho) e^{-\frac{\rho}{2}}$$

$$\text{constant} = \frac{2}{a_0^{\frac{3}{2}} \cdot 2 \cdot \sqrt{2}}$$

$$(3s) \quad R_{30} = Z^{\frac{3}{2}} \cdot (6 - 6 \cdot \rho + \rho^2) \cdot e^{-\frac{\rho}{2}}$$

$$\text{constant} = \frac{2}{a_0^{\frac{3}{2}} \cdot 9 \cdot \sqrt{3}}$$

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

$$\text{constant} = \frac{2}{a o^{\frac{3}{2}} \cdot 96}$$

$$(2p) \quad R21 = Z^{\frac{3}{2}} \cdot \rho \cdot e^{-\frac{\rho}{2}}$$

$$\text{constant} = \frac{1}{a o^{\frac{3}{2}} \cdot 2 \cdot \sqrt{6}}$$

$$(3p) \quad R31 = Z^{\frac{3}{2}} \cdot (4 - \rho) \cdot \rho \cdot e^{-\frac{\rho}{2}}$$

$$\text{constant} = \frac{1}{a o^{\frac{3}{2}} \cdot 9 \cdot \sqrt{6}}$$

$$(4p) \quad R41 = Z^{\frac{3}{2}} \cdot (20 - 10 \cdot \rho + \rho^2) \cdot \rho \cdot e^{-\frac{\rho}{2}}$$

$$\text{constant} = \frac{1}{a o^{\frac{3}{2}} \cdot 32 \cdot \sqrt{15}}$$

$$(3d) \quad R32 = Z^{\frac{3}{2}} \cdot \rho^2 \cdot e^{-\frac{\rho}{2}}$$

$$\text{constant} = \frac{1}{a o^{\frac{3}{2}} \cdot 9 \cdot \sqrt{30}}$$

$$(4d) \quad R42 = Z^{\frac{3}{2}} \cdot (6 - \rho) \cdot \rho^2 \cdot e^{-\frac{\rho}{2}}$$

$$\text{constant} = \frac{1}{a o^{\frac{3}{2}} \cdot 96 \cdot \sqrt{5}}$$

$$(4f) \quad R43 = Z^{\frac{3}{2}} \cdot \rho^2 \cdot e^{-\frac{\rho}{2}}$$

$$\text{constant} = \frac{1}{a o^{\frac{3}{2}} \cdot 9 \cdot \sqrt{30}}$$

Angular Wave Functions

(s) $X_{ml} = X_{00} = \frac{1}{2} \cdot \sqrt{2}$

(p) $X_{10} = \text{COS}(\theta)$

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

(p) $X_{11} = \text{SIN}(\theta)$

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

(d) $X_{20} = 3 \cdot \text{COS}^2(\theta) - 1$

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

(d) $X_{21} = \text{SIN}(\theta) \cdot \text{COS}(\theta)$

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

(d) $X_{22} = \text{SIN}^2(\theta)$

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

(f) $X_{30} = \frac{5}{3} \cdot \text{COS}^3(\theta) - \text{COS}(\theta)$

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

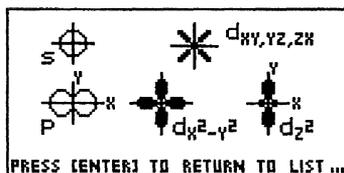
(f) $X_{31} = \text{SIN}(\theta) \cdot (5 \cdot \text{COS}^2(\theta) - 1)$

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

(f) $X_{32} = \text{SIN}^2(\theta) \cdot \text{COS}(\theta)$

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

(f) $X_{33} = \text{SIN}^3(\theta)$



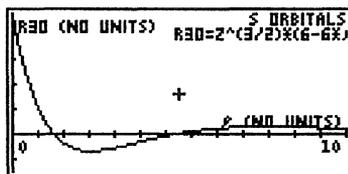
$$\text{constant} = \frac{1}{8} \cdot \sqrt{70}$$

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	°
ao	Bohr radius*	m

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

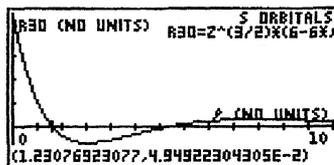
Example: At what distance from the hydrogen atom ($Z=1$) is the first node in the 3s radial function? There are two nodes in the 3s radial function.

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 = 0
x2 = 10
autoscale y

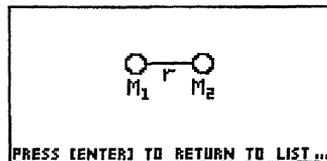


Move the cursor to the first node and press **COORD** to display the (x,y) coordinates of the node. This yields:

The first node occurs at $\rho = 1.23$. Pressing **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.



$$I = \frac{1}{NA} \cdot \frac{m1 \cdot m2}{m1 + m2} \cdot r^2$$

$$B = \frac{h}{8 \cdot \pi^2 \cdot I \cdot c}$$

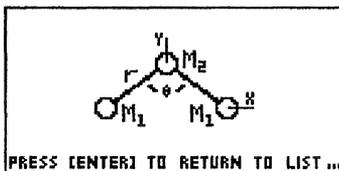
Variable	Description	Units
I	moment of inertia	kg.cm ²
m1	mass of 1	kg/mol
m2	mass of 2	kg/mol
r	internuclear distance	m
B	rotational constant	1/cm

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 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.



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

$$I_y = \left(\frac{2}{NA} \right) \cdot m_1 \cdot r^2 \cdot \text{SIN}^2 \left(\frac{\theta}{2} \right)$$

$$I_z = I_x + I_y$$

Variable	Description	Units
I_y	moment of inertia about y	kg. m ²
I_x	moment of inertia about x	kg. m ²
I_z	moment of inertia about z	kg. m ²
m_1	mass of 1	Kg/mol
m_2	mass of 2	kg/mol
r	internuclear distance	m
θ	bond angle	°

Example: What is the moment of inertia of water?

Given	Result
$r = 0.96 \text{ \AA}$	$I_x = 1.02\text{E-}40 \text{ g. m}^2$
$m_1 = 1.0079 \text{ g/mol}$	$I_y = 1.94\text{E-}40 \text{ g. m}^2$
$m_2 = 15.9994 \text{ g/mol}$	$I_z = 2.96\text{E-}40 \text{ g. m}^2$
$\theta = 104.9^\circ$	

Solids/Liquids

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

Heat Capacity
 Blackbody Radiation
 Equation of State
 Bragg Law
 Born-Haber Cycle
 Melting Point

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.

$$\text{Einstein: } C_{vE} = 3 \cdot R \cdot \left(\frac{\theta_e}{T} \right)^2 \cdot \frac{e^{-\left(\frac{\theta_e}{T}\right)}}{\left(1 - e^{-\left(\frac{\theta_e}{T}\right)} \right)^2}$$

$$\text{Debye: } C_{vD} = 9 \cdot R \cdot \left(\frac{T}{\theta_d} \right)^3 \cdot \int_0^{\frac{\theta_d}{T}} \frac{x^4 \cdot e^x}{(e^x - 1)^2} \cdot dx$$

Variable	Description	Units
C_{vE}	Einstein heat capacity	J/(mol.K)
C_{vD}	Debye heat capacity	J/(mol.K)
θ_e	Einstein characteristic temperature	K
θ_d	Debye characteristic temperature	K
T	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 $\theta = h \cdot \nu_m / k$.

Example: The Debye characteristic temperature of Pb is $\theta_d = 88\text{K}$. Estimate the heat capacity of Pb at 20K and 25°C. First enter θ_d and $T=20_K$, and solve for C_{vD} . Next enter $T=25_^\circ\text{C}$ and solve again for C_{vD} .

