

**The PocketProfessional™**

# **Chemistry Applications**

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## **Owner's Manual**

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# Notice

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## Table of Contents

<b>Chapter 1: Getting Started</b>	<b>1</b>
Welcome	1
Installing, Removing the Pocket Professional	1
To Install the Card	1
To Remove the Card	2
To Access the Chemistry Application Pac	3
Using the Main Menu	3
Moving Around the Screen	4
Viewing Items Too Wide for the Display	4
Changing the Font Size	4
Using the Search Mode	5
Editing Text Entries	5
Using the Equation Library	5
Solving a Single Equation	5
Accessing Equations	6
Selecting and Displaying Equations	6
Viewing Variable Definitions	7
Using the Solver Function	7
Converting Data to Different Units	8
Options After Solving the Equation	9
Managing Units	9
Solving Multiple Equations	10
Selecting the Equation Set	10
Solving the Equation Set	11
Tagging Variables	12
Plotting One Equation	12
Finding and Selecting the Equation	13
Tagging and Entering the Variables	13
Entering the X and Y Coordinates	14
Plotting Speed	14
Softkeys for the Plot Function	15
Plotting Multiple Equations	15
What You Should Know About the Solver	15
Speeding Up Computing Time	16
"Bad Guess" Message	16
Equations with Multiple Roots	16
Loading Values from the Stack	16
da Vinci's GCAPPD Directory	17
Summary of Softkeys	18
 <b>Chapter 2: Equation Library</b>	 <b>20</b>

In This Chapter	20
Atoms Molecules	20
Mass/Mole/Atom	21
Light	21
Quantum	21
Hydrogen Energy	22
s,p,d and f Orbitals	23
Radial Functions	23
Angular Wave Functions	25
Diatomic Moment	27
Symmetrical Moment	28
Solids/Liquids	28
Heat Capacity	29
Blackbody Radiation	30
Equation of State	30
Bragg Law	31
Born-Haber Cycle	32
Melting Point	32
Concentration	32
Raoult's Law	34
BP/FP Colligative	35
Molarity/Dilution	36
Clausius Clapyron	37
Capillary Rise	38
Gases	38
Ideal Gas	38
State Changes	39
Gas Over Water	40
Barometric Equation	41
Van der Waal Gases	42
Kinetic Theory	43
Graham's Law	44
Collision Theory	45
Acids/Bases	46
pH Function	46
Strong Acids	47
Strong Bases	48
Weak Acids/Bases	49
Henderson-Hasselbach	49
Titration (SA/SB)	50
Titration (SB/SA)	51
Titration (WA/SB)	51
Titration (WB/SA)	54
Thermo/Electrochemistry	55

Heat Transfer	55
Heat Engines	56
Free Energy	56
Thermodynamics	57
Heat Capacity	58
Nernst Law	59
Reduction	60
Precipitation	61
Kinetics	62
First Order	63
Parallel First Order	64
First Order Consecutive	65
Second Order (I)	66
Second Order (II)	67
Arrhenius Law	68
Fractional Life	69
<b>Chapter 3: Periodic Table</b>	<b>70</b>
In This Chapter	70
Using the periodic Table	70
Property of each Element	70
Moving Around the Periodic Table	71
Using Search and List Utilities	71
List Element Names and Symbols	71
Search for a Property	71
Editing Text Entries during a search	72
Using the print function	72
Summary of Softkeys	72
<b>Chapter 4: Stoichiometry</b>	<b>74</b>
In This Chapter	74
Using Stoichiometry Function	74
Selecting and Displaying a chemical reaction	74
Calculating theoretical yields	75
Entering Quantity of a reactant	75
Limiting reagents	76
Stoichiometry with solutions	77
Using the species library	77
Creating a chemical reaction	78
Entering Molecular formula	80
Summary of softkeys	81
Stoichiometric softkeys	81
Species Library softkeys	82
<b>Chapter 5: Constants Library</b>	<b>83</b>
In this Chapter	83
Using Constants Library	83

Using GCON function	84
Constant Library softkeys	84
<b>Chapter 6: Reference Library</b>	<b>85</b>
In this chapter	85
Using the Reference Library	85
Examples of using the reference Library	86
Summary of softkeys	86
 <b>Appendix A : Warranty and Service</b>	 <b>87</b>
Warranty & Service	87
PocketProfessional Support	87
If the Card requires Service	87
Environmental test Limits	88
 <b>Appendix B: Questions and Answers</b>	 <b>89</b>
Questions Commonly Asked	89
 <b>Appendix C: References</b>	 <b>91</b>
 <b>Index</b>	 <b>92</b>

# 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.

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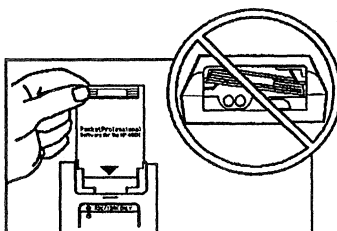
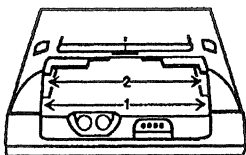
## **Installing, Removing the Pocket Professional**

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**

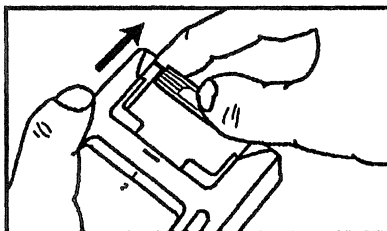
- Turn off the calculator. Do not press **[ON]** until you have completed the installation procedure.
- Remove the port cover. Press against the grip lines and push forward. Lift the cover to expose the two plug-in ports.
- Select either empty port for the Pocket Professional card.
- Position the card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

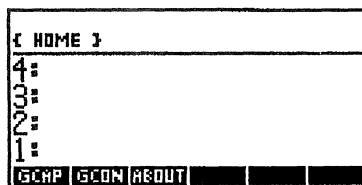
1. Turn the calculator off. Do not press **ON** until you have completed the procedure.
2. Remove the port cover. Press against the card's grip and slide the card out of the port.
3. Replace the port cover.



### **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.

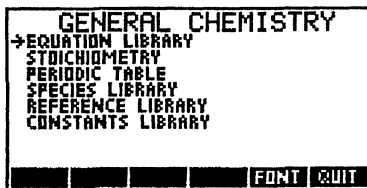
**Second Method:** Type in the letters **GCAPP** and press **ENTER**.



## Using the Main Menu

After you start the Application Pac, the main menu screen appears. The main menu lists the main categories in a “browser” menu format.

“Browser” refers to the ability to use the cursor keys  and  to move the pointer to the menu item you wish to select and to press  to call that menu item to the screen.



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





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







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

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

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

## Moving Around the Screen

Use the  and  keys to move the pointer up and down in the menu list. Pressing   moves the pointer to the bottom of the screen, or pages

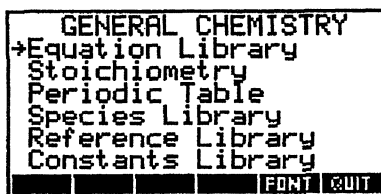
down if the pointer is already at the bottom of the screen. Pressing   moves to the top of the screen or pages up if the pointer is already at the top of the screen. Pressing   moves the pointer to the bottom of the list or   moves to the top of the list.

## 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.

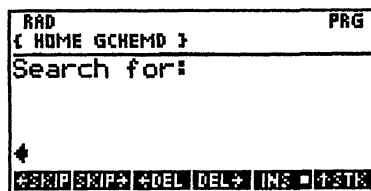
## Changing the Font Size


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 ( $\alpha$ ) 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.

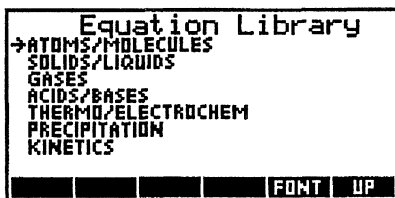
## Editing Text Entries

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:

<b>&lt;-SKIP</b>	Moves the cursor to the beginning of the current word
<b>SKIP-&gt;</b>	Moves the cursor to the beginning of the next word
<b>&lt;-DEL</b>	Deletes all characters in the current word to the left of the cursor
<b>DEL-&gt;</b>	Deletes all characters from the current position to the first character of the next word
<b>INS</b>	Toggles between insert and typeover modes
<b>-&gt;STK</b>	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:

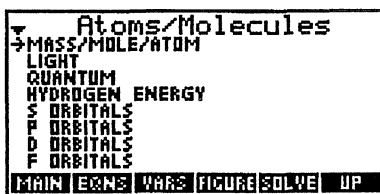


- Select the equation category and topic from the main menu.
- List all the equations in a topic.
- Solve a specific equation or a set of equations.
- View a description of the variables.
- View a figure that illustrates the problem.
- Plot the equation.

## Solving a Single Equation

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

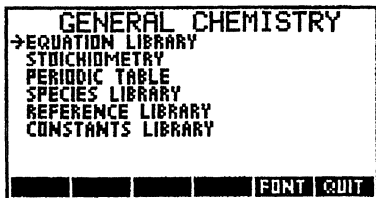
55.847\_g/mol) in a truck containing 1.5 metric tons of material.



