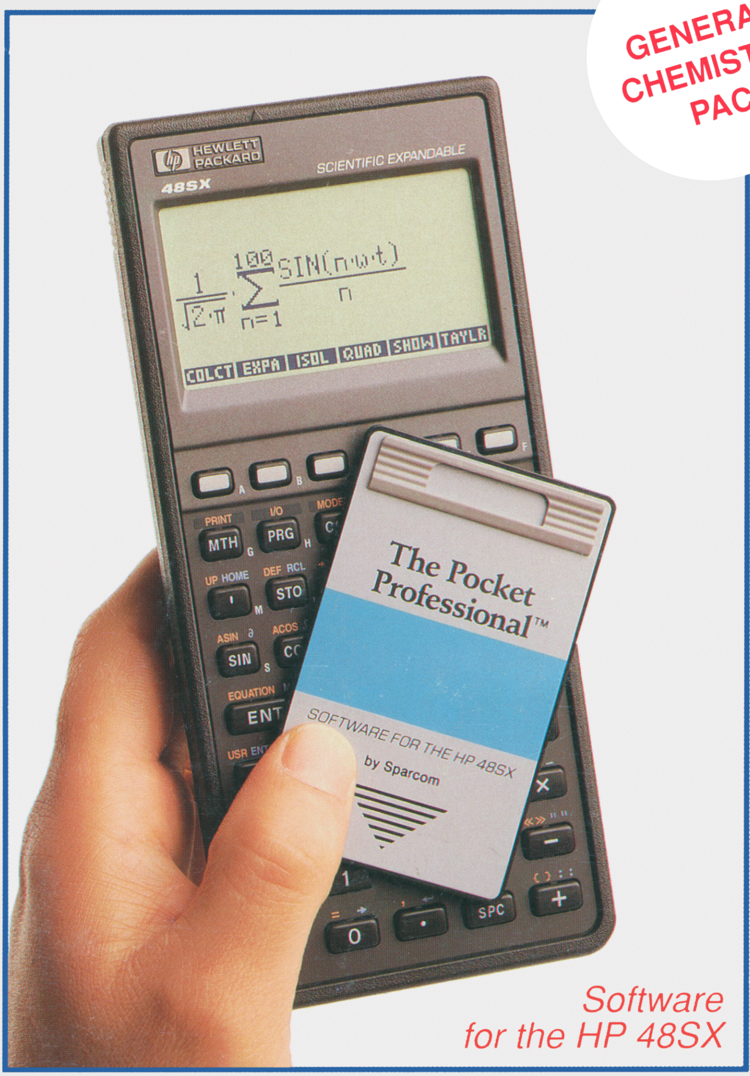
Sparcom

Pocket Professional™

OWNER'S MANUAL

GENERAL CHEMISTRY PAC



Software for the HP 48SX

The Pocket Professional™

General Chemistry Application Pac

Owner's Manual

SPARCOM®

Edition 2 November, 1991

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Notice

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General Chemistry Application Pac Changes

The following changes were made to the General Chemistry Application Pac for version 2.5:

✔ Browser: Cursor movement and scrolling speed have been increased.

✔ Constant Library: Constants have been updated to conform to latest accepted values.

<u>HP 48GX USERS ONLY</u>: You should install the application card in Port 1 for two reasons:

1. Application cards installed in Port 1 will execute ~ 20% faster than those installed in Port 2.

2. Application cards installed in Port 2 may experience long pauses (~ 5-10 seconds or more) intermittently during operation. This is not a software defect. It is caused by the new memory architecture of the extended HP 48GX Port 2, which is different from the HP 48SX Port 2. Such pauses will not occur if the application card is operated from Port 1 of the HP 48GX or if it is oporated from either port of the HP 48SX.

General Chemistry Application Pac Manual Changes

These changes apply to the General Chemistry Application Pac Manual, Edition 2, November 1991.

Changes for the HP 48GX

General: To display all libraries on the HP 48GX, press → LIBRARY instead of ← LIBRARY.

General: On the HP 48GX, the ATTN key has been replaced by CANCEL.

General: To perform a screen dump on the HP 48GX, press ON – /0 instead of ON–MTH.

General: To display an item too wide for the display on the HP 48GX, press → CMD instead of → VISIT.

Page 1-19: On the HP 48GX, COORD has been renamed to (X, Y).

Changes for Version 2.5

General: Because the constants have been updated, some of the examples may differ slightly from the manual.

Page 1-3: Accessing the General Chemistry Application Pac: Picture menu keys should read GCAP GCON ABOUT instead of GCAP GCON DERG DERUB DERUV ABOUT.

Page 1-5: Using the Main Menu: The Constant Library now includes 31 constants.

Page 1-6: Using the Search Mode: The search mode is now case-insensitive.

Page 1-10: Using the Solver Function: After pressing SOLVE, press UNITS to turn units on.

Page 2-16: Concentration: Example 1: ma=5.8E-2_mol/kg.

Page 2-21: Ideal Gas: Example: ρ=3.09E-3_g/cm^3.

Page 2-25: Barometric Equation: Before plotting, unmark h as known.

Page 2-27: Kinetic Theory: Example: cavg=445.5382_m/s. Plot equation 1. Use autoscale instead of the y1 and y2 values.

Page 2-34: Weak Acids/Bases: Example: Use equations 1, 4, and 5, not 3-5.

Page 2-42: Free Energy: Plot equation 1.

Page 2-43: Thermodynamics: Example: ΔS=28.7_cal/(mol*K).

Page 2-44: Heat Capacity: Example: ΔC=.517_J/(mol*K).

Page 2-48: First Order: Example: Ca=.01_mol/l, Cao=1_mol/l, Rate=7.7E-7_mol/(cm^3*s).

Page 2-53: Second Order (II): Example: Solve equation 2.

Page 3-3: List of Element Names and Symbols: Picture should include the title, "Elements"; 3rd picture should read GCHEMD instead of GCAPPD in status area.

Page 5-1: Using the Constants Library: The Constant Library now includes 31 constants.

Table of Contents

Chapter 1: Getting Started

Chapter 2: Equation Library

Chapter 3: Periodic Table

Chapter 4 : Stoichiometry

Chapter 5: Constants Library

Chapter 6: Reference Library

Appendix A: Warranty and Service

Appendix B: Questions and Answers

Appendix C: References

Chapter 1

Getting Started

In This Chapter

- ☐ Installing and Removing the Card
- ☐ Using the Main Menu
- ☐ Using the Equation Library
- ☐ What You Should Know About the Solver
- ☐ Sparcom's GCHEMD Directory
- ☐ Equation Library Structure
- ☐ Summary of Softkeys

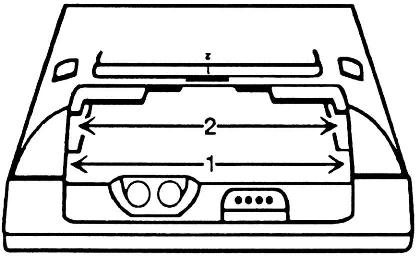
Sparcom's Pocket Professional™ software is the first of its kind, developed to provide speed, efficiency and portability to students and professionals in technical fields. When you slide the Pocket Professional™ General Chemistry Application Pac into your HP 48SX, your calculator is instantly transformed into an electronic "textbook," ready to efficiently solve your chemistry problems. The software is organized into six major sections: Equation Library, Periodic Table, Stoichiometry, Species Library, Constants Library and Reference Library. . . all in an efficient, menu-driven format.

Installing and Removing the Card

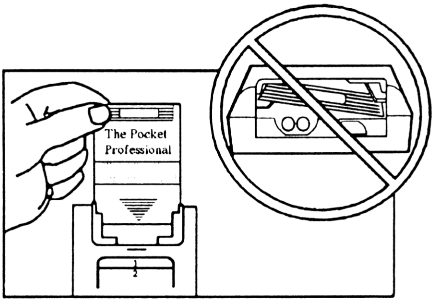
The HP 48SX has two ports for installing plug-in cards. You can install the software card in either port. Be sure to **turn off the calculator** while installing or removing the card. Otherwise, user memory may be erased.

To Install the Application Card

1. Turn off the calculator. Do not press ON until you have completed the installation procedure.
2. Remove the port cover. Press against the grip lines and push forward. Lift the cover to expose the two plug-in ports.



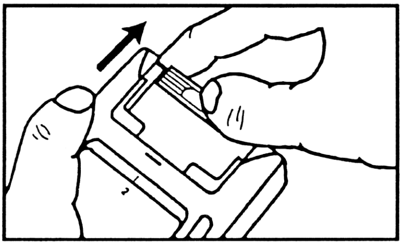
3. Select either empty port for the Pocket Professional card.
4. Position the card just outside the slot. Point the triangular arrow on the card toward the calculator port opening, as shown.
5. Slide the card firmly into the slot. After you first feel resistance, push the card about 1/4 inch further, until it is fully seated.



6. Replace the port cover.

To Remove the Application 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.

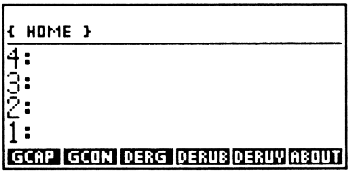


3. Replace the port cover. If you want to remove a RAM card that contains merged memory, **you must free the** merged memory before removing the card. Otherwise, you are likely to **lose data stored in user memory.** See the *HP 48SX Owner's Manual* for instructions.

Accessing the General Chemistry Application Pac

After you turn your calculator [ON], there are three ways to start the software.

First Method: Press [⬅] [LIBRARY] to display all libraries available to the HP 48SX. Find and press **GCAP** to enter the General Chemistry Application Pac library directory. The screen displays new menu keys or "softkeys" along the bottom, as shown:



```
{ HOME }
4:
3:
2:
1:
GCAP GCON DERG DERUB DERUV ABOUT
```

Press the **GCAP** softkey again to start the application.