Given	Result
$\theta_d = 88_K$	$C_{vD} = 1.1_J/(\text{mol}\cdot\text{K}) @ 20_K$

$$T = 20_K$$

$$T = 25_°C$$

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

Blackbody Radiation

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

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

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

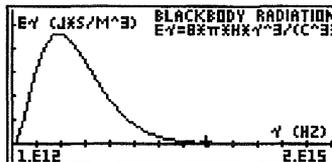
Variable	Description	Units
E_{γ}	energy density	$J \cdot s / m^3$
ET	total energy density	J / m^3
T	absolute temperature	K
γ	frequency	Hz

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

Given
T = 5000 K

Result
ET = 35439500_W/m²

To solve the second part of the problem, set T=5000 K and plot E_{γ} versus γ 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 ~8.7E12_Hz and the high frequency limit of ~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.

$$VTP = V_o \cdot (1 + \alpha_s \cdot (t_2 - 0 \text{ } ^\circ \text{C})) \cdot (1 - \rho_s \cdot (p_2 - 1 \text{ atm}))$$

Variable	Description	Units
VTP	volume at any temperature & pressure	m ³
V _o	reference volume	m ³
α _s	thermal expansion coefficient	1/K
t ₂	temperature	K
ρ _s	compressibility coefficient	1/Pa
p ₂	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?

Given

V_o = 1.000 cm³
 α_s = 1.03E-4 1/°C
 ρ_s = 2.86E-6 1/atm
 t₂ = 360 °F
 p₂ = 1800 psi

Result

VTP = 1.02 cm³

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
⊖	diffraction angle	°
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 (λd=1.44 Å) impinges on NaCl (d=5.627 Å)?

Given

d = 5.627 Å
 n = 1

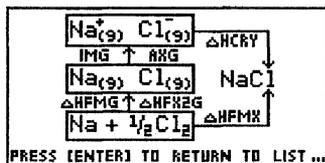
Result

⊖ = 7.35 °

$$\lambda d = 1.44 \text{ \AA}$$

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.



$$\Delta H_{lmx} = \Delta H_{cry} + \Delta H_{fmg} + \frac{1}{2} \cdot \Delta H_{fx2g} + I_{mg} + A_{xg}$$

Variable	Description	Units
ΔH_{fmx}	heat of formation of mx	J/mol
ΔH_{cry}	heat of crystallization of mx	J/mol
ΔH_{fmg}	heat of formation of gaseous m	J/mol
ΔH_{fx2g}	heat of formation of gaseous x2	J/mol
I_{mg}	ionization energy of m	J/mol
A_{xg}	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.

$$P_2 = P_1 \cdot \left(\frac{\Delta H_{fus}}{\Delta V_{fus}} \right) \cdot LN \left(\frac{T_2 m}{T_1 m} \right)$$

Variable	Description	Units
P_2	pressure	Pa
P_1	reference pressure	Pa
ΔH_{fus}	heat of fusion	J/mol
ΔV_{fus}	volume change upon fusion	m ³ /mol
$T_1 m$	reference melting point	K
$T_2 m$	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.

$$gs = gs + gb$$

$$na = \frac{ga}{MWTa}$$

$$ga = wa \cdot \frac{gs}{100}$$

$$gb = wb \cdot \frac{gs}{100}$$

$$gs = vs \cdot \rho_s$$

$$Ma = \frac{na}{vs}$$

$$ma = \frac{na}{gb}$$

$$xa = \frac{na}{na + nb}$$

$$wa + wb = 100$$

$$nb = \frac{gb}{MWTb}$$

$$ppma = \frac{ga \cdot 1E6}{gb}$$

$$gb = vb \cdot \rho_b$$

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	-
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
Ma	molarity solution	mol/m ³
ma	molality solution	mol/kg
xa	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

$g_b = 1000_g$
 $MWT_a = 79.904_g/mol$
 $ppma = 4600$

Result

$ma = 5.8E-2_mol/kg$

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.

Given

$g_a = 5.0_g$
 $g_b = 225.0_g$
 $MWT_a = 92.1402_g/mol$
 $\rho_s = 0.876_g/ml$
 $MWT_b = 78.1134_g/mol$

Result

$Ma = 0.206_mol/l$
 $xa = .0185$
 $wa = 2.17$

Other variables solved for are:

$na = 0.054_mol$
 $nb = 2.88_mol$
 $wb = 97.8$
 $ppma = 22222.2$
 $gs = 0.23_kg$
 $vs = 0.263_l$
 $ma = 0.24_mol/kg$

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.

$$P = x_b \cdot P_{in}$$

$$\Delta P = -x_a \cdot P_{in}$$

$$\Delta P = P - P_{in}$$

$$na = \frac{nb}{MWT_a}$$

$$nb = \frac{gb}{MWT_b}$$

$$xa = \frac{na}{na + nb}$$

$$xb = \frac{nb}{na + nb}$$

$$xa = 1 - xb$$

Variable	Description	Units
P	solvent partial pressure	1_Pa
x_b	solvent mole fraction	1
P_{in}	solvent initial pressure (pure)	1_Pa
ΔP	pressure difference	1_Pa

xa	solute mole fraction	1
na	moles of solute	1_mol
ga	mass of solute	1_kg
MW _{Ta}	molecular weight of solute	1_kg/mol
MW _{Tb}	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 (C₁₂H₂₂O₁₁) 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
MW _{Ta} = 342.2992_g/mol	xa = 5.24 x 10 ⁻³
MW _{Tb} = 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.

$$\Delta T_b = K_b \cdot m_a \qquad m_a = \frac{na}{gb}$$

$$nb = \frac{ga}{MW_{Ta}} \qquad \Delta T_f = -K_f \cdot m_a$$

Variable	Description	Units
ΔT _b	boiling point elevation	1_K
K _b	ebullioscopic constant	1_K·kg/mol
m _a	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
MW _{Ta}	molecular weight of solute	1_kg/mol
ΔT _f	freezing point depression	1_K
K _f	cryoscopic constant	1_K·kg/mol

Note that once calculated, the values of ΔT_b and ΔT_f may not be converted into other temperature values. When entering a value for ΔT_f , it must 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
$K_b = 0.52 \text{ K}\cdot\text{kg/mol}$	$\Delta T_b = 0.932 \text{ }^\circ\text{C}$
$g_b = 900 \text{ g}$	$m_a = 1.79 \text{ mol/kg}$
$g_a = 100 \text{ g}$	$n_a = 1.61 \text{ mol}$
$MW_{Ta} = 62 \text{ g/mol}$	$\Delta T_f = -3.33 \text{ }^\circ\text{C}$
$K_f = 1.86 \text{ K}\cdot\text{kg/mol}$	

Molarity/Dilution

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

$$M_i = \frac{na}{V}$$

$$na = \frac{ga}{MW_{Ta}}$$

$$V_f \cdot M_f = V_i \cdot M_i$$

Variable	Description	Units
M_i	initial concentration, Molarity	1 mol/m^3
na	moles of solute	1 mol
V_i	initial volume	1 m^3
ga	mass of solute	1 kg
MW_{Ta}	molecular weight of solute	1 kg/mol
V_f	final volume	1 m^3
M_f	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
$ga = 4.5060 \text{ g}$	$M_i = 0.4506 \text{ mol/l}$
$MW_{Ta} = 39.99707 \text{ g/mol}$	$M_f = 9.013 \times 10^{-3} \text{ mol/l}$
$V = 250.00 \text{ ml}$	$na = 0.1127 \text{ mol}$
$V_i = 10.00 \text{ ml}$	

$$V_f = 500_ml$$

Clausius Clapyron

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

$$LN\left(\frac{P}{P_o}\right) = \frac{RH_v}{V} \cdot \left(\frac{1}{T_o} - \frac{1}{T}\right)$$

Variable	Description	Units
P	vapor pressure	1_Pa
ΔH_v	heat of vaporization	1_J/mol
T_o	reference temperature	1_K
T	temperature	1_K
P_o	reference vapor pressure	1_Pa

Example: The vapor pressure of white phosphorus has the values: P at (76.6_°C)=1.0_mmHg, P at (197.3_°C)=100.0_mmHg. Calculate the heat of vaporization of liquid phosphorus.