## 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:



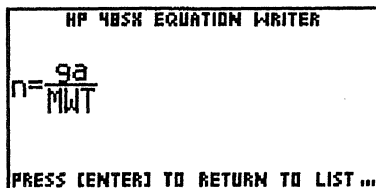
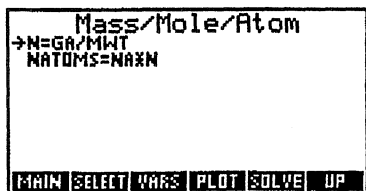
**ENTER** to display the list of topics:

## 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



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 VIEW 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
  
```

```

RAD                                     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

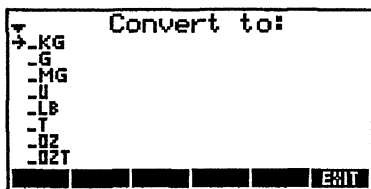
```

Mass/Mole/Atom
→*N: '26859.0971762_MOL'
→GA: '1.5_T'
→MWT: '55.847_G/MOL'

KNOW WANT CLEAR PURGE CONV UP

```

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



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

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

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

### Options After Solving the Equation

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

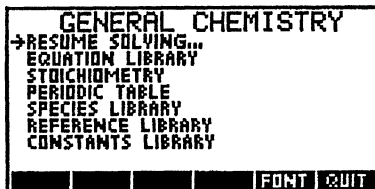
Selecting the RESUME SOLVING function returns you directly to the equation set you were working with, with all previous entries still intact.

## Managing Units

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

## Solving Multiple Equations

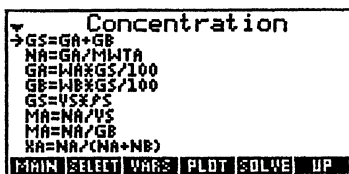
For many problems, the result of one calculation acts as the input to another. The Chemistry Application Pac is capable of solving multiple equations, sequentially and systematically.



## Selecting the Equation Set

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

To solve this problem, move to the "CONCENTRATION" topic under the "SOLIDS/LIQUIDS" category. This topic contains 12 equations which relate the various forms of concentration of solute (labeled a) in the solvent (labeled b) to the fundamental parameters of the solution. These equations are listed below:



$$gs = ga + gb$$

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

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

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

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

$$wa + wb = 100$$

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

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

$$gs = vs \cdot ps$$

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

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

$$gb = vb \cdot pb$$



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

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

Variable	Description	Units
<b>ga</b>	mass solute	kg
<b>gb</b>	mass solvent	kg
<b>na</b>	moles solute	mol
<b>nb</b>	moles solvent	mol
<b>MWta</b>	molecular weight solute	kg/mol
<b>MWtb</b>	molecular weight solvent	kg/mol
<b>wa</b>	weight % solute	-
<b>wb</b>	weight % solvent	-
<b>pb</b>	pure solvent density	kg/m <sup>3</sup>
<b>vb</b>	volume of solvent	m <sup>3</sup>
<b>gs</b>	mass solution	kg
<b>vs</b>	volume solution	m <sup>3</sup>
<b>ps</b>	density solution	kg/m <sup>3</sup>
<b>Ma</b>	molarity solution	mol/m <sup>3</sup>
<b>ma</b>	molality solution	mol/kg
<b>xa</b>	mole fraction solution	-
<b>ppma</b>	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: '0.0004284_T'	
*GB: '7.61600000002E-2_KG'	
*NA: '1.17495728301_MOL'	
*NB: '4.22754118745_MOL'	
*MWTA: '36.4609_G/MOL'	
*MWTB: '18.0152_G/MOL'	
*WA: 36	
*WB: 64.0000000002	
<b>CALC</b>	<b>EQNS</b> <b>VARs</b> <b>UNIT</b> <b>3STK</b> <b>UP</b>

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

Concentration			
*XGA:	'0.576_KG'		
*XGB:	'1024_KG'		
*XNA:	'1.57808219178_MOL'		
*XNB:	'5.67313019391_MOL'		
*MWta:	'36.5_g/MOL'		
*MWtb:	'18.05_g/MOL'		
*wa:	36		
*XNB:	84.0000000001		
*pb:	'0_KG/M^3'		
*vb:	'0_M^3'		
*GS:	'16_KG'		
*VS:	'100_ML'		
*PS:	'1.6_g/CM^3'		
*MA:	'15780.8219178_MOL/M^3'		
*MB:	'154105589041_MOL/M^3'		
*XA:	217630115882		
*XPMa:	562500		
VALUE	EXPR	UNITS	UNIT
			DOWN 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 **ENTER** to display the additional softkeys for this screen, and press **WANT**. This places a "?" tag in front of the variable you want to solve for:

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

## Plotting One Equation

Any equation in the equation library that is of the form:  $y=f(a,b,...)$  can be easily plotted using the General Chemistry Application Pac. To plot an

Concentration			
*VB:	'0_M^3'		
*GS:	'0_KG'		
*VS:	'100_ML'		
*PS:	'1.19_g/ML'		
*MA:	'0_MOL/M^3'		
*MB:	'0_MOL/M^3'		
*XA:	0		
*XPMa:	0		
CALC	EXPR	UNITS	UNIT
			DOWN UP

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/CE*VA
PH=-LOG(-(VB*CB-VA*CA)/(2*(VA+Vb...
PH=-LOG(H)
CE=GB/(M*V*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

<b>Ca</b>	acid concentration	mol/m <sup>3</sup>
<b>Cb</b>	base concentration	mol/m <sup>3</sup>
<b>Va</b>	volume of acid solution	m <sup>3</sup>
<b>Vb</b>	volume of base titrant	m <sup>3</sup>
<b>Kw</b>	water dissociation constant	mol <sup>2</sup> /m <sup>6</sup>
<b>pH</b>	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<sup>-14</sup> mol<sup>2</sup>/l<sup>2</sup>

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

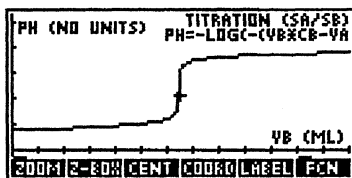
With these four variables entered, return to the equations screen by pressing **EQNS**. Move the pointer to the second equation and press **PLOT**. Since this equation is of the proper form, and all but  $V_b$  has been specified on the right hand side, it may be plotted.

## 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.

RAD	PRG
{ HOME GCHEMD }	
Enter horizontal range for Vb (m <sup>3</sup> ):	
<Min> <Max>	
*SKIP *XIP* *DEL DEL* INS *STX*	

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  $\text{m}^3$  instead of  $\text{ml}$ . The plot will also be displayed in SI units.

## Softkeys for the Plot Function

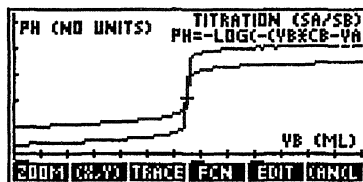
The softkeys shown in the above plot are plot function keys in the HP 48. For example, pressing **COORD** displays the (x,y) coordinates of any point on the screen indicated by the cursor. For a description of the behavior of the plot function softkeys, see the *HP 48 Owner's Manual*. Note that the **SLOPE** 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:

<b>Gcpar</b>	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 <b>CANCEL</b> to quit the General Chemistry Pac and exit to the calculator stack, 2) Pressing <b>UP</b> to return to the topic level, or 3) Pressing <b>MAIN</b> to return to the main menu level
<b>RXNS</b>	Contains user defined reactions. To eliminate all reactions, this variable may be purged. It is recreated whenever a new reaction is built
<b>SPEC</b>	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
<b>SPECCODE</b>	Contains the index of the last species added to the

USRSYMBs	Species Library. User modification or deletion of this variable will corrupt the reaction and species libraries
USRATWTS	Contains user-defined chemical symbols
	Contains user-defined atomic weights

## Summary of Softkeys

<b>CALC</b>	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 "*".
<b>CLEAR</b>	Resets the values of the current variable set to zero.
<b>EQNS</b>	Enters the equation level of the current topic.
<b>FIGURE</b>	Displays a figure for the currently selected topic or displays "No figure".
<b>FONT</b>	Toggles between small and medium display fonts of the HP 48GX.
<b>KNOW</b>	Toggles the currently selected variable between known and unknown, adding or removing the triangular tag.
<b>MAIN</b>	Returns to the main menu.
<b>PLOT</b>	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.
<b>PURGE</b>	Purges the global copies (in the GCHEMD directory) of the current variable set displayed in the solver level.
<b>QUIT</b>	Exits the Chemistry Application Pac.
<b>SELECT</b>	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.
<b>SOLVE</b>	Enters the solver level of the current topic.
<b>↑STK</b>	Copies selected entry to calculator stack.
<b>UNIT ■</b>	Toggle key. Indicates that units are on.
<b>UNITS</b>	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.
<b>UP</b>	Moves up one level in the software menu structure.
<b>VARS</b>	Enters the variable level for the current topic.
<b>VIEW</b>	Displays the full text entry for a variable description or value if the description is too wide to fit on the screen.
<b>WANT</b>	Toggles the currently selected variable between wanted



**ENTER**

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

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.