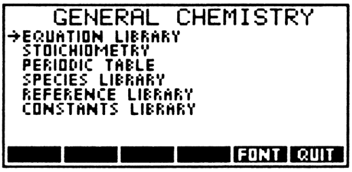
Pressing the last softkey in the row, **ABOUT**, displays a screen containing the revision number of the software. (Press [ATTN] to exit the revision screen). The **GCON** softkey accesses the Constants Library, described in Chapter 5. The other softkeys access programs required by the software and are not available to the user.

Second Method: Type in the letters GCAPP (using alpha entry mode) and press ENTER.

Third Method: Add the command "GCAPP" to the CST (custom) menu (for more information, refer to Chapter 15 of the *HP-48SX Owner's Manual,* "Customizing the Calculator"). After the command has been added, press CST, then press GCAP to start the software.

Using the Main Menu

After you start the application, the main menu screen appears:



GENERAL CHEMISTRY
→EQUATION LIBRARY
STOICHIOMETRY
PERIODIC TABLE
SPECIES LIBRARY
REFERENCE LIBRARY
CONSTANTS LIBRARY

The main menu lists the six main functions of the General Chemistry Application Pac in a "browser" menu format. "Browser" refers to the ability to use the cursor keys (▲, ▼) to move the pointer to the menu item you wish and to press ENTER to select an item or function.

Each function in the main menu is briefly described below, and is discussed in detail in the next five chapters of this manual.

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	Displays properties for each element of the Periodic Table.

Stoichiometry	Lets you enter your own chemical equation, check mass and charge balance, and perform theoretical yield and limiting reagent calculations.
Constants Library	Lists the values for 29 common constants.
Reference Library	Selected reference data useful in solving today's practical problems.

*The Species Library is discussed in Chapter 4: "Stoichiometry."

The "softkeys" located along the bottom of each screen give you options that relate to that screen. The following softkeys appear in the main menu screen. A summary of common softkeys used throughout the software program is given at the end of this chapter.

FONT	Toggles between the small and medium fonts for optimum viewing of results.
QUIT	Exits the General Chemistry Application Pac.

Moving Around the Screen

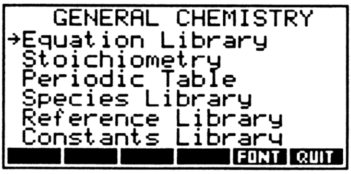
Use the ▲ and ▼ keys to move the pointer up and down in the menu list. Pressing ↰▼ moves the pointer to the bottom of the screen, or pages down (one screen at a time) if the pointer is already at the bottom of the screen. Pressing ↰▲ moves the pointer to the top of the screen, or pages up. Pressing ↱▼ moves the pointer to the bottom of the list, and ↱▲ moves the pointer 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 ↱ VISIT to display the rest of the text. Press ATTN or ENTER to return the display to the beginning of the line.

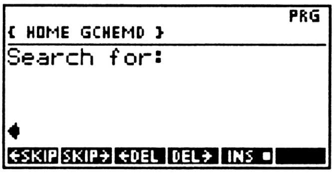
Changing the Font Size

The default font for the General Chemistry Application Pac displays information in small, uppercase letters only. Pressing **FONT** displays the information in a medium font, which is case-sensitive. The font size stays medium (shown below) until you press **FONT** again:



Using the Search Mode

When menu lists are long, it may be faster to locate an item using the search mode. To initiate a search, press the α key, which displays the following screen:



Search for:

The calculator is now in *alpha* entry mode, as indicated by the alpha (α) annunciator at the very top of the screen. 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. (See the *HP 48SX Owner's Manual*, "The Keyboard and Display", for a complete description of how the alpha mode operates). Type the first letter or letters of the name you want to search for, to create the *search string*, and press ENTER. **The search function is case-sensitive.** To enter a lower case letter in the alpha entry mode, press the ↰ key before typing in each letter.

Editing Text Entries

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

←SKIP	Moves the cursor to the beginning of the current word.
SKIP→	Moves the cursor to the beginning of the next word.

←DEL	Deletes all the characters in the current word to the left of the cursor.
DEL→	Deletes all the characters from the cursor's current position to the first character of the next word.
INS	Toggles between insert and typeover modes.
→STK	Accesses a version of the "Interactive Stack" in which only the echo function is available. (For more information on the Interactive Stack, see Chapter 3 of the *HP 48SX Owner's Manual*).

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:

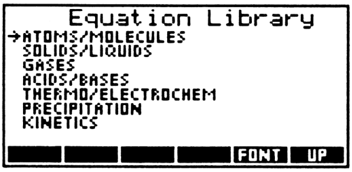
- Select the equation category and topic from the main menu.
- List all the equations in a topic.
- Solve a specific equation or a set of equations.
- View a description of the variables.
- View a figure that illustrates the problem.
- Plot the equation.

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.

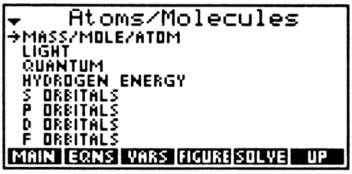
Accessing Equations

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:



```
     Equation Library
→ATOMS/MOLECULES
 SOLIDS/LIQUIDS
 GASES
 ACIDS/BASES
 THERMO/ELECTROCHEM
 PRECIPITATION
 KINETICS
```

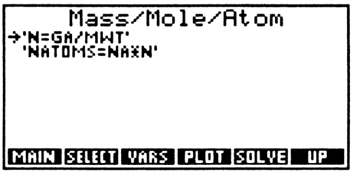
Move the pointer to the category "ATOMS/MOLECULES," and press ENTER to display the list of topics:



```
▾    Atoms/Molecules
→MASS/MOLE/ATOM
 LIGHT
 QUANTUM
 HYDROGEN ENERGY
 S ORBITALS
 P ORBITALS
 D ORBITALS
 F ORBITALS
```

Selecting and Displaying Equations

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

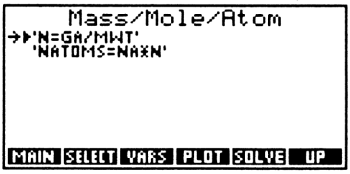


```
     Mass/Mole/Atom
→'N=GA/MWT'
 'NATOMS=NA*N'
```

This screen lists all the equations in the current topic. In the case of mass-to-mole conversions, 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:

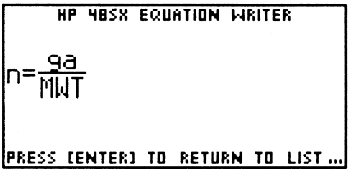


Mass/Mole/Atom

→▸'N=GA/MWT'

'NATOMS=NA*N'

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:



HP 48SX EQUATION WRITER

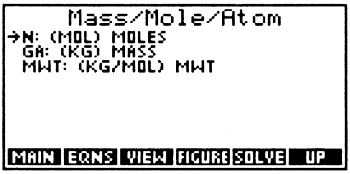
$$n=\frac{ga}{MWT}$$

PRESS [ENTER] TO RETURN TO LIST ...

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 ATTN 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

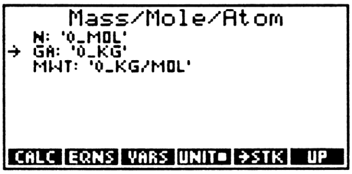
GA: (KG) MASS

MWT: (KG/MOL) MWT

Using the Solver Function

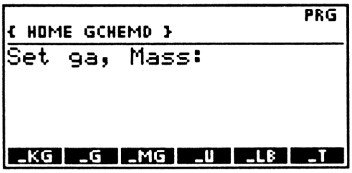
The Sparcom "solver" is a software function that simplifies the job of setting up equations to be calculated by the HP 48SX. The solver function is discussed in more detail later in this chapter, under "What You Need to Know About the Solver."

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:



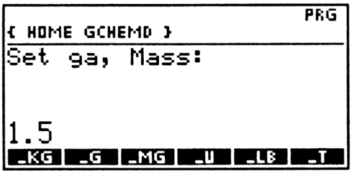
```
       Mass/Mole/Atom
   N: '0_MOL'
→  GA: '0_KG'
   MWT: '0_KG/MOL'
```

To enter the mass of iron, move the pointer to ga and press ENTER. This displays the following screen:



```
                                PRG
{ HOME GCHEMD }
Set ga, Mass:
```

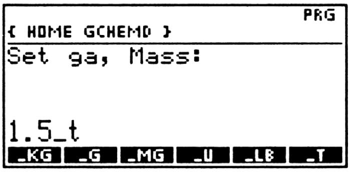
Enter the mass of iron at the prompt.



```
                                PRG
{ HOME GCHEMD }
Set ga, Mass:

1.5
```

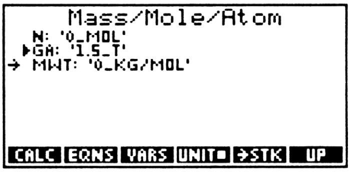
After the mass has been entered, you may assign units to your entry by pressing the appropriate unit softkey. If you choose not to add units and press ENTER at the prompt, SI units will be assumed. In some cases, more units are available than the six softkeys displayed in the first screen. In these cases, press NXT to display the next page of additional units. For a complete description of units available in the HP 48SX, see Chapter 13 of the *HP 48SX Owner's Manual*.