Given

$$P_o = 1.0_mmHg$$

$$T_o = 76.6_°C$$

$$P = 100.0_mmHg$$

$$T = 197.3_°C$$

Result

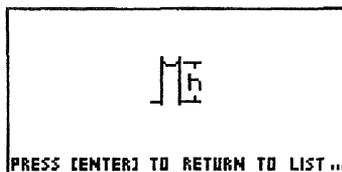
$$\Delta H_v = 12.47 \text{ kcal/mol}$$

Capillary Rise

These equations describe the capillary rise phenomenon observed with fluids. The first equation is an approximate equation, assuming no interaction between the capillary surface and the liquid ($\theta=0_°$), and no edge effects. The second equation includes these contributions.

$$h = \frac{2 \cdot \gamma}{\rho_l \cdot g \cdot r}$$

$$hex = \frac{2 \cdot \gamma \cdot \cos(\theta)}{(\rho_l - \rho_v) \cdot g \cdot r} - \frac{r}{3}$$



Variable	Description	Units
h	capillary rise	1_m

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

Example: A capillary ($r=0.100\text{ mm}$) is inserted into a fluid ($\gamma_l= 46.0\text{ dyn/cm}$) 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

$\gamma_l = 46.0\text{ dyn/cm}$
 $\rho_l = 1.06\text{ g/cm}^3$
 $r = 0.10\text{ mm}$
 $\theta = 76^\circ$
 $\rho_v = 1.0\text{ g/l}$

Result

$h = 88.5\text{ mm}$
 $hex = 21.4\text{ mm}$

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.

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

Variable	Description	Units
P	pressure	1_Pa
n	moles of gas	1_mol
T	temperature	1_K

V	volume	l_m^3
mg	mass of gas	l_kg
MWT	molecular weight	l_kg/mol
ρ	density	l_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_mmHg	n = 3.62 x 10 ⁻² _mol
V = 933_ml	ρ = 3.09 x 10 ⁻² _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)

$$\frac{P1 \cdot V1}{n1 \cdot T1} = \frac{P2 \cdot V2}{n2 \cdot T2}$$

$$\frac{P1 \cdot V1}{T1} = \frac{P2 \cdot V2}{T2} \quad (n, \text{ constant})$$

$$P1 \cdot V1 = P2 \cdot V2 \quad (n, T \text{ constant})$$

$$\frac{P1}{T1} = \frac{P2}{T2} \quad (n, V \text{ constant})$$

$$\frac{V1}{T1} = \frac{V2}{T2} \quad (P, n \text{ constant})$$

$$P1 \cdot V1 = n1 \cdot R \cdot T1$$

$$P2 \cdot V2 = n2 \cdot R \cdot T2$$

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?

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

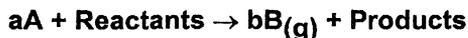
T2 = 25_°C

Result

P2 = 1.21_mmHg

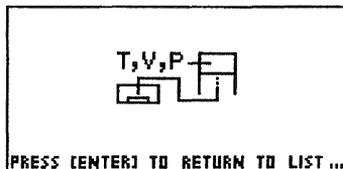
Gas Over Water

Consider the general chemical reaction:



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, P_w, 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



gb	mass b	1_kg
MWTb	molecular weight b	1_kg/mol
ga	mass a	1_kg
MWTa	molecular weight a	1_kg/mol
Pb	collected gas volume	1_m^3
T	temperature	1_K
nt	total moles collected	1_mol
nw	moles of water collected	1_mol
Pt	total pressure	1_Pa
Pw	water partial pressure	1_Pa

Example: Consider the decomposition of CaCO_3 according to the reaction:



When 4.6_g of CaCO_3 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

$$\begin{aligned} a &= b = 1 \\ \text{MWTb} &= 44.0098 \text{ _g/mol } (\text{CO}_2) \\ \text{MWTa} &= 100.0892 \text{ _g/mol } (\text{CaCO}_3) \\ ga &= 4.6 \text{ _g} \\ T &= 26 \text{ _°C} \\ Pt &= 1.0 \text{ _atm} \\ Pw &= 25.00 \text{ _torr} \end{aligned}$$

Result

$$\begin{aligned} V &= 1.17 \text{ _l} \\ nb &= 4.60 \times 10^{-2} \text{ _mol} \\ gb &= 2.02 \times 10^{-3} \text{ _kg} \\ Pb &= 0.967 \text{ _atm} \\ na &= 4.60 \times 10^{-2} \text{ _mol} \\ nt &= 4.75 \times 10^{-2} \text{ _mol} \\ nw &= 1.56 \times 10^{-3} \text{ _mol} \end{aligned}$$

Barometric Equation

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

$$P = P_o \cdot \text{EXP} \left(\frac{-MWT \cdot g \cdot h}{R \cdot T} \right)$$

$$C_o = \frac{P_o}{R \cdot T} \qquad C = \frac{P}{R \cdot T}$$

Variable	Description	Units
P	pressure at height, h	1_Pa

Po	reference pressure	1_Pa
MWT	molecular weight of gas	1_kg/mol
h	height above sea level	1_m
T	temperature	1_K
Co	reference concentration	1_mol/m^3
C	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_°F).

Given

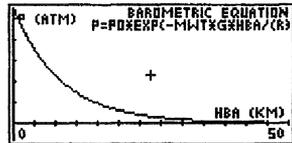
Po = 1.0_atm
MWT = 29_g/mol
h = 1_km
T = 75_°F

Result

P = 0.89_atm
Co = 4.1 E-2_mol/l
C = 3.6 E-2_mol/l

Plotting the barometric equation yields:

x1 = 0_km autoscale y
x2 = 50_km



Van der Waal Gases

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

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

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

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

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

$$Tc = \frac{8 \cdot a}{27 \cdot b \cdot R}$$

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

Variable	Description	Units
p	pressure of gas	1_Pa
n	moles of gas	1_mol
V	volume of gas	1_m^3
T	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)	
Z	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

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

Given	Result
T = 300_°C	p = 139.9_atm
V = 100_l	n = 285.7_mol
b = 0.03913_l/mol	Z = 1.04
a = 1.390_l^2_atm/mol^2	Tc = 128.3_K
ga = 8000_g	Vc = 33.54_l
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
T	absolute temperature	1 K
C	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

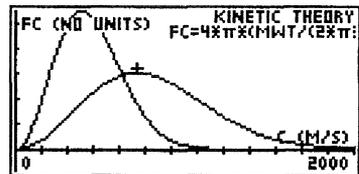
Example: What is the average velocity of an oxygen molecule at 300_K?
Use equation 3.

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 = 0
x2 = 2000
y1 = 6.0 E-4
y2 = 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.

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

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

r2

rate of effusion of gas 2 $1 \text{ m}^3/\text{s}$ **Example:** What is the enrichment factor of nitrogen compared to oxygen?**Given**

$$\text{MWT}_2 = 28.0134 \text{ g/mol}$$

$$\text{MWT}_1 = 31.9988 \text{ g/mol}$$

Result

$$f = 0.9357$$

Collision Theory

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

$$c_{avg} = \sqrt{\left(\frac{8 \cdot R \cdot T}{\pi \cdot \text{MWT}}\right)}$$

$$n = \frac{NA \cdot P}{R \cdot T}$$

$$Z = \frac{1}{4 \cdot NA} \cdot n \cdot c_{avg}$$

$$Z_1 = \frac{2 \cdot d \cdot \sqrt{\left(\frac{\pi \cdot R \cdot T}{\text{MWT}}\right)} \cdot n^2}{NA}$$

$$\lambda_{mfp} = \frac{1}{\sqrt{2} \cdot \pi \cdot d^2 \cdot n}$$

$$D = \frac{1}{2} \cdot c_{avg} \cdot \lambda_{mfp}$$

$$\rho = \frac{\text{MWT} \cdot p}{R \cdot T}$$

$$\eta = \frac{1}{2} \cdot \rho \cdot c_{avg} \cdot \lambda_{mfp}$$

$$n = \frac{\rho \cdot NA}{\text{MWT}}$$

Variable	Description	Units
cavg	average velocity	1 m/s
T	absolute temperature	1 K
MWT	molecular weight	1 kg/mol
n	particle density	1 1/m^3
P	pressure	1 Pa
Z	surface collision frequency	$1 \text{ mol}/(\text{m}^2 \cdot \text{s})$
Z1	bimolecular collision frequency	$1 \text{ mol}/(\text{m}^3 \cdot \text{s})$

d	collision diameter	1_m
λ_{mfp}	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·s)