<b><math>\pi</math></b>	$\pi$
<b><math>g</math></b>	Acceleration due to gravity
<b><math>R</math></b>	Universal gas constant
<b><math>NA</math></b>	Avogadro's number
<b><math>c</math></b>	Velocity of light
<b><math>h</math></b>	Planck's constant
<b><math>k</math></b>	Boltzmann's constant
<b><math>q</math></b>	Electron charge
<b><math>R_\infty</math></b>	Rydberg's constant
<b><math>a_0</math></b>	Bohr radius
<b><math>\sigma</math></b>	Stefan-Boltzmann
<b><math>F</math></b>	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

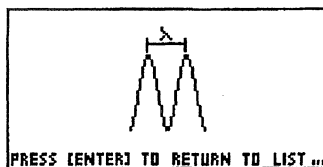
- Quantum
- Symmetrical Moment
- Hydrogen Energy

## 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
<b>n</b>	number of moles	mol
<b>ga</b>	mass of sample	kg
<b>MWT</b>	molecular weight of sample	kg/mol
<b>Natoms</b>	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
<b>ga</b> = 45_lb	<b>n</b> = 365.5 mol
<b>MWT</b> = 55.847 g/mol	<b>Natoms</b> = 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
$\lambda$	wavelength	m
$\gamma$	frequency	Hz
<b>E</b>	photon energy	J
<b>nubar</b>	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.

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

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

Variable	Description	Units
$\lambda$	de Broglie wavelength	m
<b>m</b>	mass	kg
<b>v</b>	velocity	m/s
<b>E</b>	energy	J
<b>h</b>	Plank's constant	J.s
<b>c</b>	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

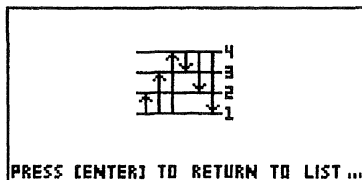
**Result**

$\lambda$  = 1.28 E-25\_nm

**E** = 2.55 E15\_J

## Hydrogen Energy

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



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

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

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

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

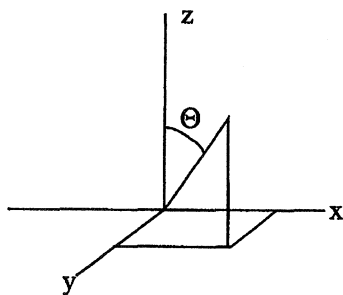
Variable	Description	Units
<b>E</b>	energy	J
<b>Z</b>	nuclear charge	-
<b>ni</b>	initial quantum number	-

$n_f$	final quantum number	-
$\Delta E$	energy change	J
$\gamma$	frequency	Hz
$\lambda$	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,  $\phi_{nlm}$ , 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)  $X_{10} = \cos(\theta)$

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

(p)  $X_{11} = \sin(\theta)$

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

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

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

(d)  $X_{21} = \sin(\theta) \cdot \cos(\theta)$

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

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

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

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

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

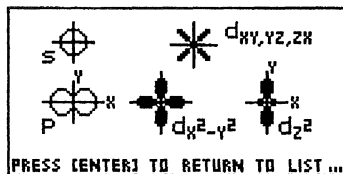
(f)  $X_{31} = \sin(\theta) \cdot (5 \cdot \cos^2(\theta) - 1)$

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

(f)  $X_{32} = \sin^2(\theta) \cdot \cos(\theta)$

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

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



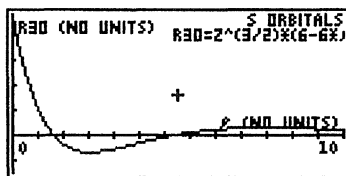
$$\text{constant} = \frac{1}{8} \cdot \sqrt{70}$$

Variable	Description	Units
$\rho$	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	-
$\Theta$	azimuthal angle	°
$a_0$	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  $\rho$ , find  $\rho$  at the first node, then solve for  $r$ .



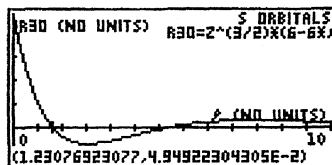


After entering Z=1, plot the R30 function (in s orbitals) from  $\rho=0$  to  $\rho=10$ , as shown below (autoscale y):

$$x1 = 0$$

$$x2 = 10$$

autoscale y

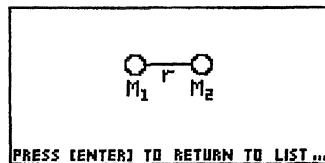


Move the cursor to the first node and press **COORD** to display the (x,y) coordinates of the node. This yields:

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 <sup>2</sup>
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

$$m1 = 1.00797 \text{ g/mol}$$

$$m2 = 35.453 \text{ g/mol}$$

$$r = 1.27460 \text{ Å}$$

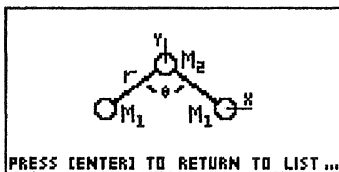
### Result

$$I = 2.644\text{E-}40 \text{ kg.cm}^2$$

$$B = 10.59 \text{ 1/cm}$$

## Symmetrical Moment

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



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

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

$$I_z = I_x + I_y$$

Variable	Description	Units
$I_y$	moment of inertia about y	kg. m <sup>2</sup>
$I_x$	moment of inertia about x	kg. m <sup>2</sup>
$I_z$	moment of inertia about z	kg. m <sup>2</sup>
$m_1$	mass of 1	Kg/mol
$m_2$	mass of 2	kg/mol
$r$	internuclear distance	m
$\theta$	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.

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

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

Variable	Description	Units
CvE	Einstein heat capacity	J/(mol.K)
CvD	Debye heat capacity	J/(mol.K)
$\theta_e$	Einstein characteristic temperature	K
$\theta_d$	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  $\theta_d = 88K$ . Estimate the heat capacity of Pb at 20K and 25°C. First enter  $\theta_d$  and  $T=20\_K$ , and solve for CvD. Next enter  $T=25\_°C$  and solve again for CvD.

Given	Result
$\theta_d = 88\_K$	$CvD = 1.1\_J/(mol \cdot K) @ 20\_K$

$$T = 20\_K$$

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

$$T = 25\_^\circ C$$

## 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
$E_\gamma$	energy density	$J \cdot s / m^3$
ET	total energy density	$J / m^3$
T	absolute temperature	K
$\gamma$	frequency	Hz

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

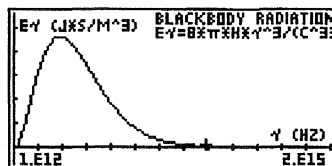
**Given**

$$T = 5000\ K$$

**Result**

$$ET = 35439500\_W / m^2$$

To solve the second part of the problem, set  $T=5000\ K$  and plot  $E_\gamma$  versus  $\gamma$  over a wide range of frequencies (this example uses  $1E12\_Hz$  to  $1E15\ Hz$ ), as shown:



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

## Equation of State

This equation is general to solids and relates volume, pressure and temperature.

$$VTP = V_o \cdot (1 + \alpha s \cdot (t2 - 0 \text{ } ^\circ \text{C})) \cdot (1 - \rho s \cdot (p2 - 1 \text{ atm}))$$

Variable	Description	Units
VTP	volume at any temperature & pressure	m <sup>3</sup>
V <sub>o</sub>	reference volume	m <sup>3</sup>
αs	thermal expansion coefficient	1/K
t2	temperature	K
ρs	compressibility coefficient	1/Pa
p2	pressure	Pa

**Example:** A 1.000\_cm<sup>3</sup> solid has a coefficient of expansion of αs=1.03E-4\_1/K and a compressibility coefficient of ρs=2.86E-6\_1/atm. What is the volume at 360 °F and pressure of 1800\_psi?