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



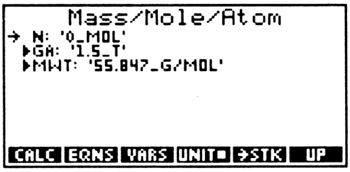
```
                                 PRG
{ HOME GCHEMD }
Set ga, Mass:

1.5_t
```

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



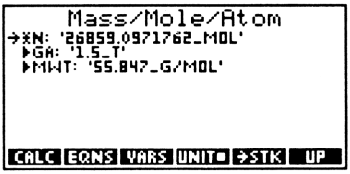
```
       Mass/Mole/Atom
  N: '0_MOL'
 ▶GA: '1.5_T'
→ MWT: '0_KG/MOL'
```

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: '0_MOL'
 ▶GA: '1.5_T'
 ▶MWT: '55.847_G/MOL'
```

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:



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

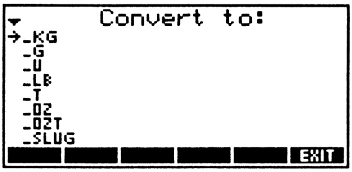
The * by n indicates that this value was calculated and was not user specified.

Converting Data to Different Units

Suppose you want to convert the mass of iron just computed to pounds. First press NXT to view a new page of softkeys:

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

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



```
▾       Convert to:
→_KG
 _G
 _U
 _LB
 _T
 _OZ
 _OZT
 _SLUG
```

Move the pointer to _lb (_LB when condensed font is used) and press ENTER.

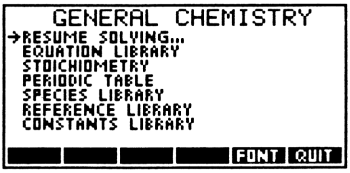
```
      Mass/Mole/Atom
 *N: '26859.0971762_MOL'
→▶GA: '3306.93393277_LB'
 ▶MWT: '55.847_G/MOL'
```

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 ATTN exits the General 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:



GENERAL CHEMISTRY
→RESUME SOLVING...
EQUATION LIBRARY
STOICHIOMETRY
PERIODIC TABLE
SPECIES LIBRARY
REFERENCE LIBRARY
CONSTANTS LIBRARY

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 General 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:

$$gs = ga + gb$$

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

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

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

$$gs = vs \cdot \rho s$$

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

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

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

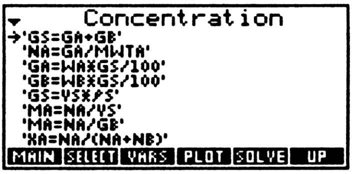
$$wa + wb = 100$$

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

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

$$gb = vb \cdot \rho b$$

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



```
▾          Concentration
→'GS=GA+GB'
 'NA=GA/MWTA'
 'GA=WA*GS/100'
 'GB=WB*GS/100'
 'GS=VS*ρS'
 'MA=NA/VS'
 'MA=NA/GB'
 'XA=NA/(NA+NB)'
```

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

Variable	Description	Units
ga	mass solute	1_kg
gb	mass solvent	1_kg
na	moles solute	1_mol
nb	moles solvent	1_mol
MWTa	molecular weight solute	1_kg/mol
MWTb	molecular weight solvent	1_kg/mol
wa	weight % solute	1

wb	weight % solvent	1
ρb	pure solvent density	1_kg/m^3
vb	volume of solvent	1_m^3
gs	mass solution	1_kg
vs	volume solution	1_m^3
ρs	density solution	1_kg/m^3
Ma	molarity solution	1_mol/m^3
ma	molality solution	1_mol/kg
xa	mole fraction solution	1
ppma	solute concentration	1

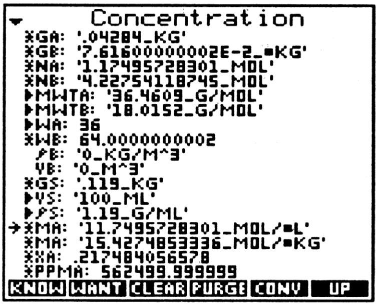
Solving the Equation Set

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.

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

Given	Result
MWTa = 36.4609_g/mol (HCl)	Ma = 11.7_mol/l
MWTb = 18.0152_g/mol (H_2O)	
wa = 36.0	
vs = 100._ml	
ρs = 1.19_g/ml	

With the information given, the solver found all variables but two, ρb 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:

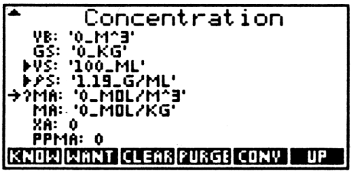


```
▼       Concentration
  *GA: '.04284_KG'
  *GB: '7.61600000002E-2_▪KG'
  *NA: '1.17495728301_MOL'
  *NB: '4.22754118745_MOL'
  ▶MWTA: '36.4609_G/MOL'
  ▶MWTB: '18.0152_G/MOL'
  ▶WA: 36
  *WB: 64.0000000002
   ρB: '0_KG/M^3'
   VB: '0_M^3'
  *GS: '.119_KG'
  ▶VS: '100_ML'
  ▶ρS: '1.19_G/ML'
→*MA: '11.7495728301_MOL/▪L'
  *MA: '15.4274853336_MOL/▪KG'
  *XA: .21748405657 8
  *PPMA: 562499.999999
```

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 NXT 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:



```
▲       Concentration
    VB: '0_M^3'
    GS: '0_KG'
   ▶VS: '100_ML'
   ▶ρS: '1.19_G/ML'
 →?MA: '0_MOL/M^3'
    MA: '0_MOL/KG'
    XA: 0
    PPMA: 0
```

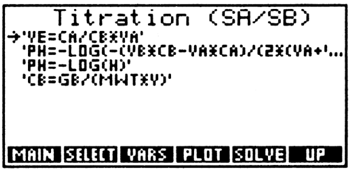
If you tag Ma (molarity) and press **CALC** the solver calculates for Ma only, rather than solving for the entire set. It is possible to tag more than one variable in the list.

Plotting One Equation

Any equation in the equation library that is of the form: y = f (a,b,. . .) can be easily plotted using the General Chemistry Application Pac. To plot an equation, the dependent variable, y (on the left), and the desired independent variable, a or b or c, etc. (on the right), must be unknown (no triangular tag). However, all other variables must be known.

Finding and Selecting the Equation

As an example, plot the titration curve (the pH versus the volume of added base) of the titration: 25_ml of a 0.1_mol/l strong acid with a 0.1_mol/l strong base at 25°C. The equations that describe strong acid/strong base titrations are filed in the ACIDS/BASES category of the Equation Library, under the topic TITRATION (SA/SB). The equation screen for this topic is shown below:



```
       Titration (SA/SB)
→'VE=CA/CB*VA'
 'PH=-LOG(-(VB*CB-VA*CA)/(2*(VA+'…
 'PH=-LOG(H)'
 'CB=GB/(MWT*V)'
```

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

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

where:

Ca	acid concentration	1_mol/m^3
Cb	base concentration	1_mol/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
pH	pH value	1

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 = 1.01×10^{-14}_mol^2/l^2

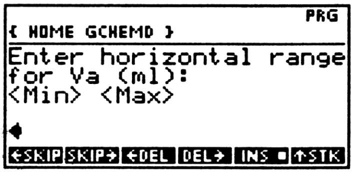
Use the **CONV** softkey to change the units of Vb to _ml for the plot.

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

Entering the X and Y Coordinates

The first prompt asks whether you want to erase the previous plot and reset the axes, **YES**, or whether you want the new plot drawn over any existing graphics already on the screen, **NO**. To continue with this example, at the prompt enter **YES** to clear all previous plots from the screen.

Now enter the minimum and maximum x coordinates for the graph, starting with the x range as x1 x2. Type the coordinates for the plot on the same line, separated by a space (use the SPC key). Plot between 0 and 50 milliliters of added base, since this is approximately twice the equivalent volume:

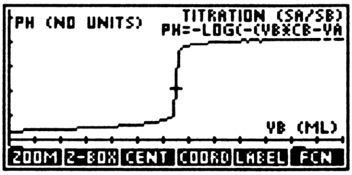