Example: Calculate the surface collision frequency, bimolecular collision frequency, mean free path, and viscosity coefficient of O₂ (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_mol/(cm^2·s)
d = 3.61_Å	Z1 = 1.29 E5_mol/(cm^3·s)
	$\lambda_{\text{mfp}} = 701_Å$
	D = 0.156_cm^2/s
	$\rho = 1.31 E-3_g/cm^3$
	$\eta = 2.04 E-4_g(cm·s)$

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, pK_b, pK_a and pK_w 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.

$$pH = -\text{LOG}(H)$$

$$pOH = -\text{LOG}(OH)$$

$$pK_w = -\text{LOG}(K_w)$$

$$pK_a = -\text{LOG}(K_a)$$

$$pK_b = -\text{LOG}(K_b)$$

$$K_w = K_a \cdot K_b$$

$$K_w = H \cdot OH$$

Variable	Description	Units
H	hydrogen ion concentration	1_mol/m^3
OH	hydroxide ion concentration	1_mol/m^3
K _w	water dissociation constant	1_mol^2/m^6
K _a	acid dissociation constant	1_mol/m^3
K _b	base dissociation constant	1_mol/m^3
pH	pH function	1
pOH	pOH function	1
pK _w	pK _w function	1
pK _a	pK _a function	1
pK _b	pK _b function	1

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

Given

$$H = 0.01_mol/l$$

$$K_w = 1.01 \text{ E-}14_mol^2/l^2$$

$$pOH = 12.0$$

$$pK_w = 14.0$$

Result

$$pH = 2$$

$$OH = 1.01 \times 10^{-12}_mol/l$$

Strong Acids

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

$$H = n \cdot \frac{ga}{MWT_a \cdot V} \quad pH = -\text{LOG}(H)$$

Variable	Description	Units
H	hydrogen ion concentration	1_mol/m^3
ga	mass of acid	1_kg
MWT _a	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

ga = 0.50_g
 V = 100_ml
 MWTa = 98.0734_g/mol
 n = 2

Result

H = 0.101_mol/l
 pH = 0.991

Strong Bases

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

$$OH = n \cdot \frac{gb}{MWT \cdot V}$$

$$H = \frac{Kw}{OH}$$

$$pH = -LOG(H)$$

Variable	Description	Units
OH	hydroxide ion concentration	1_mol/m^3
H	hydrogen ion concentration	1_mol/m^3
gb	mass of base	1_kg
MWTb	molecular weight of base	1_kg/mol
V	volume of solution	1_m^3
pH	pH function	1
Kw	water dissociation constant	1_mol^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

gb = 4.5617_g
 MWTb = 39.99707_g/mol
 V = 500_ml
 Kw = 1.01 X 1E-14_mol^2/l^2
 n = 1

Result

pH = 13.35
 H = 4.43 x 1E-14_mol/l
 OH = 0.228_mol/l

Weak Acids/Bases

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

$$H^3 + K_a \cdot H^2 - (C_a \cdot K_a + K_w) \cdot H - K_a \cdot K_w = 0$$

$$OH^3 + K_b \cdot OH^2 - (C_b \cdot K_b + K_w) \cdot OH - K_b \cdot K_w = 0$$

$$K_w = H \cdot OH \quad pH = -\text{LOG}(H)$$

$$C_a = \frac{g_a}{MWT \cdot V} \quad C_b = \frac{g_b}{MWT \cdot V}$$

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
H	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	1_l

Example: 0.3862 grams of iodic acid, HIO₃ (K_a = 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 x 10E-3_mol/l
Ka = 0.162_mol/l	H = 2.17 x 10E-3_mol/l
V = 1.0_l	pH = 2.66
MWT = 175.9106_g/mol	
Kw = 1.01 X 10-14_mol^2/l^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.

$$Ca = \frac{ga}{MWTa \cdot V} \quad Ccb = \frac{gb}{MWTb \cdot V}$$

$$pKa = -\text{LOG}(Ka) \quad pH = pKa - \text{LOG}\left(\frac{Ca}{Ccb}\right)$$

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_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

gb = 0.45_g
 MWTb = 110.04467_g/mol
 V = 100_ml
 Ca = 0.01_mol/l
 Ka = 1.78 x 1E-5_mol/l

Result

pKa = 4.75
 Ccb = 4.09 x 1E-2_mol/l
 pH = 5.36

Note that the Henderson-Hasselbach equation is valid when the acid to base concentration is 10 << acid/base << 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.

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

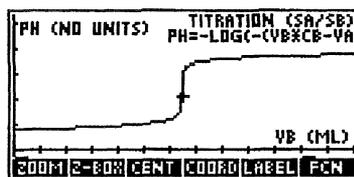
$$pH = -\text{LOG}\left(\frac{-(Vb \cdot Cb - Va \cdot Ca)}{2(Va + Vb)} + \frac{1}{2} \cdot \left(\left(\frac{Vb \cdot Cb - Va \cdot Ca}{Va + Vb}\right)^2 + 4 \cdot Kw\right)^{\frac{1}{2}}\right)$$

$$pH = -\text{LOG}(H)$$

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

Variable	Description	Units
Ca	acid concentration	1_mol/m^3
Cb	base (titrant) concentration	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	water dissociation constant	1_mol^2/m^6
H	hydrogen ion concentration	1_mol/m^3
pH	pH value	1
gb	mass of base primary standard	1_Kg
MWT	molecular weight of base	1_kg/mol
V	primary standard volume	1_m^3

Example: A primary standard solution was made by adding 0.3986_g of NaOH (MWT = 39.99707_g/mol) to 1.000_l 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

$gb = 0.3986_g$
 $MWT = 39.99707_g/mol$
 $V = 1.000_l$
 $Kw = 1.01 \times 1E-14_mol^2/l^2$
 $Ve = 49.68_ml$
 $Va = 100_ml$

Result

$Ca = 4.951 \times E-3_mol/l$
 $Cb = 9.966 \times 1E-3_mol/l$

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):

$x1 = 0_ml$
 $y1 = -3$

$x2 = 100_ml$
 $y2 = 16$

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

acid.

$$V_e = \frac{C_b}{C_a} \cdot V_b$$

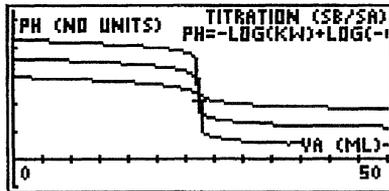
$$pH = -\text{LOG}(K_w) + \text{LOG} \left(\frac{-(V_a \cdot C_a - V_b \cdot C_b)}{2 \cdot (V_a + V_b)} + \frac{1}{2} \cdot \left(\frac{V_a \cdot C_a - V_b \cdot C_b}{V_a + V_b} \right) \right)$$

$$pH = -\text{LOG}(H)$$

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

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
pH	pH value	1
ga	mass primary standard	1_kg
MWT	molecular weight	1_kg/mol
V	primary standard volume	1_m^3

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.

$$H^3 + \left(\frac{C_b \cdot V_b}{V_a + V_b} + K_a \right) \cdot H^2 - \left(\frac{C_a \cdot V_a - C_b \cdot V_b}{V_a + V_b} \cdot K_a + K_w \right) \cdot H - K_w = 0$$

$$V_b = V_a \cdot \frac{\frac{C_a \cdot K_a}{K_a + H} - H + \frac{K_w}{H}}{C_b + H - \frac{K_w}{H}}$$

$$pH = -\text{LOG}(H)$$

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
H	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 = 2.67x1E-5_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_ml	H = 1.78x1E-5_mol/l
Vb = 10.0_ml	pH = 4.75
	15.0_ml
	H = 1.19x1E-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.