#### Given

$$V_o = 1.000 \text{ cm}^3$$

$$\alpha s = 1.03\text{E-}4 \text{ 1/ } ^\circ \text{C}$$

$$\rho s = 2.86\text{E-}6 \text{ 1/atm}$$

$$t2 = 360 \text{ } ^\circ \text{F}$$

$$p2 = 1800 \text{ psi}$$

#### Result

$$VTP = 1.02 \text{ cm}^3$$

## Bragg Law

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

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

Variable	Description	Units
Θ	diffraction angle	°
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

$$d = 5.627 \text{ } _\text{\AA}$$

$$n = 1$$

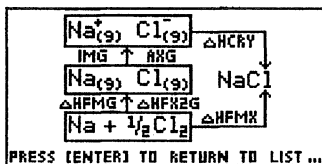
#### Result

$$\Theta = 7.35 \text{ } _\circ$$

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

## 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.



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

Variable	Description	Units
$\Delta H_{fmx}$	heat of formation of mx	J/mol
$\Delta H_{cry}$	heat of crystalization of mx	J/mol
$\Delta H_{fmg}$	heat of formation of gaseous m	J/mol
$\Delta H_{fx2g}$	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
$\Delta H_{fus}$	heat of fusion	J/mol
$\Delta V_{fus}$	volume change upon fusion	m <sup>3</sup> /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	-
pb	pure solvent density	kg/m <sup>3</sup>
vb	volume of solvent	m <sup>3</sup>
gs	mass solution	kg
vs	volume solution	m <sup>3</sup>
ps	density solution	kg/m <sup>3</sup>
Ma	molarity solution	mol/m <sup>3</sup>
ma	molality solution	mol/kg
xa	mole fraction solution	-
ppma	solute concentration	-

**Example 1:** Calculate the molality of Br<sup>-</sup> in a 1000\_g solution containing 4600 ppm of the ion.

**Given**

gb = 1000\_g  
 MWTa = 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**

ga = 5.0\_g  
 gb = 225.0\_g  
 MWTa = 92.1402\_g/mol  
 ps = 0.876\_g/ml  
 MWTb = 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

**Raoult's 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.

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

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

$$n_b = \frac{g_b}{MWT_b}$$

$$x_b = \frac{n_b}{n_a + n_b}$$

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

$$n_a = \frac{n_b}{MWT_a}$$

$$x_a = \frac{n_a}{n_a + n_b}$$

$$x_a = 1 - x_b$$

Variable	Description	Units
P	solvent partial pressure	1_Pa
x <sub>b</sub>	solvent mole fraction	1
P <sub>in</sub>	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
MWTa	molecular weight of solute	1_kg/mol
MWTb	molecular weight of solvent	1_kg/mol
nb	moles of solvent	1_mol
gb	mass of solvent	1_kg

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

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

### BP/FP Colligative

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

$$\Delta T_b = K_b \cdot m_a$$

$$m_a = \frac{n_a}{g_b}$$

$$n_b = \frac{g_a}{MWT_a}$$

$$\Delta T_f = -K_f \cdot m_a$$

Variable	Description	Units
$\Delta T_b$	boiling point elevation	1_K
$K_b$	ebullioscopic constant	1_K·kg/mol
ma	solute concentration in molality	1_mol/kg
na	moles of solute	1_mol
gb	mass of solvent	1_kg
ga	mass of solute	1_kg
MWTa	molecular weight of solute	1_kg/mol
$\Delta T_f$	freezing point depression	1_K
$K_f$	cryoscopic constant	1_K·kg/mol

Note that once calculated, the values of  $\Delta T_b$  and  $\Delta T_f$  may not be converted into other temperature values. When entering a value for  $\Delta T_f$ , 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**

$$K_b = 0.52 \text{ K}\cdot\text{kg/mol}$$

$$g_b = 900 \text{ _g}$$

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

$$MWT_a = 62 \text{ _g/mol}$$

$$K_f = 1.86 \text{ K}\cdot\text{kg/mol}$$

**Result**

$$\Delta T_b = 0.932 \text{ }^\circ\text{C}$$

$$m_a = 1.79 \text{ _mol/kg}$$

$$n_a = 1.61 \text{ _mol}$$

$$\Delta T_f = -3.33 \text{ }^\circ\text{C}$$

## Molarity/Dilution

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

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

$$n_a = \frac{g_a}{MWT_a}$$

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

Variable	Description	Units
$M_i$	initial concentration, Molarity	1 _mol/m <sup>3</sup>
$n_a$	moles of solute	1 _mol
$V_i$	initial volume	1 _m <sup>3</sup>
$g_a$	mass of solute	1 _kg
$MWT_a$	molecular weight of solute	1 _kg/mol
$V_f$	final volume	1 _m <sup>3</sup>
$M_f$	final concentration	1 _mol/m <sup>3</sup>
$V$	solution volume	1 _m <sup>3</sup>

**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**

$$g_a = 4.5060 \text{ _g}$$

$$MWT_a = 39.99707 \text{ _g/mol}$$

$$V = 250.00 \text{ _ml}$$

$$V_i = 10.00 \text{ _ml}$$

**Result**

$$M_i = 0.4506 \text{ _mol/l}$$

$$M_f = 9.013 \times 10^{-3} \text{ _mol/l}$$

$$n_a = 0.1127 \text{ _mol}$$

$$V_f = 500\_ml$$

## 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
$\Delta H_v$	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**

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

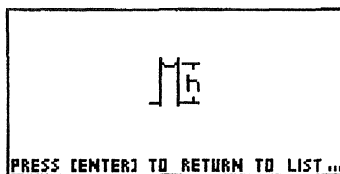
## Capillary Rise

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

$\gamma_l$	surface tension	1_N/m
$\rho_l$	liquid density	1_kg/m^3
$r$	capillary radius	1_m
$\theta$	meniscus angle	1_°
$\rho_v$	vapor density	1_kg/m^3
hex	capillary rise (exact)	1_m

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

#### Given

$$\gamma_l = 46.0\_dyn/cm$$

$$\rho_l = 1.06\_g/cm^3$$

$$r = 0.10\_mm$$

$$\theta = 76\_°$$

$$\rho_v = 1.0\_g/l$$

#### Result

$$h = 88.5\_mm$$

$$hex = 21.4\_mm$$

## 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.

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

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

$$\rho = \frac{mg}{V}$$

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
$\rho$	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 <sup>-2</sup> _mol
V = 933_ml	$\rho = 3.09 \times 10^{-2}$ _g/cm <sup>3</sup>
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)

$$\frac{P_1 \cdot V_1}{n_1 \cdot T_1} = \frac{P_2 \cdot V_2}{n_2 \cdot T_2}$$

$$\frac{P_1 \cdot V_1}{T_1} = \frac{P_2 \cdot V_2}{T_2} \quad (n, \text{ constant})$$

$$P_1 \cdot V_1 = P_2 \cdot V_2 \quad (n, T \text{ constant})$$

$$\frac{P_1}{T_1} = \frac{P_2}{T_2} \quad (n, V \text{ constant})$$

$$\frac{V_1}{T_1} = \frac{V_2}{T_2} \quad (P, n \text{ constant})$$

$$P_1 \cdot V_1 = n_1 \cdot R \cdot T_1$$

$$P_2 \cdot V_2 = n_2 \cdot R \cdot T_2$$

**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

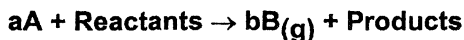
T2 = 25\_°C

**Result**

P2 = 1.21\_mmHg

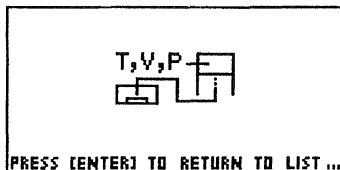
## Gas Over Water

Consider the general chemical reaction:



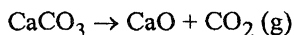
Often, the gaseous product is collected by displacing liquid from a graduated cylinder filled with water. The following equations relate the volume, temperature, pressure, and number of moles of gas to the quantity of reactant consumed in the reaction. Note that the vapor pressure of water at the temperature 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  $\text{CaCO}_3$  according to the reaction:



When 4.6\_g of  $\text{CaCO}_3$  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

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

#### Result

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

### 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

$$P_o = 1.0\_atm$$

$$MWT = 29\_g/mol$$

$$h = 1\_km$$

$$T = 75\_°F$$

#### Result

$$P = 0.89\_atm$$

$$C_o = 4.1\ E-2\_mol/l$$

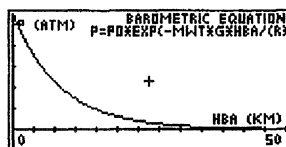
$$C = 3.6\ E-2\_mol/l$$

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 (N<sub>2</sub>) is compressed in a vessel to 100\_l at 300\_°C. What is the pressure?

#### Given

T = 300\_°C  
V = 100\_l  
b = 0.03913\_l/mol  
a = 1.390\_l^2\_atm/mol^2  
ga = 8000\_g  
MWT = 28.0134\_g/mol

#### Result

p = 139.9\_atm  
n = 285.7\_mol  
Z = 1.04  
Tc = 128.3\_K  
Vc = 33.54\_l  
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) .

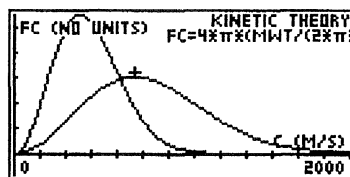
This yields:

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.