```
                                  PRG
{ HOME GCHEMD }
Enter horizontal range
for Va (ml):
<Min> <Max>
```

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.

NOTE: When the independent variable has units of °C or °F, plots may not autoscale correctly.

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 48SX unit manager. **If the units are turned off** (by pressing **UNIT■** at the solver screen) **the plot takes only 40 seconds** (plus 10 seconds for autoscaling).

However, as described earlier in this chapter under "Managing Units," when you turn off units, all user entered values are converted to SI units. Therefore, when you enter the x-axis coordinates, you need to enter them as "0 0.000050" to account for concentration units of $\_m^3$ instead of _ml. The plot will also be displayed in SI units.

Softkeys for the Plot Function

The softkeys shown in the above plot are plot function keys in the HP 48SX. 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 Chapter 18 of the *HP 48SX Owner's Manual.*

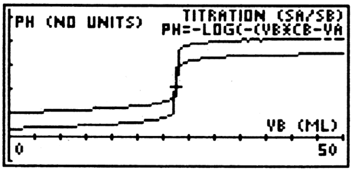
Note that the **SLOPE** and **F** keys, inside the HP 48SX **FCN** submenu, are supported by the General Chemistry Application Pac only when SI units are used (units are off).

You can remove the softkeys from the plot to expose more of the graph by pressing NXT NXT and **KEYS**. Press ATTN 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 48SX 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 48SX numerical root-finder. For the selected equations(s), the solver screen lists all the variables, shows whether they are known (triangular tag), unknown (no tag), wanted ("?" tag), or already calculated (*); and whether units are on or off.

Once you set these parameters, pressing **CALC** activates the HP 48SX 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 Chapter 17 of the *HP 48SX 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 48SX'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.

Sparcom's GCHEMD Directory

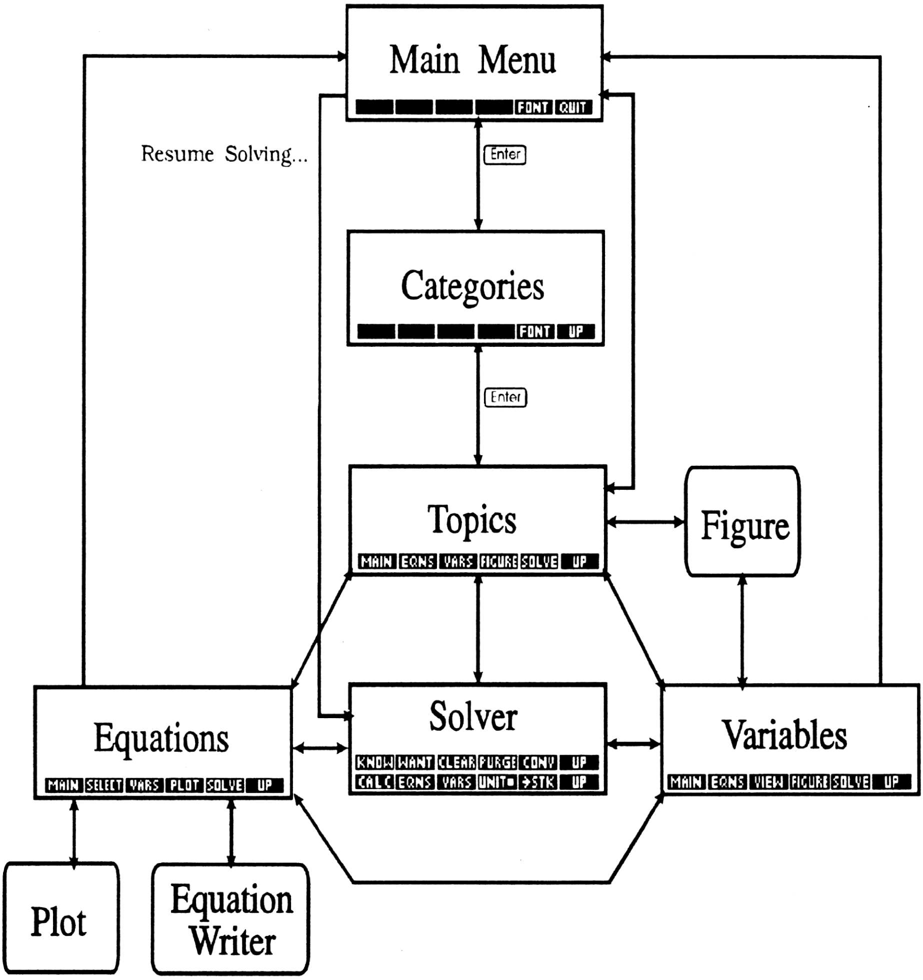
When you plug in the General Chemistry Application Pac for the first time, the software creates its own directory, GCHEMD, in the HOME directory of the HP 48SX. ALL operations performed by the software take place in the GCHEMD directory. It is, therefore, the only place where global variables are created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

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

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

Equation Library Structure

The following figure diagrams the basic flow and function of each level of the Equation Library and Sparcom's solver interface. On the following page, the softkeys available at each level are explained in more detail.



Summary of Softkeys

CALC	Stores all variable values and iterates through the set of selected equations in an attempt to find values for all wanted variables. After completion of the solver process, the user is returned to the solver level, where newly found variables are marked with "*".
CLEAR	Resets the values of the current variable set to zero.
EQNS	Enters the equation level of the current topic.
FIGURE	Displays a figure for the currently selected topic or displays "No figure".
FONT	Toggles between small and medium display fonts of the HP 48SX.
KNOW	Toggles the currently selected variable between known and unknown, adding or removing the triangular tag.
MAIN	Returns to the main menu.
PLOT	Prompts the user for x-axis and y-axis values (with option for autoscale y). This feature only works for equations of the form y = f(a,b, ...) where y and one variable on the right are unknown.
PURGE	Purges the global copies (in the GCHEMD directory) of the current variable set displayed in the solver level.
QUIT	Exits the General Chemistry Application Pac.
SELECT	Marks or unmarks the currently selected equation with the triangular tag. Only variables in the marked equations will appear in the solver and variable levels. If no equations are selected, all will be used.
SOLVE	Enters the solver level of the currrent topic.
↑STK	Copies selected entry to calculator stack.
UNIT■	Toggle key. Indicates that units are on.

UNITS	Toggle key. Indicates units are off. When off, all variables are assumed to be SI if entered with no units or are converted to SI units.
UP	Moves up one level in the software menu structure.
VARS	Enters the variable level for the current topic.
VIEW	Displays the full text entry for a variable description or value if the description is too wide to fit on the screen.
WANT	Toggles the currently selected variable between wanted and not wanted, adding or removing the symbol "?". If no variables are marked "wanted," all variables are assumed to be wanted.
ENTER	Prompts for the value of the currently selected variable. If the selected variable already contains a value, that value is copied to the command line for editing. Pressing ATTN clears the command line, or returns you to the variables screen if the command line is already empty.
ATTN	Generally used to exit a function or application.

Notes:

Chapter 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
- ☐ Solids/Liquids
- ☐ Gases
- ☐ Acids/Bases
- ☐ Thermo/Electrochemistry
- ☐ Precipitation
- ☐ Kinetics

In the Equation Library, the following constants are used:

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

Atoms/Molecules

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

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

Mass/Mole/Atom

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

1) $n = \frac{ga}{MWT}$ 2) $Natoms = NA \cdot n$

Variable	Description	Units
n	number of moles	1_mol
ga	mass of sample	1_kg
MWT	molecular weight of sample	1_kg/mol
Natoms	number of atoms	1

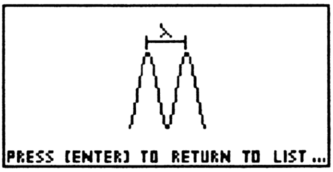
Example: How many atoms and moles are contained in a 45_lb sample of iron (molecular weight = 55.847_g/mol)?

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

Light

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

1) $\lambda = \frac{c}{\gamma}$ 2) $E = h \cdot \gamma$ 3) $nubar = \frac{1}{\lambda}$



PRESS [ENTER] TO RETURN TO LIST ...

Variable	Description	Units
λ	wavelength	1_m
γ	frequency	1_Hz
E	photon energy	1_J
nubar	wavenumber	1_1/m

Example: Calculate the frequency, photon energy, and wavenumber of light from a He-Ne laser ($\lambda = 6328$_Å).

Given	Result
$\lambda = 6328$_Å	$\gamma = 4.738$ E14_Hz E = 3.139 E-19_J nubar = 15803_1/cm

Quantum

Two fundamental equations of quantum mechanics are included here. The first equation relates the de Broglie wavelength of a particle to its momentum, and the second equation relates particle mass to its inherent energy.

1) $\lambda l = \dfrac{h}{m \cdot v}$ 2) $E = m \cdot c^2$

Variable	Description	Units
λl	de Broglie wavelength	1_m
m	mass	1_kg
v	velocity	1_m/s
E	energy	1_J
h	Planck's constant	1_J·s
c	speed of light	1_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 ?

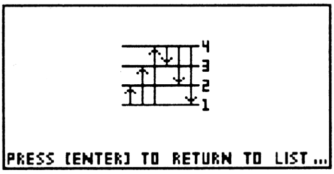
Given	Result
m = 1.0_oz	λl = 1.28 E-25_nm
v = 600_ft/s	E = 2.55 E15_J

Hydrogen Energy

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

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

3) $\gamma = \frac{\Delta E}{h}$ 4) $\lambda l = \frac{c}{\gamma}$



PRESS [ENTER] TO RETURN TO LIST ...

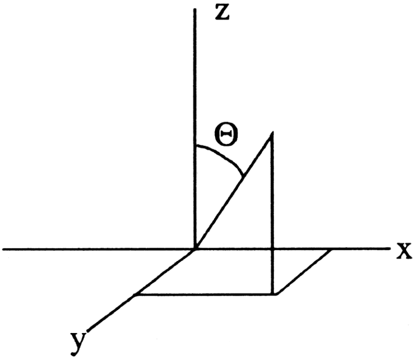
Variable	Description	Units
E	energy	1_J
Z	nuclear charge	1
ni	initial quantum number	1
nf	final quantum number	1
ΔE	energy change	1_J
γ	frequency	1_Hz
λl	wavelength	1_m

Example: What is the wavelength and frequency of the blue emission line (nf = 2 and ni = 4) in the Balmer series of hydrogen? Use all four equations.

Given	Result
Z = 1	E = -1.36 E-19_J
ni = 4	ΔE = -4.09 E-19_J
nf = 2	γ = 6.17 E14_Hz
	λl = 486_nm

s,p,d and f Orbitals

These equations describe the angular and radial portions of the Schroedinger one-electron atom. They are grouped by azimuthal quantum number (s, p, d or f). Note that the wavefunction, φ_{nlm}, is given by: $\varphi_{nlm} = R_{nl} \cdot X_{lm}$ The normalization constant given below is provided for reference only and guarantees that the integrated probability over all space is unity.



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

Radial Functions:

(1s) $Rnl = R10 = Z^{3/2} \cdot e^{-\rho/2}$

$$\text{constant} = \frac{2}{ao^{3/2}}$$

(2s) $R20 = Z^{3/2} \cdot (2 - \rho) \cdot e^{-\rho/2}$

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

(3s) $R30 = Z^{3/2} \cdot (6 - 6 \cdot \rho + \rho^2) \cdot e^{-\rho/2}$

$$\text{constant} = \frac{1}{ao^{3/2} \cdot 9 \cdot \sqrt{3}}$$

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

$$\text{constant} = \frac{1}{ao^{3/2} \cdot 96}$$

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