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

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

$$Kw = H \cdot OH \quad pH = -\text{LOG}(H)$$

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
Cb	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
H	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 ($Kb=1.80 \times 1E-5$ _mol/l). What is the pH?

Given

Ca = 0.100_mol/l
 Cb = 0.100_mol/l
 Kb = 1.80 x 1E-5_mol/l
 Kw = 1.01 1E-14_mol^2/l^2
 Va = 10.0_ml

Result

H = 2.81 x 1E-10_mol/l
 OH = 3.59 x 1E-5_mol/l
 pH = 9.55

$$V_b = 30.0 \text{ ml}$$

Thermo/Electrochemistry

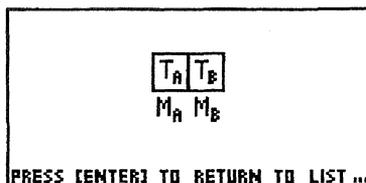
Seven topics in this category focus on thermal and thermodynamic properties, and electrochemical reactions.

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.



$$q_a = m_a \cdot c_{pa} \cdot (T_f - T_a)$$

$$q_b = m_b \cdot c_{pb} \cdot (T_f - T_b)$$

$$q_a = -q_b$$

$$T_f = \frac{m_b \cdot c_{pb} \cdot T_b + m_a \cdot c_{pa} \cdot T_a}{m_a \cdot c_{pa} + m_b \cdot c_{pb}}$$

$$c_{pa} = \frac{C_{pa}}{MWT_a}$$

$$c_{pb} = \frac{C_{pb}}{MWT_b}$$

Variable	Description	Units
q _a	heat flow in or out of material a	1_J
q _b	heat flow in or out of material b	1_J
m _a	mass of a	1_kg
m _b	mass of b	1_kg
c _{pa}	specific heat of a	1_J/(kg·K)
c _{pb}	specific heat of b	1_J/(kg·K)
C _{pa}	molar heat capacity of a	1_J/(mol·K)
C _{pb}	molar heat capacity of b	1_J/(mol·K)
T _f	final temperature	1_K
T _a	temperature of a	1_K
T _b	temperature of b	1_K
MWT _a	molecular weight of a	1_kg/mol

MWTb

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

$$c_{pa} \text{ (copper)} = 0.385 \text{ _J/(g}\cdot\text{K)}$$

$$m_a = 20 \text{ _g}$$

$$T_a = 90 \text{ _}^\circ\text{C}$$

$$c_{pb} \text{ (water)} = 4.184 \text{ _J/(g}\cdot\text{K)}$$

$$m_b = 100 \text{ _g}$$

$$T_b = 25 \text{ _}^\circ\text{C}$$

Result

$$q_a = -491 \text{ _J}$$

$$q_b = 491 \text{ _J}$$

$$T_f = 26 \text{ _}^\circ\text{C}$$

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

Heat Engines

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

$$\eta = 1 - \frac{T_c}{T_h}$$

$$C_{op} = \frac{T_c}{T_h - T_c}$$

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

$$T_h = 459 \text{ _}^\circ\text{F}$$

$$T_c = 25 \text{ _}^\circ\text{C}$$

Result

$$\eta = 0.42$$

$$C_{op} = 1.4$$

Free Energy

The following equations define free energy.

$$\Delta G = \Delta H - T \cdot \Delta S$$

$$\Delta G = -R \cdot T \cdot \text{LN}(K_{eq})$$

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

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

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

Variable	Description	Units
C _p	heat capacity	1_J/(mol·K)
ΔH	enthalpy at T	1_J/mol
ΔS	entropy at T	1_J/(mol·K)
A	empirical constant	1_J/(mol·K)
B	empirical constant	1_J/(mol·K ²)
C	empirical constant	1_J/(mol·K ³)
D	empirical constant	1_J·K/mol
T	absolute temperature	1_K
H ₂₉₈	enthalpy at 298_K	1_J/mol
S ₂₉₈	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:

Given

A = 26.12_cal/(mol·K)

B = 4.388 x 1E-3_cal/(mol·K²)

C = 0

D = -7.269 x 1E5_cal·K/mol

T = 600_K

H₂₉₈ = 10.422_kcal/mol

S₂₉₈ = 142.03_cal/(mol·K)

Results

C_p = 26.73_cal/(mol·K)

ΔH = 7.251_kcal/mol

ΔS = 28.43_cal/(mol·K)

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.

$$\Delta C = \frac{\alpha^2 \cdot V \cdot T}{\epsilon}$$

$$\Delta C = C_p - C_v$$

Variable	Description	Units
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ΔC	heat capacity difference	$1 \text{ J}/(\text{mol}\cdot\text{K})$
α	expansion coefficient	$1 \text{ } / \text{K}$
V	molar volume	$1 \text{ m}^3/\text{mol}$
T	temperature	1 K
ϵ	compressibility coefficient	$1 \text{ } / \text{Pa}$
C_p	heat capacity (constant pressure)	$1 \text{ J}/(\text{mol}\cdot\text{K})$
C_v	heat capacity (constant volume)	$1 \text{ J}/(\text{mol}\cdot\text{K})$

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

Given

$$\alpha = 2.07 \times 10^{-4} \text{ } / \text{K}$$

$$V = 18.087 \text{ cm}^3/\text{mol}$$

$$T = 25 \text{ }^\circ\text{C}$$

$$\epsilon = 45.3 \times 10^{-6} \text{ } / \text{atm}$$

Result

$$\Delta C = .517 \times 10^{-3} \text{ J}/(\text{mol}\cdot\text{K})$$

Nernst Law

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

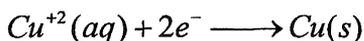
$$E = E_o - 2.303 \cdot \frac{R \cdot T}{n \cdot F} \cdot \text{LOG}(Q) \quad Q = \frac{(C)^c \cdot (D)^d}{(A)^a \cdot (B)^b}$$

$$E_o = 2.303 \cdot \frac{R \cdot T}{n \cdot F} \cdot \text{LOG}(K) \quad \Delta G = -n \cdot F \cdot E$$

$$\Delta G_o = -n \cdot F \cdot E_o$$

Variable	Description	Units
E	cell potential	1 V
E_o	standard cell potential	1 V
T	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	$1 \text{ mol}/\text{m}^3$
ΔG	free energy change	$1 \text{ J}/\text{mol}$
ΔG_o	standard free energy change	$1 \text{ J}/\text{mol}$
K	equilibrium constant	1

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



Given

$E_0 = 0.34 \text{ V}$
 $T = 49 \text{ } ^\circ\text{C}$
 $n = 2$
 $A = 5$
 $a = 1$
 $B = C = D = 1$
 $b = c = d = 0$

Result

$E = 0.36 \text{ V}$
 $Q = 0.2$
 $\Delta G = -16.7 \text{ kcal/mol}$
 $\Delta G_0 = -15.7 \text{ kcal/mol}$
 $K = 4.3 \times 10^1$

Reduction

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



$$Q = A \cdot t$$

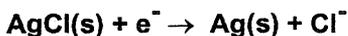
$$ne = \frac{Q}{F}$$

$$na = \left(\frac{a}{n}\right) \cdot ne$$

$$ma = MWTa \cdot na$$

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
a	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



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

Given

t = 4.5_h
 A = 50.0_mA
 a = n = 1
 MWTa = 107.87_g/mol

Result

Q = 810_C
 ne = 8.40 x 1E-3_mol
 na = 8.40 x 1E-3_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.

$K_{sp} = fa \cdot fb \cdot s^2$ AB

$K_{sp} = 4 \cdot fa^2 \cdot fb \cdot s^3$ A2B

$K_{sp} = 4 \cdot fa \cdot fb^2 \cdot s^3$ AB2

$K_{sp} = 27 \cdot fa^3 \cdot fb \cdot s^4$ A3B

$K_{sp} = 27 \cdot fa \cdot fb^3 \cdot s^4$ AB3

$K_{sp} = 108 \cdot fa^2 \cdot fb^3 \cdot s^5$ A2B3

$K_{sp} = 108 \cdot fa^3 \cdot fb^2 \cdot s^5$ 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 K_{sp} depend on the stoichiometric ratios within the dissolving species.