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

$$f = \frac{r1}{r2}$$

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\_m^3/s

**Example:** What is the enrichment factor of nitrogen compared to oxygen?**Given****Result**

MWT2 = 28.0134\_g/mol

f = 0.9357

MWT1 = 31.9988\_g/mol

### Collision Theory

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

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

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

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

$$Z1 = \frac{2 \cdot d \cdot \sqrt{\left( \frac{\pi \cdot R \cdot T}{MWT} \right)} \cdot n^2}{NA}$$

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

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

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

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

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

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_mol/(m^2.s)
Z1	bimolecular collision frequency	1_mol/(m^3.s)

d	collision diameter	1_m
$\lambda_{\text{mfp}}$	mean free path	1_m
D	self diffusion coefficient	1_m^2/s
$\rho$	density of gas	1_kg/m^3
$\eta$	viscosity coefficient	1_kg/(m·s)

**Example:** Calculate the surface collision frequency, bimolecular collision frequency, mean free path, and viscosity coefficient of O<sub>2</sub> (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.  $[\text{H}^+]$ , 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<sub>b</sub>, pK<sub>a</sub> and pK<sub>w</sub> 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 <sub>w</sub>	water dissociation constant	1_mol^2/m^6
K <sub>a</sub>	acid dissociation constant	1_mol/m^3
K <sub>b</sub>	base dissociation constant	1_mol/m^3
pH	pH function	1
pOH	pOH function	1
pK <sub>w</sub>	pK <sub>w</sub> function	1
pK <sub>a</sub>	pK <sub>a</sub> function	1
pK <sub>b</sub>	pK <sub>b</sub> function	1

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

Given	Result
H = 0.01_mol/l	pH = 2
K <sub>w</sub> = 1.01 E-14_mol^2/l^2	OH = 1.01 x 10^-12_mol/l
pOH = 12.0	
pK <sub>w</sub> = 14.0	

## 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 <sub>a</sub>	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.

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

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

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

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.

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

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

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

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

Variable	Description	Units
Ca	acid concentration	1_mol/m^3
Cb	base concentration	1_mol/m^3
Ka	acid dissociation constant	1_mol/m^3
Kb	base dissociation constant	1_mol/m^3
Kw	water dissociation constant	1_mol^2/l^2
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, HIO<sub>3</sub> (Ka = 0.162), is dissolved in 1.0 liter of water. What is the pH? Use equations 3-5.

Given	Result
ga = 0.3862_g	Ca = 2.20 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 NaCH<sub>3</sub>COCOO 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  $10 \ll \text{acid/base} \ll 0.1$ .

### Titration (SA/SB)

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

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

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

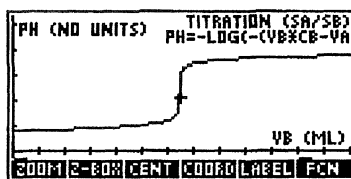


$$pH = -\text{LOG}(H)$$

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

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 x 1E-14\_mol^2/l^2  
Ve = 49.68\_ml  
Va = 100\_ml

### Result

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

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

x1 = 0\_ml  
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.

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

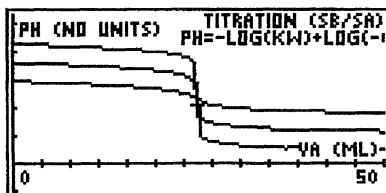
$$pH = -\text{LOG}(K_w) + \text{LOG} \left( \frac{-(V_a \cdot C_a - V_b \cdot C_b)}{2 \cdot (V_a + V_b)} + \frac{1}{2} \cdot \left( \frac{V_a \cdot C_a - V_b \cdot C_b}{V_a + V_b} \right) \right)$$

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

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

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.

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

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

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

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.

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

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

$$Kw = H \cdot OH$$

$$pH = -\log(H)$$

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

Variable	Description	Units
Ca	concentration of acid titrant	1_mol/m^3
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 ( $Kb = 1.80 \times 10^{-5}$ \_mol/l). What is the pH?

### Given

$$Ca = 0.100\_mol/l$$

$$Cb = 0.100\_mol/l$$

$$Kb = 1.80 \times 10^{-5}\_mol/l$$

$$Kw = 1.01 \times 10^{-14}\_mol^2/l^2$$

$$Va = 10.0\_ml$$

### Result

$$H = 2.81 \times 10^{-10}\_mol/l$$

$$OH = 3.59 \times 10^{-5}\_mol/l$$

$$pH = 9.55$$

$$V_b = 30.0\_ml$$

## Thermo/Electrochemistry

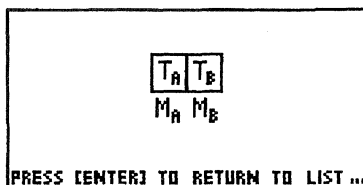
Seven topics in this category focus on thermal and thermodynamic properties, and electrochemical reactions.

Heat Transfer  
Heat Capacity  
Heat Engines  
Nernst Law

Free Energy  
Reduction  
Thermodynamics

### Heat Transfer

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



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

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

$$q_a = -q_b$$

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

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

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

Variable	Description	Units
q <sub>a</sub>	heat flow in or out of material a	1_J
q <sub>b</sub>	heat flow in or out of material b	1_J
m <sub>a</sub>	mass of a	1_kg
m <sub>b</sub>	mass of b	1_kg
c <sub>pa</sub>	specific heat of a	1_J/(kg·K)
c <sub>pb</sub>	specific heat of b	1_J/(kg·K)
C <sub>pa</sub>	molar heat capacity of a	1_J/(mol·K)
C <sub>pb</sub>	molar heat capacity of b	1_J/(mol·K)
T <sub>f</sub>	final temperature	1_K
T <sub>a</sub>	temperature of a	1_K
T <sub>b</sub>	temperature of b	1_K
MWT <sub>a</sub>	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**

cpa (copper) = 0.385\_J/(g·K)

ma = 20\_g

Ta = 90\_°C

cpb (water) = 4.184\_J/(g·K)

mb = 100\_g

Tb = 25\_°C

**Result**

qa = -491\_J

qb = 491\_J

Tf = 26\_°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
$\eta$	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**

Th = 459\_°F

Tc = 25\_°C

**Result** $\eta = 0.42$ C<sub>op</sub> = 1.4**Free Energy**

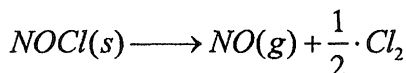
The following equations define free energy.

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

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

Variable	Description	Units
$\Delta G$	free energy change	1_J/mol
$\Delta H$	enthalpy change	1_J/mol
T	temperature	1_K
$\Delta S$	entropy change	1_J/(mol.K)
Keq	equilibrium constant	1

**Example:** The reaction below has a  $\Delta H$  and a  $\Delta S$  of +37.6 kJ/mol and 58.5 J/mol·K at 25 °C.



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

Given	Result
$\Delta H = 37.6 \text{ kJ/mol}$	$\Delta G = 20.2 \text{ kJ/mol}$
$\Delta S = 58.5 \text{ J/(mol}\cdot\text{K)}$	$K_{eq} = 2.94042\text{E-4}$
$T = 25 \text{ }^{\circ}\text{C}$	$(\ln K_{eq} = -8.13)$

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

Given	Result
$\Delta G = 0$	$T = 369\text{ }^{\circ}\text{C}$
$\Delta H = 37.6\text{ kJ/mol}$	$K_{eq} = 1$
$\Delta S = 58.5\text{ J/(mol}\cdot\text{K)}$	$(\ln K_{eq} = 0)$

Note: To solve this problem the temperature "T" must be "Unknown"

$\Delta G$  vs.  $T$  is plotted below (Note: Temperature variable  $T$  must be converted to K before this plot is generated):

**x1 = 200**

$$x_2 = 800$$

**y = autoscale**

## Thermodynamics

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

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

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

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

Variable	Description	Units
C <sub>p</sub>	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 <sub>298</sub>	enthalpy at 298_K	1_J/mol
S <sub>298</sub>	entropy at 298_K	1_J/(mol·K)

**Example:** What is the heat capacity, enthalpy and entropy of Al<sub>2</sub>O<sub>3</sub>(s) at 600\_K? The appropriate constants are given below:

#### Given

$$A = 26.12\_ \text{cal}/(\text{mol} \cdot \text{K})$$

$$B = 4.388 \times 10^{-3} \_ \text{cal}/(\text{mol} \cdot \text{K}^2)$$

$$C = 0$$

$$D = -7.269 \times 10^5 \_ \text{cal} \cdot \text{K}/\text{mol}$$

$$T = 600\_ \text{K}$$

$$H_{298} = 10.422\_ \text{kcal}/\text{mol}$$

$$S_{298} = 142.03\_ \text{cal}/(\text{mol} \cdot \text{K})$$

#### Results

$$C_p = 26.73\_ \text{cal}/(\text{mol} \cdot \text{K})$$

$$\Delta H = 7.251\_ \text{kcal}/\text{mol}$$

$$\Delta S = 28.43\_ \text{cal}/(\text{mol} \cdot \text{K})$$

## 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.

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

$$\Delta C = C_p - C_v$$

Variable	Description	Units
----------	-------------	-------



$\Delta C$	heat capacity difference	$1 \text{ J}/(\text{mol} \cdot \text{K})$
$\alpha$	expansion coefficient	$1 \text{ } 1/\text{K}$
$V$	molar volume	$1 \text{ m}^3/\text{mol}$
$T$	temperature	$1 \text{ K}$
$\epsilon$	compressibility coefficient	$1 \text{ } 1/\text{Pa}$
$C_p$	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

$$\begin{aligned}\alpha &= 2.07 \times 10^{-4} \text{ } 1/\text{K} \\ V &= 18.087 \text{ cm}^3/\text{mol} \\ T &= 25 \text{ } ^\circ\text{C} \\ \epsilon &= 45.3 \times 10^{-6} \text{ } 1/\text{atm}\end{aligned}$$