$$\text{constant} = \frac{1}{ao^{3/2} \cdot 2 \cdot \sqrt{6}}$$

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

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

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

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

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

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

(4d) $R42 = z^{3/2} \cdot (6 - \rho) \cdot \rho^2 \cdot e^{-\rho/2}$

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

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

$$\text{constant} = \frac{1}{ao^{3/2} \cdot 96 \cdot \sqrt{35}}$$

Angular Wave Functions

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

(p) $X10 = COS\ (\Theta)$ constant $= \frac{1}{2} \cdot \sqrt{6}$

(p) $X11 = SIN(\Theta)$ constant $= \frac{1}{2} \cdot \sqrt{3}$

(d) $X20 = 3 \cdot COS^2(\Theta) - 1$ constant $= \frac{1}{4} \cdot \sqrt{10}$

(d) $X21 = SIN(\Theta) \cdot COS(\Theta)$ constant $= \frac{1}{2} \cdot \sqrt{15}$

(d) $X22 = SIN^2(\Theta)$ constant $= \frac{1}{4} \cdot \sqrt{15}$

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

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

(f) $X31 = SIN(\Theta) \cdot (5 \cdot COS^2(\Theta) - 1)$

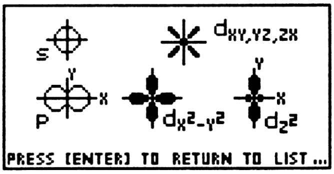
constant $= \frac{1}{8} \cdot \sqrt{42}$

(f) $X32 = SIN^2(\Theta) \cdot COS(\Theta)$

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

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

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



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Variable	**Description**	**Units**
ρ	normalized distance	1

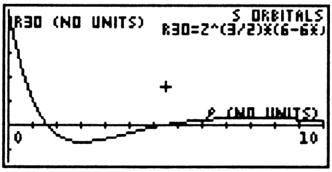
r	distance from nuclei	1_m
Z	nuclear charge	1
R10	1s radial function	1
R20	2s radial function	1
R30	3s radial function	1
R40	4s radial function	1
R21	2p radial function	1
R31	3p radial function	1
R41	4p radial function	1
R32	3d radial function	1
R42	4d radial function	1
R43	4f radial function	1
X10	p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

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

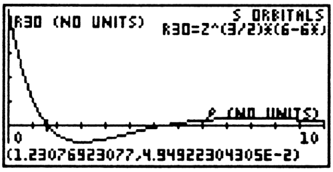
Example: At what distance from the hydrogen atom ($Z = 1$) is the first node in the 3s radial function? There are two nodes in the 3s radial function. The easiest way to solve this problem is to plot the 3s function versus ρ, find ρ at the first node, then solve for r.

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

x1 = 0
x2 = 10
autoscale y



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



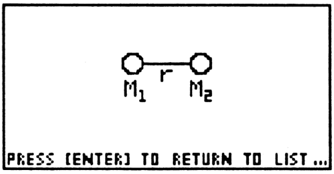
```
(1.23076923077,4.94922304305E-2)
```

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

$$I = \frac{1}{NA} \cdot \left(\frac{m1 \cdot m2}{m1 + m2}\right) \cdot r^2 \qquad B = \frac{h}{8\pi^2 \cdot I \cdot c}$$



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Variable	**Description**	**Units**
I	moment of inertia	1_kg·cm^2
m1	mass of 1	1_kg/mol
m2	mass of 2	1_kg/mol
r	internuclear distance	1_m
B	rotational constant	1_1/cm

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

Given	**Result**
m1 = 1.00797_g/mol	I = 2.644E-40_g·cm^2
m2 = 35.453_g/mol	B = 10.59_1/cm
r = 1.27460_Å	

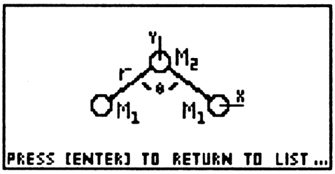
Symmetrical Moment

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

$$Ix = \left(\frac{2}{NA}\right) \cdot \left(\frac{m1 \cdot m2}{2 \cdot m1 + m2}\right) \cdot r^2 \cdot COS^2\left(\frac{\theta}{2}\right)$$

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

$$Iz = Ix + Iy$$



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Variable	Description	Units
Iy	moment of inertia about y	1_kg·m^2
Ix	moment of inertia about x	1_kg·m^2
Iz	moment of inertia about z	1_kg·m^2
m1	mass of 1	1_kg/mol
m2	mass of 2	1_kg/mol
r	internuclear distance	1_m
Θ	bond angle	1_°

Example: What is the moment of inertia of water?

Given	**Result**
r = 0.96_Å	Ix = 1.02E-40_g·cm^2
m1 = 1.0079_g/mol	Iy = 1.94E-40_g·cm^2
m2 = 15.9994_g/mol	Iz = 2.96E-40_g·cm^2
Θ = 104.9_°	

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

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

*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 the Debye or Einstein temperatures. Both the Debye and Einstein temperatures are defined by the equation: $\Theta = h\,\nu_m/k$.

Variable	Description	Units
CvE	Einstein heat capacity	1_J/(mol·K)
CvD	Debye heat capacity	1_J/(mol·K)
Θe	Einstein characteristic temperature	1_K
Θd	Debye characteristic temperature	1_K
T	temperature	1_K

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

Given	Result
Θd = 88_K	CvD = 11.1_J/(mol·K) @ 20_K
T = 20_K	CvD = 24.8_J/(mol·K) @ 25_°C
T = 25_°C	

Blackbody Radiation

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

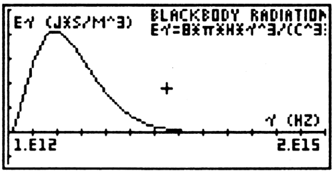
$$E\gamma = \frac{8\pi \cdot h \cdot \gamma^3}{c^3 \cdot (e^{h \cdot \gamma / k \cdot T} - 1)} \qquad ET = \sigma \cdot T^4$$

Variable	Description	Units
$E\gamma$	energy density	1_J·s/m^3
ET	total energy density	1_W/m^3
T	absolute temperature	1_K
γ	frequency	1_Hz

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

Given	Result
T = 5000_K	ET = 35439500_W/m^2

To solve the second part of the problem, set T = 5000_K and plot $E\gamma$ versus γ over a wide range of frequencies (this example uses 1E12_Hz to 2E15_Hz), as shown:



Move the cursor to the low frequency and high frequency intersection (where intensity is zero) and press **COORD**. This displays the approximate coordinates of the low frequency limit of ~ 8.7E12_Hz and the high frequency limit of ~ 1.2E15_Hz. Note that a more accurate determination of the intercept may be obtained by using a more expanded graph.

Equation of State

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

$$VTP = Vo \cdot (1 + \alpha s \cdot (t2 - 0\_°C)) \cdot (1 - \rho s \cdot (p2 - 1\_atm))$$

Variable	Description	Units
VTP	volume at any temperature & pressure	1_m^3
Vo	reference volume	1_m^3
αs	thermal expansion coefficient	1_1/K
t2	temperature	1_K
ρs	compressibility coefficient	1_1/Pa
p2	pressure	1_Pa

Example: A 1.000_cm^3 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	Result
Vo = 1.000_cm^3	VTP = 1.02_cm^3
αs = 1.03E-4_1/°C	
ρs = 2.86E-6_1/atm	
t2 = 360_°F	
p2 = 1800_psi	

Bragg Law

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

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

Variable	Description	Units
Θ	diffraction angle	1_°
n	order	1
λd	wavelength	1_m
d	distance between planes	1_m

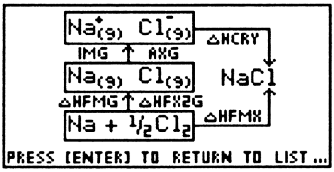
Example: At what angle does the (hkl = 100) first-order diffraction occur when Cu α radiation (λd = 1.44_Å) impinges on NaCl (d = 5.627_Å)?

Given	Result
d = 5.627_Å	Θ = 7.35_°
n = 1	
λd = 1.44_Å	

Born-Haber Cycle

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

$$\Delta Hfmx = \Delta Hcry + \Delta Hfmg + \frac{1}{2}\Delta Hfx2g + Img + Axg$$



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Variable	Description	Units
ΔHfmx	heat of formation of mx	1_J/mol
ΔHcry	heat of crystalization of mx	1_J/mol
ΔHfmg	heat of formation of gaseous m	1_J/mol
ΔHfx2g	heat of formation of gaseous x2	1_J/mol
Img	ionization energy of m	1_J/mol
Axg	electron affinity of x	1_J/mol

Example: Given the energies of each step in the Born-Haber Cycle, calculate the heat of formation of NaCl (s).

Given	Result
ΔHcry = -779.0_kJ/mol	DHfmx = -421.0_kJ/mol
ΔHfmg = 108.4_kJ/mol	
ΔHfx2g = 243.3_kJ/mol	
Img = 495.7_kJ/mol	
Axg = -367.7_kJ/mol	

Melting Point

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

$$P2 = P1 \cdot \left(\frac{\Delta Hfus}{\Delta Vfus}\right) \cdot LN\left(\frac{T2m}{T1m}\right)$$

Variable	**Description**	**Units**
P2	pressure	1_Pa
P1	reference pressure	1_Pa
ΔHfus	heat of fusion	1_J/mol
ΔVfus	volume change upon fusion	1_m^3/mol
T1m	reference melting point	1_K
T2m	new melting point	1_K

Example: What is the melting point of water under 3400_atm, given the values of ΔHfus and ΔVfus below ?

Given	**Result**
P2 = 3400_atm	T2m = 249.1_K
P1 = 1.0_atm	
ΔHfus = 1.4363_kcal/mol	
T1m = 273.16_K	
ΔVfus = -1.61_cm^3/mol	

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.

1) $gs = ga + gb$

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

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

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

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

6) $wa + wb = 100$

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

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

9) $gs = vs \cdot \rho s$

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

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

12) $gb = vb \cdot \rho b$

Variable	Description	Units
ga	mass solute	1_kg
gb	mass solvent	1_kg
na	moles solute	1_mol
nb	moles solvent	1_mol
MWTa	molecular weight solute	1_kg/mol