**Activity coefficients are equal to 1 if ideal.

Example: What is the solubility of $\text{BiI}_3(\text{s})$ (AB_3 , $K_{sp}=8.1 \times 10^{-19}$ in a solution such that, at equilibrium, $f_{\text{Bi}^{+3}}=0.110$ and $f_{\text{I}^-}=0.200$. How many grams of BiI_3 are dissolved in 100 ml at equilibrium? Compare your results assuming ideality and non-ideality.

Case 1: Non-Ideal

Given

$$fb = 0.200$$

$$fa = 0.110$$

$$K_{sp} = 8.1 \times 10^{-19} \text{ mol}^4/\text{l}^4$$

$$V = 100 \text{ ml}$$

$$MWT = 589.6939 \text{ g/mol}$$

Result

$$s = 7.6 \times 10^{-5} \text{ mol/l}$$

$$ga = 4.5 \text{ mg}$$

Case 2: Ideal

Given

$$fb = 1$$

$$fa = 1$$

$$K_{sp} = 8.14 \times 10^{-19} \text{ mol}^4/\text{l}^4$$

$$V = 100 \text{ ml}$$

$$MWT = 589.6939 \text{ g/mol}$$

Result

$$s = 1.3 \times 10^{-5} \text{ mol/l}$$

$$ga = 0.776 \text{ mg}$$

Kinetics

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

Arrhenius 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.

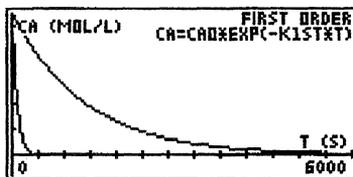
$$\text{Rate} = k_{1st} \cdot C_a$$

$$C_a = C_{a0} \cdot e^{-k_{1st} \cdot t}$$

$$t_{half} = \frac{\text{LN}(2)}{k_{1st}}$$

Variable	Description	Units
Rate	rate of reaction	1_mol/(m^3·s)
k1st	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

Ca = 1.0_mol/l (assumed)
 Cao = 0.01_mol/l (assumed)
 thalf = 15_min

Result

k1st = 7.7 x 1E-4_1/s
 t = 5979_s
 Rate = 7.7 x 1E-6_mol/(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
 autoscale y

x2 = 6000_s

Given

thalf = 1.0_min

Result

k1st = 1.16 x 1E-2_1/s

$$C_{A0} = 1.0 \text{ mol/l}$$

$$C_A = 0.01 \text{ mol/l}$$

$$t = 398 \text{ s}$$

Parallel First Order

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

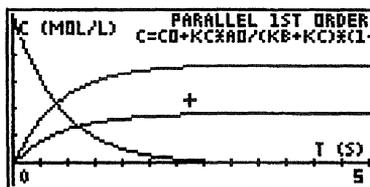
$$A = A_0 \cdot e^{-(k_b+k_c)t}$$

$$B = B_0 + \frac{k_b \cdot A_0}{k_b + k_c} \left(1 - e^{-(k_b+k_c)t}\right)$$

$$C = C_0 + \frac{k_c \cdot A_0}{k_b + k_c} \left(1 - e^{-(k_b+k_c)t}\right)$$

Variable	Description	Units
B	concentration B (t)	1 mol/m ³
B ₀	concentration B (t=0)	1 mol/m ³
k _b	rate constant for reaction B	1/s
A ₀	concentration A (t=0)	1 mol/m ³
k _c	rate constant for reaction C	1/s
t	time	s
C	concentration C (t)	1 mol/m ³
C ₀	concentration C (t=0)	1 mol/m ³
A	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

$$B_0 = 0 \text{ mol/l}$$

$$k_b = 1.0 \text{ 1/s}$$

$$A_0 = 1.0 \text{ mol/l}$$

$$k_c = 0.5 \text{ 1/s}$$

$$C_0 = 0 \text{ mol/l}$$

and

$$x_1 = 0$$

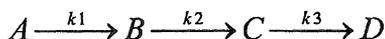
$$y_1 = -0.1363$$

$$x_2 = 5 \text{ s}$$

$$y_2 = 1.0$$

First Order Consecutive

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



These four equations describe the kinetics of such a system.

$$A = A_0 \cdot e^{-k_1 t}$$

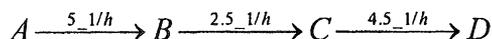
$$B = B_0 \cdot e^{-k_2 t} + \frac{k_1 \cdot A_0}{k_2 - k_1} \cdot (e^{-k_1 t} - e^{-k_2 t})$$

$$C = C_0 \cdot e^{-k_3 t} + B_0 \cdot \left(\frac{k_2 \cdot e^{-k_2 t}}{k_3 - k_2} - \frac{k_2 \cdot e^{-k_3 t}}{k_3 - k_2} \right)$$

$$+ A_0 \cdot \left(\frac{k_1 \cdot k_2 \cdot e^{-k_1 t}}{(k_3 - k_1) \cdot (k_2 - k_1)} - \frac{k_1 \cdot k_2 \cdot e^{-k_2 t}}{(k_3 - k_2)(k_2 - k_1)} + \frac{k_1 \cdot k_2 \cdot e^{-k_3 t}}{(k_3 - k_2)(k_3 - k_1)} \right)$$

Variable	Description	Units
A	concentration A (t)	1_mol/m ³
A ₀	concentration A (t=0)	1_mol/m ³
B	concentration B (t)	1_mol/m ³
B ₀	concentration B (t=0)	1_mol/m ³
C	concentration C (t)	1_mol/m ³
C ₀	concentration C (t=0)	1_mol/m ³
k ₁	rate constant for A → B	1_1/s
k ₂	rate constant for B → C	1_1/s
k ₃	rate constant for C → 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:



where A(t=0) = 1.0_mol/l and B₀=C₀=0_mol/l. Plot the concentration

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

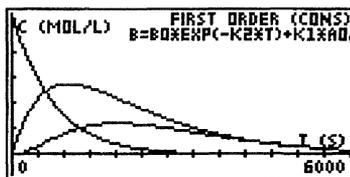
$$x1 = 0_s \quad x2 = 6000_s$$

$$y1 = -0.1363 \quad y2 = 1$$

$$A \text{ (maximum)} = 0.00_s$$

$$B \text{ (maximum)} = 0.50_mol/l, \\ \sim 969_s$$

$$C \text{ (maximum)} = 0.22_mol/l, \sim 1800_s$$



Second Order (I)

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

$$\text{Rate} = k_{2nd} \cdot Ca^2$$

$$Ca = \frac{Cao}{(1 + a \cdot k_{2nd} \cdot t \cdot Cao)}$$

$$t_{half} = \frac{1}{a \cdot Cao \cdot k_{2nd}}$$

Variable	Description	Units
Rate	rate of reaction	1_mol/(m ³ ·s)
k _{2nd}	rate constant	1_m ³ /(mol·s)
Ca	concentration A (t)	1_mol/m ³
Cao	concentration A (t=0)	1_mol/m ³
a	stoichiometric coefficient	1
t	time	1_s
t _{half}	half life	1_s

Example: The thermal decomposition of HI ($2HI \rightarrow H_2 + I_2$) 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

$$Cao = 0.10_mol/l$$

$$Ca = 0.08_mol/l$$

$$t = 10.0_min$$

Result

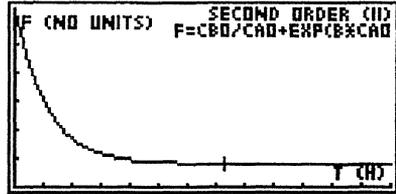
$$k_{2nd} = 2.08 \times 1E-3_l/(mol \cdot s)$$

$$t_{half} = 40_min$$

$$a = 2$$

Second Order (II)

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



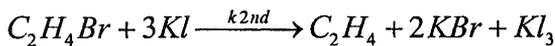
$$\text{Rate} = k_{2nd} \cdot C_a \cdot C_b$$

$$f = \left(\frac{C_{bo}}{C_{ao}} \right) \cdot \exp((a \cdot C_{bo} - b \cdot C_{ao}) \cdot k_{2nd} \cdot t)$$

$$f = \frac{CB}{CA}$$

Variable	Description	Units
Rate	rate of reaction	1_mol/(m ³ ·s)
k _{2nd}	rate constant	1_m ³ /(mol·s)
C _a	concentration A (t)	1_mol/m ³
C _b	concentration B (t)	1_mol/m ³
f	reactant ratio	1
C _{ao}	concentration A (t=0)	1_mol/m ³
C _{bo}	concentration B (t=0)	1_mol/m ³
a	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:



At 59.72 °C, k_{2nd} is reported to be 5.0 × 10⁻³ 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 h.