#### 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:  $aA + bB \rightarrow cC + dD$ .

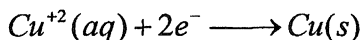
$$E = E_o - 2.303 \cdot \frac{R \cdot T}{n \cdot F} \cdot \text{LOG}(Q) \quad Q = \frac{(C)^c \cdot (D)^d}{(A)^a \cdot (B)^b}$$

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

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

Variable	Description	Units
$E$	cell potential	$1 \text{ V}$
$E_o$	standard cell potential	$1 \text{ V}$
$T$	temperature	$1 \text{ K}$
$n$	moles electrons	$1$
$Q$	reaction quotient	$1$
$a, b, c, d$	product/reactant coefficients	$1$
$A, B, C, D$	product/reactant concentrations	$1 \text{ mol}/\text{m}^3$
$\Delta G$	free energy change	$1 \text{ J}/\text{mol}$
$\Delta G_o$	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**

$$E_0 = 0.34\_V$$

$$T = 49\_<198>^{\circ}\text{C}$$

$$n = 2$$

$$A = 5$$

$$a = 1$$

$$B = C = D = 1$$

$$b = c = d = 0$$

**Result**

$$E = 0.36\_V$$

$$Q = 0.2$$

$$\Delta G = -16.7\_ \text{kcal/mol}$$

$$\Delta G_0 = -15.7\_ \text{kcal/mol}$$

$$K = 4.3 \times 10^{10}$$

## Reduction

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



$$Q = A \cdot t$$

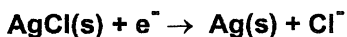
$$ne = \frac{Q}{F}$$

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

$$ma = MWTa \cdot na$$

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**

$$Q = 810\_C$$

$$ne = 8.40 \times 1E-3\_mol$$

$$na = 8.40 \times 1E-3\_mol$$

$$ma = 0.906\_g$$

**Precipitation**

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

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

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

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

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

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

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

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

$$K_{sp} = 108 \cdot fa^3 \cdot fb^2 \cdot s^5 \quad A3B2$$

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

**Variable**

$K_{sp}$

$fa$

**Description**

solubility product

activity coefficient of a

**Units**

\*

\*\*

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

### Case 1: Non-Ideal

#### Given

$$fb = 0.200$$

$$fa = 0.110$$

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

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

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

#### Result

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

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

### Case 2: Ideal

#### Given

$$fb = 1$$

$$fa = 1$$

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

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

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

#### 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:  $A \xrightarrow{k_{1st}} \text{Products}$ , which proceeds in first order, behaves according to the following equations.

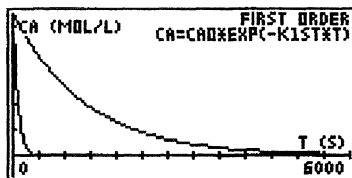
$$\text{Rate} = k_{1st} \cdot C_a$$

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

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

Variable	Description	Units
Rate	rate of reaction	$\text{l\_mol}/(\text{m}^3 \cdot \text{s})$
$k_{1st}$	rate constant	$\text{l\_1/s}$
$C_a$	concentration A (t)	$\text{l\_mol}/\text{m}^3$
$C_{a0}$	concentration A (t=0)	$\text{l\_mol}/\text{m}^3$
t	time	$\text{l\_s}$
$t_{half}$	half life	$\text{l\_s}$

**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

$C_a = 1.0 \text{ mol/l}$  (assumed)  
 $C_{a0} = 0.01 \text{ mol/l}$  (assumed)  
 $t_{half} = 15 \text{ min}$

### Result

$k_{1st} = 7.7 \times 10^{-4} \text{ 1/s}$   
 $t = 5979 \text{ s}$   
 $\text{Rate} = 7.7 \times 10^{-6} \text{ mol}/(\text{m}^3 \cdot \text{s})$

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.

$x1 = 0 \text{ s}$   
 autoscale y

$x2 = 6000 \text{ s}$

### Given

$t_{half} = 1.0 \text{ min}$

### Result

$k_{1st} = 1.16 \times 10^{-2} \text{ 1/s}$

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

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

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

## Parallel First Order

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

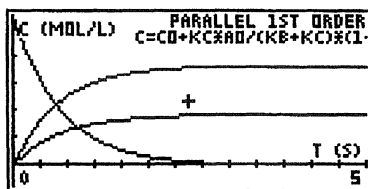
$$A = A_o \cdot e^{-(kb+kc)t}$$

$$B = B_o + \frac{kb \cdot A_o}{kb + kc} (1 - e^{-(kb+kc)t})$$

$$C = C_o + \frac{kc \cdot A_o}{kb + kc} (1 - e^{-(kb+kc)t})$$

Variable	Description	Units
B	concentration B (t)	1 mol/m <sup>3</sup>
B <sub>o</sub>	concentration B (t=0)	1 mol/m <sup>3</sup>
kb	rate constant for reaction B	1/s
A <sub>o</sub>	concentration A (t=0)	1 mol/m <sup>3</sup>
kc	rate constant for reaction C	1/s
t	time	s
C	concentration C (t)	1 mol/m <sup>3</sup>
C <sub>o</sub>	concentration C (t=0)	1 mol/m <sup>3</sup>
A	concentration A (t)	1 mol/m <sup>3</sup>

**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

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

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

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

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

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

and

$$x1 = 0$$

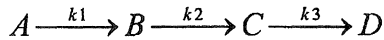
$$y1 = -0.1363$$

$$x2 = 5 \text{ s}$$

$$y2 = 1.0$$

## 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.

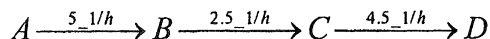
$$A = A_o \cdot e^{-k_1 t}$$

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

$$C = C_o \cdot e^{-k_3 t} + B_o \cdot \left( \frac{k_2 \cdot e^{-k_2 t}}{k_3 - k_2} - \frac{k_2 \cdot e^{-k_3 t}}{k_3 - k_2} \right) + A_o \cdot \left( \frac{k_1 \cdot k_2 \cdot e^{-k_1 t}}{(k_3 - k_1) \cdot (k_2 - k_1)} - \frac{k_1 \cdot k_2 \cdot e^{-k_2 t}}{(k_3 - k_2)(k_2 - k_1)} + \frac{k_1 \cdot k_2 \cdot e^{-k_3 t}}{(k_3 - k_2)(k_3 - k_1)} \right)$$

Variable	Description	Units
A	concentration A (t)	1_mol/m^3
Ao	concentration A (t=0)	1_mol/m^3
B	concentration B (t)	1_mol/m^3
Bo	concentration B (t=0)	1_mol/m^3
C	concentration C (t)	1_mol/m^3
Co	concentration C (t=0)	1_mol/m^3
k1	rate constant for A → B	1_1/s
k2	rate constant for B → C	1_1/s
k3	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  $B_o = C_o = 0\_mol/l$ . Plot the concentration

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

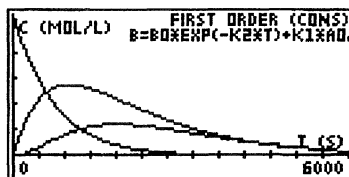
$$x1 = 0\_s \quad x2 = 6000\_s$$

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

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

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

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



## 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)
k2nd	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
thalf	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

$$Cao = 0.10\_ \text{mol/l}$$

$$Ca = 0.08\_ \text{mol/l}$$

$$t = 10.0\_ \text{min}$$

### Result

$$k_{2nd} = 2.08 \times 10^{-3} \_ \text{l/(mol.s)}$$

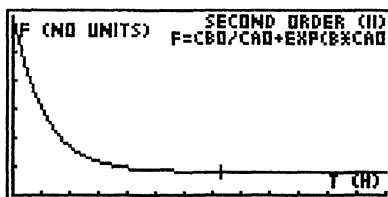
$$t_{half} = 40\_ \text{min}$$



$$a = 2$$

## Second Order (II)

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



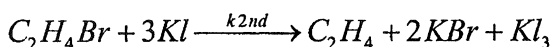
$$\text{Rate} = k_{2nd} \cdot C_a \cdot C_b$$

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

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

Variable	Description	Units
Rate	rate of reaction	1_mol/(m^3·s)
k2nd	rate constant	1_m^3/(mol·s)
Ca	concentration A (t)	1_mol/m^3
Cb	concentration B (t)	1_mol/m^3
f	reactant ratio	1
Cao	concentration A (t=0)	1_mol/m^3
Cbo	concentration B (t=0)	1_mol/m^3
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, k2nd is reported to be 5.0 x 1E-3 1/(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

$$f(0.1\_h) = 6.03$$

Cbo = 0.1531 mol/l  
 k2nd = 5.0 x 1E-3 l/(mol·s)  
 a = 1  
 b = 3  
 t = 0.5 h  
 x1 = 0  
 x2 = 10  
 y = autoscale

f(0.5\_h) = 9.78  
 f(1\_h) = 17.9  
 f(10\_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 x 1E-5 1/s and 3.16 x 1E-3 1/s at 189.7 °C and 251.2 °C respectively. From this data, calculate the activation energy and pre-exponential for this reaction.