MWTb	molecular weight solvent	1_kg/mol
wa	weight % solute	1
wb	weight % solvent	1
ρb	pure solvent density	1_kg/m^3
vb	volume of solvent	1_m^3
gs	mass solution	1_kg
vs	volume solution	1_m^3
ρs	density solution	1_kg/m^3
Ma	molarity solution	1_mol/m^3
ma	molality solution	1_mol/kg
xa	mole fraction solution	1
ppma	solute concentration	1

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

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

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

Given	Result
ga = 5.0_g	Ma = 0.206_mol/l

gb = 225.0_g
MWTa = 92.1402_g/mol
ρs = 0.876_g/ml
MWTb = 78.1134_g/mol

xa = .0185
wa = 2.17

Other variables solved for are:

na = 0.054_mol
nb = 2.88_mol
wb = 97.8

gs = 0.23_kg
vs = 0.263_l
ma = 0.24_mol/kg
ppma = 22222.2

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.

1) $P = xb \cdot Pin$ 2) $\Delta P = -xa \cdot Pin$ 3) $\Delta P = P - Pin$

4) $na = \frac{ga}{MWTa}$ 5) $nb = \frac{gb}{MWTb}$ 6) $xa = \frac{na}{na + nb}$

7) $xb = \frac{nb}{na + nb}$ 8) $xa = 1 - xb$

Variable	Description	Units
P	solvent partial pressure	1_Pa
xb	solvent mole fraction	1
Pin	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	ΔP = -0.125_torr
ga = 100_g	P = 23.68_torr
MWTa = 342.2992_g/mol	xa = 5.24×10^{-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.

1) $\Delta Tb = Kb \cdot ma$

2) $ma = \dfrac{na}{gb}$

3) $na = \dfrac{ga}{MWTa}$

4) $\Delta Tf = -Kf \cdot ma$

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

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

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

Given	**Result**
Kb = 0.52_K·kg/mol	ΔTb = 0.932_°C
gb = 900_g	ma = 1.79_mol/kg
ga = 100_g	na = 1.61_mol
MWTa = 62_g/mol	ΔTf = -3.33_°C
Kf = 1.86_K·kg/mol	

Molarity/Dilution

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

1) $Mi = \frac{na}{V}$ 2) $na = \frac{ga}{MWTa}$ 3) $Vf \cdot Mf = Vi \cdot Mi$

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

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

Given	Result
ga = 4.5060_g	Mi = 0.4506_mol/l
MWTa = 39.99707_g/mol	Mf = 9.013×10^{-3}_mol/l
V = 250.00_ml	na = 0.1127_mol
Vi = 10.00_ml	
Vf = 500_ml	

Clausius Clapyron

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

$$LN\left(\frac{P}{Po}\right) = \frac{\Delta Hv}{R} \cdot \left(\frac{1}{To} - \frac{1}{T}\right)$$

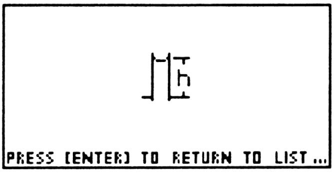
Variable	Description	Units
P	vapor pressure	1_Pa
ΔHv	heat of vaporization	1_J/mol
To	reference temperature	1_K
T	temperature	1_K
Po	reference vapor pressure	1_Pa

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	Result
Po = 1.0_mmHg	ΔHv = 12.47 kcal/mol
To = 76.6_°C	
P = 100.0_mmHg	
T = 197.3_°C	

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 (Θ = 0_°), and no edge effects. The second equation includes these contributions.



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

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

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

Given	Result
γl = 46.0_dyn/cm	h = 88.5_mm
ρl = 1.06_g/cm^3	hex = 21.4_mm
r = 0.10_mm	

Θ = 76_°
ρv = 1.0_g/l

Gases

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

- Ideal Gas
- State Changes
- Gas Over Water
- Barometric Equation
- Van der Waals Gas
- Kinetic Theory
- Graham's Law
- Collision Theory

Ideal Gas

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

$$1)\ P = \frac{n \cdot R \cdot T}{V} \qquad 2)\ n = \frac{mg}{MWT} \qquad 3)\ \rho = \frac{mg}{V}$$

Variable	Description	Units
P	pressure	1_Pa
n	moles of gas	1_mol
T	temperature	1_K
V	volume	1_m^3
mg	mass of gas	1_kg
MWT	molecular weight	1_kg/mol
ρ	density	1_kg/m^3

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

Given	Result
P = 735_mmHg	n = 3.62×10^{-2}_mol
V = 933_ml	ρ = 3.09×10^{-2}_g/cm^3
T = 31_°C	MWT = 79.9_g/mol
mg = 2.889_g	

State Changes

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

(complete state change)

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

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

3) $P1 \cdot V1 = P2 \cdot V2$ (n, T constant)

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

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

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

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

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

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

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

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

Given	Result
P1 = 1.68_mmHg	P2 = 1.21_mmHg
V1 = 45_ml	
T1 = 246_°C	
V2 = 36_ml	
T2 = 25_°C	

Gas Over Water

Consider the general chemical reaction:

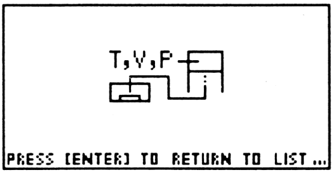
$$aA + \text{Reactants} \rightarrow bB_{(g)} + \text{Products}$$

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

$$1)\ na = \frac{a}{b} \cdot nb \qquad 2)\ nb = \frac{gb}{MWTb} \qquad 3)\ na = \frac{ga}{MWTa}$$

$$4)\ Pb \cdot V = nb \cdot R \cdot T \qquad 5)\ nt = nb + nw$$

$$6)\ Pt = Pb + Pw \qquad 7)\ Pt \cdot V = nt \cdot R \cdot T$$



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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	partial pressure of gas	1_Pa
V	collected gas volume	1_m^3
T	temperature	1_K
nt	total moles collected	1_mol
nw	moles of water collected	1_mol
Pt	total pressure	1_Pa
Pw	water partial pressure	1_Pa

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

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

When 4.6_g of $CaCO_3$ decomposes, what volume of gas is collected at 1.0_atm and 26_°C? Note that the partial pressure of water at 26_°C is 25.0_torr. Use all seven equations.

Given	**Result**
a = b = 1	V = 1.17_l
MWTb = 44.0098_g/mol (CO_2)	nb = 4.60×10^{-2}_mol
MWTa = 100.0892_g/mol ($CaCO_3$)	gb = 2.02×10^{-3}_kg
ga = 4.6_g	Pb = 0.967_atm
T = 26_°C	na = 4.60×10^{-2}_mol
Pt = 1.0_atm	nt = 4.75×10^{-2}_mol
Pw = 25.00_torr	nw = 1.56×10^{-3}_mol

Barometric Equation

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

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

2) $$Co = \frac{Po}{R \cdot T}$$

3) $$C = \frac{P}{R \cdot T}$$

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	Result
Po = 1.0_atm	P = 0.89_atm
MWT = 29_g/mol	Co = 4.1 E-2_mol/l
h = 1_km	C = 3.6 E-2_mol/l
T = 75_°F	

Plotting the barometric equation yields:

x1 = 0_km
x2 = 50_km

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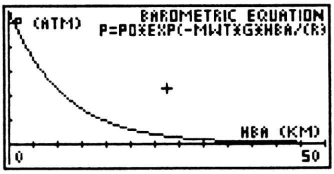


Van der Waal Gases

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

$$1)\ p=\frac{n\cdot R\cdot T}{V-n\cdot b}-\frac{n^2\cdot a}{V^2}$$

$$2)\ Z = P\cdot\frac{V}{n\cdot R\cdot T}$$

$$3)\ Tc = \frac{8\cdot a}{27\cdot b\cdot R}$$

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

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

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

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 (repulsive)	1_m^3/mol
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_2) is compressed in a vessel to 100_l at 300_°C. What is the pressure?

Given	**Result**
T = 300_°C	p = 139.9_atm
V = 100_l	n = 285.7_mol
b = 0.03913_l/mol	Z = 1.04
a = 1.390_l^2·atm/mol^2	Tc = 128.3_K
ga = 8000_g	Vc = 33.54_l
MWT = 28.0134_g/mol	Pc = 33.6_atm

Kinetic Theory

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

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

2) $$cmp = \left(\frac{2 \cdot R \cdot T}{MWT}\right)^{1/2}$$

3) $$cavg = \left(\frac{8 \cdot R \cdot T}{\pi \cdot MWT}\right)^{1/2}$$

4) $$crms = \left(\frac{3 \cdot R \cdot T}{MWT}\right)^{1/2}$$

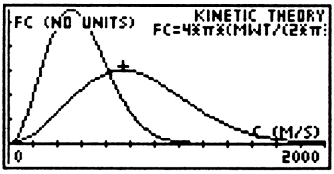
Variable	**Description**	**Units**
fC	probability that velocity is within dC	1
MWT	molecular weight of gas	1_kg/mol
T	absolute temperature	1_K
C	velocity of molecules	1_m/s
dC	velocity range	1_m/s
cmp	most probable velocity	1_m/s
cavg	average velocity	1_m/s
crms	root mean-square velocity	1_m/s

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.

Grahams' Law

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

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

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

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).

1) $cavg = \left(\frac{8 \cdot R \cdot T}{\pi \cdot MWT}\right)^{1/2}$

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

3) $Z = \frac{1}{4 \cdot NA} \cdot n \cdot cavg$

4) $Z1 = \frac{2 \cdot d^2 \cdot \left(\left(\frac{\pi \cdot R \cdot T}{MWT}\right)^{1/2}\right) \cdot n^2}{NA}$

5) $\lambda mfp = \frac{1}{\sqrt{2} \cdot \pi \cdot d^2 \cdot n}$

6) $D = \frac{1}{2} \cdot cavg \cdot \lambda mfp$

7) $\rho = \frac{MWT \cdot P}{R \cdot T}$

8) $\eta = \frac{1}{2} \cdot \rho \cdot cavg \cdot \lambda mfp$

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

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