Given

$$C_{ao} = 0.02864 \text{ mol/l}$$

Result

$$f(0.1 \text{ h}) = 6.03$$

$C_{bo} = 0.1531 \text{ mol/l}$
 $k_{2nd} = 5.0 \times 10^{-3} \text{ l/(mol}\cdot\text{s)}$
 $a = 1$
 $b = 3$
 $t = 0.5 \text{ h}$
 $x_1 = 0$
 $x_2 = 10$
 $y = \text{autoscale}$

$f(0.5 \text{ h}) = 9.78$
 $f(1 \text{ h}) = 17.9$
 $f(10 \text{ h}) = 9.5E5$

Arrhenius Law

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

$$k_1 = A \cdot e^{-\left(\frac{E_a}{R \cdot T}\right)}$$

$$LN\left(\frac{k_1}{k_2}\right) = \left(\frac{-E_a}{R}\right) \cdot \left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

Variable	Description	Units
k1	rate constant at T1	1
k2	rate constant at T2	1
A	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 $2.52 \times 10^{-5} \text{ 1/s}$ and $3.16 \times 10^{-3} \text{ 1/s}$ at $189.7 \text{ }^\circ\text{C}$ and $251.2 \text{ }^\circ\text{C}$ respectively. From this data, calculate the activation energy and pre-exponential for this reaction.

Given

$k_1 = 2.52 \times 10^{-5}$
 $k_2 = 3.16 \times 10^{-3}$
 $T_1 = 189.7 \text{ }^\circ\text{C}$
 $T_2 = 251.2 \text{ }^\circ\text{C}$

Result

$E_a = 159 \text{ kJ/mol}$
 $A = 1.96 \times 10^{13}$

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

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

$$t_{\text{fract}} = \frac{\left(\frac{1}{1-f}\right)^{\text{no}-1} - 1}{(\text{no}-1) \cdot a \cdot k_{\text{gen}} \cdot C_{\text{ao}}^{\text{no}-1}} \quad \text{If no} \neq 0$$

$$t_{\text{fract}} = \frac{-\text{LN}(1-f)}{k_{\text{gen}}} \quad \text{If no} = 1$$

Variable	Description	Units
tfract	fractional life	1_s
no	reaction order	1
kgen	general rate constant	1_1/s*
Cao	general concentration	1
a	stoichiometric coefficient	1
f	fractional order	1

*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 → 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

no = 2
 kgen = 1.03 x 1E-3 1/h
 Cao = 0.01
 a = 2
 f = 0.10

Result

tfract = 1.94 E7_s 10%
 tfract = 5.82 E7_s 25%
 tfract = 17.5 E7_s 50%
 tfract = 52.4 E7_s 75%

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.

The screenshot shows a periodic table with the element Hydrogen (H) selected. The element name 'HYDROGEN' is displayed at the top. The atomic number '1' is shown in the top left corner. The symbol 'H' is in the center, and the mass number '1.0079' is at the bottom left. The bottom of the screen features a menu with options: PROPS, FIND, ATW, LET, FAST, and UP.

Properties of Each Element

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 **ENTER** places the data on the calculator stack. The properties listed for each element (if available) are:

The screenshot displays the properties for Hydrogen. The title is 'Hydrogen'. The properties listed are: DENSITY: 8.98E-5, OX STATES: 1, ELEC CFG: 1S1, STATE: GAS, MELTING PT: 14.025, BOILING PT: 20.268, GROUP: 1(A), and FAMILY: -. The bottom of the screen features a menu with options: MAIN, STR, PRINT, UNITS, FONT, and EXIT.

- 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

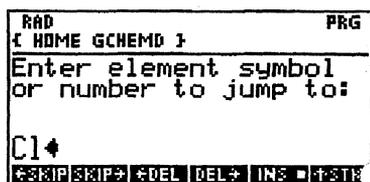
Moving Around the Periodic Table

Use the cursor keys (   ) to move the pointer to any element. Pressing the  key 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.



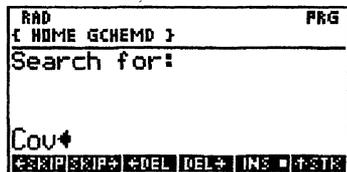
Using Search and List Utilities

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  before typing in the letter. Press **ENTER** 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  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.

The following screen displays:

Press **EXIT** to return to the Periodic Table screen.

Editing Text Entries During a Search

The search mode softkeys (**<-SKIP** , **<-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:

<-SKIP	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 **PRINT** 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 **ENTER** 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 **◀** and **▶** keys to scroll

```

      STOICHIOMETRY
    →METHANE COMBUSTION
      PERMANGANATE

    ADD  DELETE  EDIT  CHEM  STOIC  UP
  
```

the display to the right or to the left. Press **ON** key to return to the STOICHIOMETRY menu screen.

```

SPARCOM CHEMICAL EQUATION WRITER

CH4g + 2O2g ⇌ 2H2Ol + CO2g

PRESS [ENTER] TO RETURN TO LIST...
  
```

```

SPARCOM CHEMICAL EQUA

8H+1aq + MnO4-1aq + 5Fe+2aq ⇌ Mn

PRESS ◀ AND ▶ TO SCRL
PRESS [ATTN] 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 **STOIC**. This displays all reactants (labeled R) and products (labeled P) in the reaction, as shown:

```

      STOICHIOMETRY
    →METHANE COMBUSTION
      PERMANGANATE

    ADD  DELETE  EDIT  CHEM  STOIC  UP
  
```

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 **ENTER**. 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:

```

      PRG
    { HOME GCAPPD }
  Enter quantity of
  1CH4[g]:
  1_g
  _G  _KG  _MDL  _LE  _L  _ML
  
```

```

      METHANE COMBUSTION
    R: 1[1_g] 1CH4[G]
    →R: 1[ ] 2O2[G]
    P: 1[ ] 2H2O[L]
    P: 1[ ] 1CO2[G]

    CALC  COMM  CLEAR  VIEW  →STOIC  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.

```

METHANE COMBUSTION
R: {1.9999999999_G} 1CH4[G]
→R: {8.79474378866E-3_L} 2O2[G]
P: {2.24592023736_G} 2H2O[L]
P: {2.74330844127_G} 1CO2[G]

CALC CONV CLEAR VIEW →STK EXIT
  
```

```

Convert to:
GRAMS
MOLES
LITERS
KILOGRAMS
→POUNDS
MILLILITERS

EXIT
  
```

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 convert (in this case, O₂) and press **CONV**. This displays a list of available units:

```

METHANE COMBUSTION
R: {1.99999999999_G} 1CH4[G]
→R: {3.98922867864_G} 2O2[G]
P: {2.24592023736_G} 2H2O[L]
P: {2.74330844127_G} 1CO2[G]

CALC CONV CLEAR VIEW →STK EXIT
  
```

Move the cursor to pounds and press **ENTER**. 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:

```

METHANE COMBUSTION
R: {1_G} 1CH4[G]
R: {1_G} 2O2[G]
→P: {} 2H2O[L]
P: {} 1CO2[G]

CALC CONV CLEAR VIEW →STK EXIT
  