### Given

k1 = 2.52 x 1E-5  
 k2 = 3.16 x 1E-3  
 T1 = 189.7 °C  
 T2 = 251.2 °C

### Result

Ea = 159 kJ/mol  
 A = 1.96 x 1E13

## Fractional Life

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

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

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

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

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)<sup>-1</sup>, 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.

		2		HYDROGEN										3 4 5 6 7			
1				3	4	5	6	7	8	9	10	11	12				
	H																
	1																
				1.0079													
PROPS FIND ATW LIST FAST 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:

Hydrogen	
DENSITY: 8.98E-5	
OX STATES: 1	
ELEC CFG: 1S1	
STATE: GAS	
MELTING PT: 14.025	
BOILING PT: 20.268	
GROUP: 1(A)	
FAMILY: -	
MAIN STK PRINT UNITS FONT 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.

```

35  2  CHLORINE  34567
C1  3456789012
17
35.453
PROPS FIND RTW+ LIST FAST UP

```

## 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:

```

RAD                                     PRG
{ HOME GCHEMD }
Enter element symbol
or number to jump to:

C14
SKIP SKIP+ *DEL DEL+ INS = TEST

```

Elements	
Actinium	(Ac)
Aluminum	(Al)
Americium	(Am)
Antimony	(Sb)
Argon	(Ar)
Arsenic	(As)

PROPS FIND ATW+ TABLE FONT UP

## List of Element Names and Symbols

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


```

RAD                                     PRG
( HOME GCHEMD )
Search for:

Cov
SKIP SKIP DEL DEL INS TEST

```

## 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:

```

Hydrogen
Group: 1(1A)
Family: -
At Rad: 0.79
→Cov Rad: 0.32

```

```

Hydrogen
Group: 1(IA)
Family: -
At Rad: 0.79
→Cov Rad: 0.32
1st Ion Pot: 13.598
Electroneg: 2.2
MAIN → STE PRINT UNITS FONT EXIT

```

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:

<b>&lt;-SKIP</b>	Moves the cursor to the beginning of the current word.
<b>SKIP-&gt;</b>	Moves the cursor to the beginning of the next word.
<b>&lt;-DEL</b>	Deletes all the characters in the current word to the left of the cursor.
<b>DEL-&gt;</b>	Deletes all the characters from the cursor's current position to the first character of the next word.
<b>INS</b>	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***

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

<b>FIND</b>	Initiates a search for an element name, number, symbol or property.
<b>LIST</b>	Displays an alphabetical listing of elements and symbols.
<b>FAST</b>	Toggles fast display mode on and off.
<b>FAST •</b>	Indicates that fast mode is on.
<b>DEF</b>	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 CHEW 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 O<sub>2</sub> required to react with 1\_g of CH<sub>4</sub> 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 CHEW 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 CH<sub>4</sub>:

```

      { HOME GCAPPD }      PRG
Enter quantity of
1CH4[g]:

1_g
 _G _KG _MDL _LE _L _ML
  
```

```

      METHANE COMBUSTION
R: {1_g} 1CH4[G]
→R: {0} 2O2[G]
P: {0} 2H2O[L]
P: {0} 1CO2[G]

CALC CONN CLEAR VIEW →STK 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: {1.999999999999}_G 1CH4[G]
→R: {0.79474378866E-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, O<sub>2</sub>) and press **CONV**. This displays a list of available units:

```

METHANE COMBUSTION
R: {1.999999999999}_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 CH<sub>4</sub> and 1\_g of O<sub>2</sub>. 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: {250675025312}_G 1CH4[G]
R: {999999999999}_G 2O2[G]
→P: {562996112352}_G 2H2O[L]
P: {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 O<sub>2</sub> is consumed in the reaction (it's the limiting reagent) whereas only 0.25\_g of CH<sub>4</sub> 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**.

```

PRG
[ HOME GCAPPD ]
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: (.06980875_G) 5FE(AQ)+2
P: (.0137345_G) 1MNI(AQ)+2
P: (.06980875_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: (.06980875_G) 5FE(AQ)+2
P: (.0137345_G) 1MNI(AQ)+2
P: (.06980875_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 <sub>4</sub> (g)	CO <sub>2</sub> (g)
Fe <sup>+2</sup> (aq)	Fe <sup>+3</sup> (aq)
H <sub>2</sub> O(l)	H <sup>+1</sup> (aq)
MnO <sub>4</sub> <sup>-1</sup> (aq)	Mn <sup>+2</sup> (aq)
O <sub>2</sub> (g)	OH <sup>-1</sup> (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 MWT% UP
  
```

```

ALG PRG
{ HOME GCAPPD }
Enter chemical species
Formula[State]±Charge:
[GS] [LL] [CS] [AQ] [C] [ ]
  
```

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
[GS] [LL] [CS] [AQ] [C] [ ]
  
```

```

SPECIES LIBRARY
↑
FE(AQ)+3
H2O(L)
HCl(AQ)+1
MnO4(AQ)-1
Mn(AQ)+2
→ NaOH
  CO2(G)
  CH4(G)
  HCl(AQ)-1
ADD DELETE EDIT CHEW MWT% UP
  
```

```

MnO4[Aq]-1
118.9356_g/mol
0 53.8% MN 46.2%
PRESS [STOI] TO SAVE TO STACK ...
PRESS [ENTER] TO RETURN TO LIST ...
  
```

To evaluate the molecular weight of any species in the list, for example MnO<sub>4</sub>-1(aq), simply move the pointer to that species and press **MWT%**. The molecular weight and the percent

composition are then displayed on the screen, as shown:

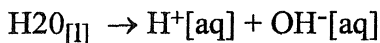
Press **STOI** to store the molecular weight on the calculator stack. Pressing **ENTER** returns you to the Species Library. Press **CHEW** to display the species on the screen:

## 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

{ HOME GCAPPD }	PRG
Edit reaction name:	
WATER DISSOCIATION	
←SKIP←SKIP←←DEL←DEL←INS←←STK	

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 F DELETE EDIT STOIC UP

Pick species:	
CH4(G)	
CO2(G)	
Fe(AQ)+2	
Fe(AQ)+3	
→H2O(L)	
HCl(AQ)+1	
MnO4(AQ)-1	
Mn(AQ)+2	
ADD	DELETE EDIT CHEM MWTS EXIT

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 H<sub>2</sub>O[L] and press **ENTER**.

{ HOME GCAPPD }	PRG
Enter coefficient:	
1	
←SKIP←SKIP←←DEL←DEL←INS←←STK	

WATER DISSOCIATION	
→R: 1H2O(L)	
ADD R	ADD F 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 H<sub>2</sub>O 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

```

**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 [ENTER] 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:

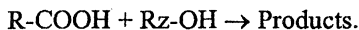
## Entering Molecular Formulas

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 <sub>3</sub>	HNO3
Ca(NO <sub>3</sub> ) <sub>2</sub>	C  A   NO3   2

After unlocking alpha-entry mode to enter parentheses or to move the cursor, it is necessary to press  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 RCO<sub>2</sub>H, Rz-OH, and Pro into the Species Library. After these are entered, you will be prompted for the molecular weight (in -g/mol only) of the unknown symbols R, Rz, and Pro. Once defined, these symbols are accessible to all species in the Species Library.

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

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

**EDIT**

**ENTER**

**EXIT**

**→STK**

**STOIC**

**UP**

**VIEW**

a chemical reaction.

Edits a chemical reaction or a reactant or a product.

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

Exits the Stoichiometry solving screen.

Copies selected entry to calculator stack.

Enters the stoichiometry solving screen after the selected chemical reaction is mass and charge balanced.

Moves up one level in the menu structure.

Displays entries too wide to fit on the screen. It is not nctional if the line does fit on the screen.

## ***Species Library Softkeys***

**ADD**

Adds a new chemical species to the Species Library.

**CHEW**

Displays a chemical species on the screen in the da Vinci's chemical Equation Writer format.

**DELETE**

Deletes a chemical species from the Species Library.

**EDIT**

Edits a chemical species.

**MWT%**

Displays the molecular weight and percent composition of the selected species.

**UP**

Returns to the main menu.