λmfp	mean free path	1_m
D	self diffusion coefficient	1_m^2/s
ρ	density of gas	1_kg/m^3
η	viscosity coefficient	1_kg/(m·s)

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

Given

P = 1.0_atm
T = 25_°C
MWT = 31.9988_g/mol
d = 3.61_Å

Result

cavg = 444_m/s
n = 2.46 E19_1/cm^3
Z = 0.454_mol/(cm^2·s)
Z1 = 1.29 E5_mol/(cm^3·s)
λmfp = 701_Å
D = 0.156_cm^2/s
ρ = 1.31 E-3_g/cm^3
η = 2.04 E-4_g(cm·s)

Acids/Bases

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

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

Note that in the equation library, SA indicates a strong acid, SB a strong base, WB a weak base, and WA a weak acid. Although it is common to denote concentrations of ions in solution with brackets, i.e $[H^+]$, this notation is not supported by the HP 48SX. Therefore, all concentrations are enclosed by parenthesis.

pH Function

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

1) $pH = -LOG\,(H)$

2) $pOH = -LOG\,(OH)$

3) $pKw = -LOG\,(Kw)$

4) $pKa = -LOG\,(Ka)$

5) $pKb = -LOG\,(Kb)$

6) $Kw = Ka \cdot Kb$

7) $Kw = H \cdot OH$

Variable	Description	Units
H	hydrogen ion concentration	1_mol/m^3
OH	hydroxide ion concentration	1_mol/m^3
Kw	water dissociation constant	1_mol^2/m^6
Ka	acid dissociation constant	1_mol/m^3
Kb	base dissociation constant	1_mol/m^3
pH	pH function	1
pOH	pOH function	1
pKw	pKw function	1
pKa	pKa function	1

pKb	pKb function	1

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

Given	Result
H = 0.01_mol/l	pH = 2
Kw = 1.01 E-14_mol^2/l^2	OH = 1.01 x 10^{-12}_mol/l
	pOH = 12.0
	pKw = 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.

$$H = n \cdot \frac{ga}{MWTa \cdot V}$$

$$pH = -LOG(H)$$

Variable	Description	Units
H	hydrogen ion concentration	1_mol/m^3
ga	mass of acid	1_kg
MWTa	molecular weight of acid	1_kg/mol
V	volume of solution	1_m^3
pH	pH function	1
n	Number of hydrogen ions per molecule	1

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

Given	Result
ga = 0.50_g	H = 0.101_mol/l
V = 100_ml	pH = 0.991
MWTa = 98.0734_g/mol	
n = 2	

Strong Bases

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

1) $OH = n \cdot \dfrac{gb}{MWTb \cdot V}$

2) $H = \dfrac{Kw}{OH}$

3) $pH = -LOG\,(H)$

Variable	Description	Units
OH	hydroxide ion concentration	1_mol/m^3
H	hydrogen ion concentration	1_mol/m^3
gb	mass of base	1_kg
MWTb	molecular weight of base	1_kg/mol
V	volume of solution	1_m^3
pH	pH function	1
Kw	water dissociation constant	1_mol^2/m^6
n	Number of hydroxide ions per molecule	1

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

Given	Result
gb = 4.5617_g	pH = 13.35
MWTb = 39.99707_g/mol	H = 4.43×10^{-14}_mol/l
V = 500_ml	OH = 0.228_mol/l
Kw = 1.01×10^{-14}_mol^2/l^2	
n = 1	

Weak Acids/Bases

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

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

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

3) $Kw = H \cdot OH$

4) $pH = -LOG\,(H)$

5) $Ca = \dfrac{ga}{MWT \cdot V}$

6) $Cb = \dfrac{gb}{MWT \cdot V}$

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_3 (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 = 2.20×10^{-3}_mol/l
Ka = 0.162_mol/l	H = 2.17×10^{-3}_mol/l
V = 1.0_l	pH = 2.66
MWT = 175.9106_g/mol	
Kw = 1.01×10^{-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.

$$1)\ Ca = \frac{ga}{MWTa \cdot V} \qquad 2)\ Ccb = \frac{gb}{MWTb \cdot V}$$

$$3)\ pKa = -LOG\,(Ka) \qquad 4)\ pH = pKa - LOG\left(\frac{Ca}{Ccb}\right)$$

Variable	Description	Units
Ca	acid concentration	1_mol/m^3
ga	mass acid	1_kg
MWTa	acid molecular weight	1_kg/mol

V	volume	1_kg/m^3
Ccb	base concentration	1_mol/m^3
gb	mass base	1_kg
MWTb	molecular weight of base	1_kg/mol
pKa	pKa function	1
Ka	acid dissociation constant	1_mol/m^3
pH	pH value	1

Example: 0.45 grams of $\mathrm{NaCH_3COCOO}$ are 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 10^{-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 10^{-5}_mol/l

Result

pKa = 4.75
Ccb = 4.09 x 10^{-2}_mol/l
pH = 5.36

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

Titration (SA/SB)

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

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

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

3) $pH = -LOG\,(H)$ 4) $Cb = \dfrac{gb}{MWT \cdot V}$

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

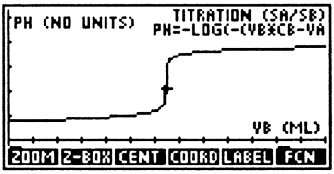
gb = 0.3986_g
MWT = 39.99707_g/mol
V = 1.000_l
Kw = 1.01 x 10^{-14}_mol^2/l^2
Ve = 49.68_ml
Va = 100_ml

Result

Ca = 4.951 x 10^{-3}_mol/l
Cb = 9.966 x 10^{-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
x2 = 100_ml
y1 = -3
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.

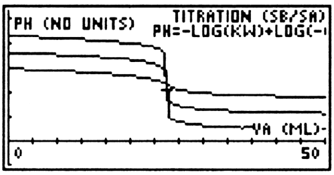
$$1)\ Ve = \frac{Cb}{Ca} \cdot Vb$$

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

$$3)\ pH = -LOG\,(H) \qquad 4)\ Ca = \frac{ga}{MWT \cdot V}$$

Variable	Description	Units
Ca	concentration of acid titrant	1_mol/m^3
Cb	concentration of base	1_mol/m^3
Ve	equilibrium volume	1_m^3
Va	volume of acid solution	1_m^3
Vb	volume of base titrant	1_m^3
Kw	dissociation constant of water	1_mol^2/l^2
H	hydrogen concentration	1_mol/m^3
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.

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

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

3) $$pH = -LOG(H)$$

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

Variable	**Description**	**Units**
Ca	acid concentration	1_mol/m^3
Cb	base (titrant) concentration	1_mol/m^3
Ka	acid dissociation constant	1_mol/m^3
Kw	water dissociation constant	1_mol^2/l^2
Va	volume acid solution	1_m^3
Vb	volume base titrant	1_m^3
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 10^{-5}_mol/l) with 10.00_ml of 0.10_mol/l NaOH? How much does the pH change if 2.50_ml of additional NaOH are added? 2.50_ml more?

Given	**Result**
Ca = 0.1_mol/l	10.0_ml
Cb = 0.1_mol/l	H = 2.67 x 10^{-5}_mol/l
Kw = 1.01 E-14_mol2/l2	pH = 4.57
Ka = 1.78 E-5_mol/l	12.50_ml
Va = 25.0_ml	H = 1.78 x 10^{-5}_mol/l
Vb = 10.0_ml	pH = 4.75
	15.0_ml
	H = 1.19 x 10^{-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.

1)

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

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

$$3)\ Kw = H \cdot OH \qquad 4)\ pH = -LOG\,(H)$$

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 NH_4OH (Kb = 1.80×10^{-5}_mol/l). What is the pH?

Given	Result
Ca = 0.100_mol/l	H = 2.81×10^{-10}_mol/l
Cb = 0.100_mol/l	OH = 3.59×10^{-5}_mol/l
Kb = 1.80×10^{-5}_mol/l	pH = 9.55
Kw = 1.01 E-14_mol^2/l^2	

Va = 10.0_ml
Vb = 30.0_ml

Thermo/Electrochemistry

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

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

Heat Transfer

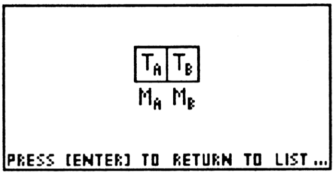
The following relations describe the heat flow equations which govern the flow of heat between two bodies of different temperatures with no phase change.

1) $qa = ma \cdot cpa \cdot (Tf - Ta)$
2) $qb = mb \cdot cpb \cdot (Tf - Tb)$

3) $qa = -qb$

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

5) $$cpa = \frac{Cpa}{MWTa}$$
6) $$cpb = \frac{Cpb}{MWTb}$$



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Variable	Description	Units
qa	heat flow in or out of material a	1_J
qb	heat flow in or out of material b	1_J
ma	mass of a	1_kg
mb	mass of b	1_kg

cpa	specific heat of a	1_J/(kg·K)
cpb	specific heat of b	1_J/(kg·K)
Cpa	molar heat capacity of a	1_J/(mol·K)
Cpb	molar heat capacity of b	1_J/(mol·K)
Tf	final temperature	1_K
Ta	temperature of a	1_K
Tb	temperature of b	1_K
MWTa	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	Result
cpa (copper) = 0.385_J/(g·K)	qa = -491_J
ma = 20_g	qb = 491_J
Ta = 90_°C	Tf = 26_°C
cpb (water) = 4.184_J/(g·K)	
mb = 100_g	
Tb = 25_°C	

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

Heat Engines

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

1) $\eta = 1 - \frac{Tc}{Th}$ 2) $Cop = \frac{Tc}{Th - Tc}$

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

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

Given	Result
Th = 459_°F	η = 0.42
Tc = 25_°C	Cop = 1.4

Free Energy

The following equations define free energy.

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

Variable	Description	Units
ΔG	free energy change	1_J/mol
ΔH	enthalpy change	1_J/mol
T	temperature	1_K
ΔS	entropy change	1_J/(mol·K)
Keq	equilibrium constant	1

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

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

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

Given	Result
ΔH = 37.6_kJ/mol	ΔG = 20.2_kJ/mol
ΔS = 58.5_J/(mol·K)	Keq = 2.94042E-4
T = 25_°C	(Ln Keq = -8.13)

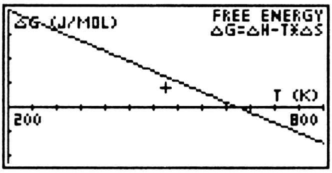
The reaction is non-spontaneous at 25_°C, solving for the equilibrium temperature where ΔG = 0.

Given	Result
ΔG = 0	T = 369_°C