```

```

METHANE COMBUSTION
R: {0.250675025312_G} 1CH4[G]
R: {0.999999999996_G} 2O2[G]
→P: {0.562996112952_G} 2H2O[L]
P: {0.687678912956_G} 1CO2[G]

CALC CONV CLEAR VIEW →STK EXIT
  
```

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 **ENTER**. Type in 25_ml and press **ENTER**.

```

{ HOME GCAPPD }          PRG
Enter molarity of
1MnO4[aq]-1:

.01_mol/l
  
```

```

PERMANGANATE
R: (.0020158_G) BH(AQ)+1
→R: (25_ML, .01_MOL/L) 1MNO4(AQ)...
R: (.06880875_G) 5FE(AQ)+2
P: (.0137345_G) 1MNI(AQ)+2
P: (.06880875_G) 5FE(AQ)+3
P: (.0180152_G) 4H2O(L)
  
```

```

PERMANGANATE
R: (.0020158_G) BH(AQ)+1
R: (25_ML, .01_MOL/L) 1MNO4(AQ)...
→R: (.06880875_G) 5FE(AQ)+2
P: (.0137345_G) 1MNI(AQ)+2
P: (.06880875_G) 5FE(AQ)+3
P: (.0180152_G) 4H2O(L)
  
```

The next screen asks you to enter the molarity of the permanganate solution. Type in 0.01_mol/l at the prompt: Press **ENTER** 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:

CH ₄ (g)	CO ₂ (g)
Fe ⁺² (aq)	Fe ⁺³ (aq)
H ₂ O(l)	H ⁺¹ (aq)
MnO ₄ ⁻¹ (aq)	Mn ⁺² (aq)
O ₂ (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 **ADD** 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:

Press **ENTER** to place NaOH into the Species Library:

```

SPECIES LIBRARY
↓ CH4(G)
CO2(G)
Fe(AQ)+2
Fe(AQ)+3
H2O(L)
HCl(AQ)+1
MnO4(AQ)-1
Mn(AQ)+2
ADD DELETE EDIT CHEW MWTT% UP
    
```

```

ALG PRG
{ HOME GCAPPD }
Enter chemical species
Formula[State]±Charge:
[CG] [LJ] [CS] [CR] [C] [J]
    
```

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.

```

ALG PRG
{ HOME GCAPPD }
Enter chemical species
Formula[State]±Charge:
NaOH
[CG] [LJ] [CS] [CR] [C] [J]
    
```

```

^ SPECIES LIBRARY
Fe(AQ)+3
H2O(L)
HCl(AQ)+1
MnO4(AQ)-1
Mn(AQ)+2
→ NaOH
O2(G)
OH(AQ)-1
ADD DELETE EDIT CHEW MWTT% UP
    
```

```

MnO4[Aq]-1
118.9356_g/mol
0 53.8% MN46.2%
PRESS [STO] TO SAVE TO STACK ...
PRESS [ENTER] TO RETURN TO LIST ...
    
```

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 **MWTT%**. The molecular weight and the percent

composition are then displayed on the screen, as shown:

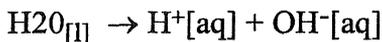
Press **STO** to store the molecular weight on the calculator stack. Pressing **ENTER** returns you to the Species Library. Press **CHEW** to display the species on the screen:

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:



```

STOICHIOMETRY
→METHANE COMBUSTION
PERMANGANATE

ADD DELETE EDIT CHEM STOIC UP
  
```

```

PRG
{ HOME GCAPPD }
Edit reaction name:

WATER DISSOCIATION
*SKIP *SKIP* *DEL DEL* INS * * *
  
```

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

```

WATER DISSOCIATION
→PRESS ADD

ADD R ADD P DELETE EDIT STOIC UP
  
```

```

Pick species:
CH4G1
CO2G1
FeAQ1+2
FeAQ1+3
→H2O[L]
H2AQ1+1
MnO4AQ1-1
MnIAQ1+2
ADD DELETE EDIT CHEM MWRT EDIT
  
```

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 species in the list. Scroll down the list until you find H2O[L] and press **ENTER**.

```

PRG
{ HOME GCAPPD }
Enter coefficient:

1
*SKIP *SKIP* *DEL DEL* INS * * *
  
```

```

WATER DISSOCIATION
→R: 1H2O[L]

ADD R ADD P DELETE EDIT STOIC UP
  
```

The prompt then asks for the stoichiometric coefficient, which in this case is 1. Type 1 at the prompt and press **ENTER**. This places H2O on the reaction list, labeled R for reactant. The coefficient 1 precedes the species entry on the list.

```

WATER DISSOCIATION
→R: 1H2O(L)
P: 1H+(AQ)+1
P: 1OH(AQ)-1
ADD R  ADD P  DELETE  EDIT  STOIC  UP

```

Press **ADD P** to add a product species. Once again, scroll down the list until you find OH[aq]-1 and press **ENTER**. 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:

```

STOICHIOMETRY
→WATER DISSOCIATION
METHANE COMBUSTION
PERMANGANATE
ADD  DELETE  EDIT  CHEW  STOIC  UP

```

```

SPARCOM CHEMICAL EQUATION WRITER

MnO4-1aq

PRESS CENTER] 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:

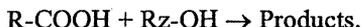
Entering Molecular Formulas

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 **☑** and pressing the appropriate softkey. Charges must be preceded by the sign (either + or -). Parentheses may be entered by either pressing **☐±** or the two softkeys shown in the display. (Note that **☐±** does not require unlocking alpha-entry mode. Some examples of acceptable chemical formulas are:

Compound	Input
HCl	HC☐L
HNO ₃	HNO3
Ca(NO ₃) ₂	C☐A ☐± NO3 ☐☑☐± 2

After unlocking alpha-entry mode to enter parentheses or to move the cursor, it is necessary to press α 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 be 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:



To enter this reaction, you must enter the species RCO₂H, R_z-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, R_z, 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 USRSYMB 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

ADD	Adds a new chemical reaction to the list.
ADD R	Adds a reactant from the Species Library and a stoichiometric coefficient to the selected chemical reaction.
ADD P	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.
DELETE	Deletes a chemical reaction or a reactant or product from

EDIT

a chemical reaction.

Edits a chemical reaction or a reactant or a product.

ENTER

Allows you to specify the quantity of a reactant or product.

EXIT

Exits the Stoichiometry solving screen.

→STK

Copies selected entry to calculator stack.

STOIC

Enters the stoichiometry solving screen after the selected chemical 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 functional 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

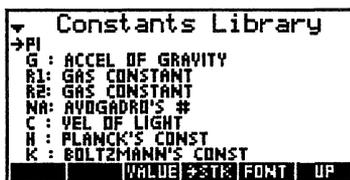
In This Chapter

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:



π	π
g	Acceleration of gravity
R1	Universal gas constant - J/(mol*K)
R2	Gas constant - atm/(mol*K)
NA	Avogadro's number
c	Velocity of light
h	Planck's constant
k	Boltzmann's constant
h_b	Dirac's constant
q	Electron charge
ϵ_0	Permittivity of vacuum
m_e	Electron mass
r_e	Classical electron radius
m_p	Proton rest mass
R_∞	Rydberg's constant
α	Fine structure constant
a_0	Bohr radius
μ_B	Bohr magneton
λ	Wavelength for 1eV
λ_c	Compton's wavelength
α	Stefan-Boltzmann
c_1	First radiation constant
c_2	Second radiation constant
V_t	Thermal voltage at 300_K
μ_0	Permeability of free space

ϕ_0	Magnetic flux quantum
F	Faraday constant
μ_e	Electron magnetic moment
μ_p	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    4. 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)'  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 .

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.

Constants Library Softkeys

VALUE	Displays the value of the constant with units on the screen. Press  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.

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 **ENTER**. 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.
Expansion/Compressibility	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.

Summary of Softkeys

FONT	Toggles the display 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.

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, Suite 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 **GCAP** 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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