# 5 Constants Library

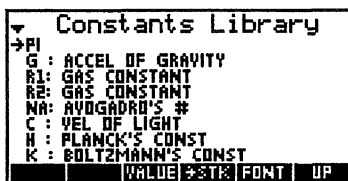
## In This Chapter

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

- Using the Constants Library
- Constants Library Softkeys

## Using the Constants Library




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




$\pi$	$\pi$
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
hb	Dirac's constant
q	Electron charge
eo	Permittivity of vacuum
me	Electron mass
re	Classical electron radius
mp	Proton rest mass
R $\infty$	Rydberg's constant
$\alpha$	Fine structure constant
ao	Bohr radius
$\mu_B$	Bohr magneton
$\lambda$	Wavelength for 1eV
$\lambda_c$	Compton's wavelength
$\alpha$	Stefan-Boltzmann
c1	First radiation constant
c2	Second radiation constant
Vt	Thermal voltage at 300_K
$\mu_0$	Permeability of free space

$\phi_0$	Magnetic flux quantum
F	Faraday constant
$\mu_e$	Electron magnetic moment
$\mu_p$	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

<b>VALUE</b>	Displays the value of the constant with units on the screen. Press  to return to the constants list.
<b>-&gt;STK</b>	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.
<b>FONT</b>	Toggles between large and small display font.
<b>UP</b>	Exits to the main menu.
<b>MAIN</b>	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 <sub>2</sub> 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 - H<sub>2</sub>O 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

<b>FONT</b>	Toggles the display font between condensed and large sizes.
<b>UP</b>	Moves up one level in the menu structure.
<b>MAIN</b>	Exits to the main menu.
<b>-&gt;STK</b>	Copies selected entry to calculator stack.
<b>PRINT</b>	Allows you to print a data field or the entire list of data to an IR printer.
<b>ALL</b>	Sends all the data in a list to an IR printer.
<b>ONE</b>	Sends the data in the field selected by the pointer to an IR printer
<b>UNITS</b>	Toggles key. Indicates units are off. When off, all variables are assumed to be SI.
<b>UNIT</b>	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@dvvg.com](mailto:support@dvvg.com)  
Website URL <http://www.dvvg.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  $360^\circ$ . 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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# Index

Accessing Available Libraries, 3  
 Accessing equations, 6  
 Accessing the General Chemistry Pac, 3  
 Acids/Bases, 46  
     Henderson-Hasselbach  
     equation, 49  
     pH Function, 46  
     Strong Acids, 47  
     Strong Bases, 48  
     Titration (SA/SB), 50  
     Titration (SB/SA), 51  
     Titration (WA/SB), 51  
     Titration (WB/SA), 54  
     Weak Acids/Bases, 49  
 Activity Coefficient, 61  
 Adding Products, 78  
 Adding Reactants, 78  
 Adding Stoichiometric coefficients, 79  
 Adding units, 8  
 Additional Units Softkeys, 9  
 Atomic Number, 70  
 Atomic Radii, 70  
 Atomic Weight, 70  
 Atoms/Molecules, 20  
     Diatomic Moment, 27  
     Hydrogen Energy, 22  
     Light, 22  
     Mass/Mole/Atom, 21  
     Quantum, 21  
     s, p, d and f orbitals, 23  
         Radial functions, 23  
         Angular wave  
         functions, 25  
         Symmetric Moment, 28  
 Autoscaling Y, 14  
 Average velocity, 44  
 Azimuthal quantum number, 26  
  
 Bad guesses, 16  
 Bent Molecules, 38  
 Boiling point elevation, 32  
 Boiling point of elements, 70  
 Born-Haber Cycle, 32  
  
 Calculating Molecular weights, 81

Capillary rise, 37  
 Chemical Equation Writer, 74  
 Clausius-Clapyron equation, 37  
 Colligative Properties, 35  
 Compressibility Coefficient, 31  
 Conjugate base, 33  
 Constants Library, 83  
 Covalent Radii, 70  
  
 de Broglie wavelength, 22  
 Debye Heat Capacity Model, 29  
 Default units, 8  
 DEL, 5, 72  
 Density of elements, 70  
 Displaying a constant on the screen, 84  
 Displaying equations, 6  
  
 Editing Text Entries, 5  
 Editing the Browser, 5  
 Einstein Heat Capacity Model, 29  
 Electron Configuration, 70  
 Electronegativity, 70  
 Element mass number, 70  
 Element Physical State, 70  
 Ellipsis ..., 4  
 Environmental limits of card, 88  
 Equation Library, 5, 20  
  
 Family, 70  
 Font size, 4  
 Freezing point lowering, 35  
  
 Gases, 38  
     Barometric equation, 41  
     Collision Theory, 45  
     Graham's Law, 44  
     Ideal Gas, 38  
     Kinetic Theory, 43  
     State Changes, 39  
     Van der Waal equation, 42  
     Gas over water, 40  
 GCAPPD Directory, 17  
 GCpar Variable, 17  
 Global Variables, 17  
 Group, 70

HP 48 equationwriter, 6  
Hydrogen wave functions, 22

Initializing, 17  
Installing an Application Card, 1  
Ionization Potential, 70

Kinetics, 62  
    Arrhenius Law, 68  
    Consecutive First Order, 65  
    First Order, 63  
    Fractional Life, 69  
    Parallel First Order, 64  
    Second Order (I), 66  
    Second Order (II), 67

Main Menu, 3  
Managing Units, 9  
Maxwell-Boltzman, 43  
Mean Free Path, 73  
Melting point of elements, 70  
Merged Memory, 2  
Molality, 36  
Molarity, 33  
Mole-fraction, 33  
Moment of Inertia, 27  
Most probable velocity, 43  
Moving around the screen, 4

ON key, 2  
Operating Efficiency of heat engines, 56  
Oxidation State, 70

Periodic Table, 70  
    Finding Properties, 71  
    Moving around, 71  
    Searching for an property, 70

Plotting -Proper form of equations, 16  
Plotting equations, 12  
Plotting multiple graphs, 15  
Precipitation, 61

    A2B molecule, 61  
    A2B3 molecule, 61  
    A3B molecule, 61  
    A3B2 molecule, 61  
    AB molecule, 61  
    AB2 molecule, 61  
    AB3 molecule, 61

Print function, 72  
Putting constants on the stack, 84

Reference Data  
    pKas of common acids, 85

Reference Library, 85  
    Air Composition, 85  
    Bond Distances, 85  
    Bond Energies, 85  
    Common Anions, 85  
    Expansion Coefficients, 85  
    Solubility Products, 85  
    Van der Waals Constants of

Gases, 85  
    Vapor Pressure of water, 85  
    Water Dissociation constants,

85  
References, 91  
Removing an Application Card, 2  
Root-mean-square velocity, 44

Search Mode, 5  
Seeding the Solver, 16  
Selecting equations, 6  
Service

    Service charge, 87  
    Shipping instructions, 88  
Service (if card requires), 87

SI units, 9  
Softkey

    ABOUT, 2  
    ADD, 81  
    ALL, 6-3  
    CALC, 7  
    ChEW, 74  
    CLEAR, 76  
    CONV, 9, 76  
    COORD, 14  
    ECHO, 17  
    EQNS, 6  
    FAST, 71  
    FIND, 71  
    FONT, 4  
    GCON, 2  
    INS, 5, 72  
    KEYS, 15  
    KNOW, 16  
    MAIN, 86  
    MWT%, 78  
    ON, 1  
    ONE, 81  
    PLOT, 15

PRINT, 86  
 PROP, 70  
 QUIT, 4  
 SKIP, 4, 72  
 SOLVE, 11  
 STK, 5  
 STOIC, 75  
 UNITS, 72  
 UP, 8  
 VARS, 7  
 WANT, 12  
 Solids/Liquids, 28  
     Blackbody Radiation, 30  
     Born-Haber Cycle, 32  
     BP/FP Colligative, 35  
     Bragg Law, 31  
     Capillary rise, 38  
     Clausius-Clapyron equation,  
 37  
     Concentration, 32  
     Equation of State, 30  
     Heat Capacity, 29  
     Melting Point, 31  
     Raoult's Law, 34  
 Solving a single equation, 5  
 Solving equations, 10  
 Solving multiple equations, 11  
 SPEC Variable, 17  
 SPECCODE Variable, 17  
 Species Library, 76  
 Stoichiometry, 74  
     Creating Chemical  
 Equations, 78  
     Limiting Reagents, 76  
     Selecting chemical equations,  
 74  
     Stoichiometry with solutions,  
 77  
     Theoretical Yields, 75  
 Summary of Functions  
     Periodic Table, 72  
     Reference Library, 86  
     Stoichiometry, 81  
 Tagging Variables (calculated), 12  
 Tagging variables (knowns), 12  
 Tagging variables (want), 12  
 Thermo/Electrochemistry, 55  
     Free Energy, 56  
     Heat Capacity, 58  
     Heat Engines, 56  
     Heat Transfer, 55  
     Nernst law, 59  
     Reduction, 60  
     Thermodynamics  
         (Calculations), 57  
     Unit conversion, 88  
     Variable Definitions, 7  
     Viewing Wide Entries, 4  
     Warranty, 87