ΔH = 37.6_kJ/mol	Keq = 1
ΔS = 58.5_J/(mol·K)	(Ln Keq = 0)

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

ΔG vs. T is plotted below (Note: Temperature variable T must be converted to _K before this plot is generated):

x1 = 200
x2 = 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.

$$1)\ Cp = A + B \cdot T + C \cdot T^2 + \frac{D}{T^2}$$

$$2)\ \Delta H = A \cdot T + \frac{B}{2} \cdot T^2 + \frac{C}{3} \cdot T^3 - \frac{D}{T} - H298$$

$$3)\ \Delta S = 2.303 \cdot A \cdot LOG\,(T) + B \cdot T + \frac{C}{2} \cdot T^2 - \frac{1}{2} \cdot \frac{D}{T^2} - S298$$

Variable	Description	Units
Cp	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
H298	enthalpy at 298_K	1_J/mol
S298	entropy at 298_K	1_J/(mol*K)

Example: What is the heat capacity, enthalpy and entropy of Al_2O_3(s) at 600_K? The appropriate constants are given below:

Given

A = 26.12_cal/(mol*K)
B = 4.388 x 10^{-3} _cal/(mol*K^2)
C = 0
D = -7.269 x 10^5_cal·K/mol
T = 600_K
H298 = 10.422_kcal/mol

Results

Cp = 26.73_cal/(mol·K)
ΔH = 7.251_kcal/mol
ΔS = 28.43_cal/(mol·K)

S298 = 142.03_cal/(mol·K)

Heat Capacity

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

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

Variable	Description	Units
ΔC	heat capacity difference	1_J/(mol·K)
α	expansion coefficient	1_1/K
V	molar volume	1_m^3/mol
T	temperature	1_K
ε	compressibility coefficient	1_1/Pa
Cp	heat capacity (constant pressure)	1_J/(mol·K)
Cv	heat capacity (constant volume)	1_J/(mol·K)

Example: What is the difference in the heat capacities at constant volume and pressure for water at 25_°C?

Given	Result
$\alpha = 2.07 \times 10^{-4}$_1/K	ΔC = $.517 \times 10^{-3}$_J/(mol·K)
V = 18.087_cm^3/mol	
T = 25_°C	
$\varepsilon = 45.3 \times 10^{-6}$_1/atm	

Nernst Law

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

1) $E = Eo - 2.303 \cdot \frac{RT}{n \cdot F} \cdot LOG\ (Q)$

2) $Q = \frac{(C)^c \cdot (D)^d}{(A)^a \cdot (B)^b}$

3) $Eo = 2.303 \cdot \frac{RT}{n \cdot F} \cdot LOG(K)$

4) $\Delta G = -n \cdot F \cdot E$

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

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

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

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

if Eo = 0.34_V and $[Cu^{+2}]$ = 5.0_mol/l.

Given	Result
Eo = 0.34_V	E = 0.36_V
T = 49_°C	Q = 0.2
n = 2	ΔG = -16.7_kcal/mol
A = 5	ΔGo = -15.7_kcal/mol
a = 1	K = 4.3×10^{10}
B = C = D = 1	
b = c = d = 0	

Reduction

The following equations describe the quantity of *a* produced by electrolytic reduction for time *t* by the chemical equation: Reactant + n e^{-} → aA.

$$1)\ Q = A \cdot t$$

$$2)\ ne = \frac{Q}{F}$$

$$3)\ na = \left(\frac{a}{n}\right) \cdot ne$$

$$4)\ ma = MWTa \cdot na$$

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

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

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

Given	**Result**
t = 4.5_h	Q = 810_C
A = 50.0_mA	ne = 8.40×10^{-3}_mol
a = n = 1	na = 8.40×10^{-3}_mol
MWTa = 107.87_g/mol	ma = 0.906_g

Precipitation

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

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

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

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

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

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

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

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

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

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

Variable	Description	Units
Ksp	solubility product	*
fa	activity coefficient of a	**
fb	activity coefficient of b	1
s	solubility	1_mol/m^3
ga	mass of a	1_kg
MWT	molecular weight of a	1_kg/mol
V	volume	1_m^3

* Units of Ksp depend on the stoichiometric ratios within the dissolving species.
**Activity coefficients are equal to 1 if ideal.

Example: What is the solubility of BiI_3(s) (AB3, Ksp = 8.1×10^{-19}) in a solution such that, at equilibrium, $fBi^{+3} = 0.110$ and $fI^- = 0.200$. How many grams of BiI_3 are dissolved in 100_ml at equilibrium? Compare your results assuming ideality and non-ideality.

Case 1: Non-Ideal

Given	Result
fb = 0.200	s = 7.6×10^{-5}_mol/l
fa = 0.110	ga = 4.5_mg
Ksp = 8.1×10^{-19}_mol^4/l^4	
V = 100 _ml	
MWT = 589.6939_g/mol	

Case 2: Ideal

Given	Result
fb = 1	s = 1.3×10^{-5}_mol/l
fa = 1	ga = 0.776_mg
Ksp = 8.14×10^{-19}_mol^4/l^4	
V = 100_ml	
MWT = 589.6939_g/mol	

Kinetics

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

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

First Order

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

$$1)\ Rate = k1st \cdot Ca$$

$$2)\ Ca = Cao \cdot e^{-k1st \cdot t}$$

$$3)\ thalf = \frac{LN\,(2)}{k1st}$$

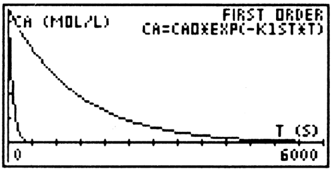
Variable	**Description**	**Units**
Rate	rate of reaction	1_mol/(m^3·s)
k1st	rate constant	1_1/s
Ca	concentration A (t)	1_mol/m^3
Cao	concentration A (t=0)	1_mol/m^3
t	time	1_s
thalf	half life	1_s

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

Given	**Result**
Ca = 1.0_mol/l (assumed)	k1st = 7.7 x 10^{-4}_1/s
Cao = 0.01_mol/l (assumed)	t = 5979_s –
thalf = 15_min	Rate = 7.7 X 10^{-6}_mol/(m^3*s)

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

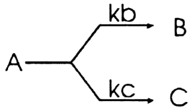
x1 = 0_s
x2 = 6000_s
autoscale y



Given	**Result**
thalf = 1.0_min	k1st = 1.16×10^{-2}_1/s
Cao = 1.0_mol/l	t = 398_s
Ca = 0.01_mol/l	

Parallel First Order

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



$$1)\ A = Ao \cdot e^{-(k\,b + k\,c)\cdot t}$$

$$2)\ B = Bo + \frac{k\,b \cdot Ao}{(k\,b + kc)} \cdot \left[1 - e^{-(k\,b + k\,c)\cdot t}\right]$$

$$3)\ C = Co + \frac{kc \cdot Ao}{(k\,b + kc)} \cdot \left[1 - e^{-(kb + kc)\cdot t}\right]$$

Variable	**Description**	**Units**
B	concentration B (t)	1_mol/m^3
Bo	concentration B (t=0)	1_mol/m^3
kb	rate constant for reaction B	1_1/s

Ao	concentration A (t=0)	1_mol/m^3
kc	rate constant for reaction C	1_1/s
t	time	1_s
C	concentration C (t)	1_mol/m^3
Co	concentration C (t=0)	1_mol/m^3
A	concentration A (t)	1_mol/m^3

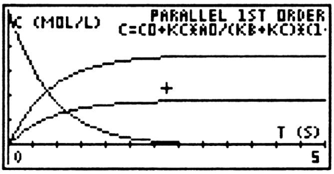
Example: A parallel reaction can produce two products with rate constants of 1.0_1/s and 0.5_1/s. Starting with 1_mol/l of initial reactant, plot the concentration profiles of A, B and C vs. time.

Given

Bo = 0_mol/l
kc = 0.5_1/s
kb = 1.0_1/s
Co = 0_mol/l
Ao = 1.0_mol/l

and

x1 = 0
x2 = 5_s
y1 = -0.1363
y2 = 1.0



First Order Consecutive

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

$$A \xrightarrow{k1} B \xrightarrow{k2} C \xrightarrow{k3} D$$

These four equations describe the kinetics of such a system.

1) $A = Ao \cdot e^{-k1 \cdot t}$

$$2)\ B = Bo \cdot e^{-k2 \cdot t} + \frac{k1 \cdot Ao}{k2 - k1} \cdot \left(e^{-k1 \cdot t} - e^{-k2 \cdot t}\right)$$

$$3)\ C = Co\ e^{-k3 \cdot t} + Bo \cdot \left(\frac{k2 \cdot e^{-k2 \cdot t}}{k3 - k2} - \frac{k2\ e^{-k3 \cdot t}}{k3 - k2}\right) +$$

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

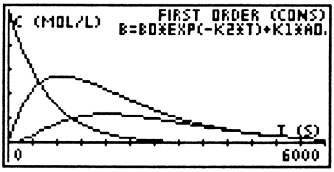
Variable	**Description**	**Units**
A	concentration A (t)	1_mol/m^3
Ao	concentration A (t=0)	1_mol/m^3
B	concentration B (t)	1_mol/m^3
Bo	concentration B (t=0)	1_mol/m^3
C	concentration C (t)	1_mol/m^3
Co	concentration C (t=0)	1_mol/m^3
k1	rate constant for A → B	1_1/s
k2	rate constant for B → C	1_1/s
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:

$$A \xrightarrow{5.0\_1/h} B \xrightarrow{2.5\_1/h} C \xrightarrow{4.5\_1/h} D$$

where A(t=0) = 1.0_mol/l and Bo=Co=0_mol/l. Plot the concentration of B and C vs. time, and determine the point where the maximum concentration of each material occurs.

x1 = 0_s
x2 = 6000_s
y1 = -0.1363
y2 = 1



A (maximum) = 0.00_s
B (maximum) = 0.50_mol/l, ~969_s
C (maximum) = 0.22_mol/l, ~1800_s

Second Order (I)

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

1) $Rate = k2nd \cdot Ca^2$

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

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

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 → H2 + I2) proceeds in second order in HI. In this reaction, a 0.10_mol/l of HI sample reacts for 10 minutes in a spectrophotometer. After 10 minutes the concentration is 0.08_mol/l. What is the rate constant and half life?

Given	**Result**
Cao = 0.10_mol/l	k2nd = 2.08×10^{-3}_l/(mol·s)
Ca = 0.08_mol/l	thalf = 40_min
t = 10.0_min	

a = 2

Second Order (II)

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

1) $Rate = k2nd \cdot Ca \cdot Cb$

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

3) $f = \left(\frac{CB}{CA}\right)$

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:

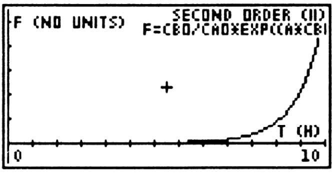
$$C_2H_4Br + 3KI \xrightarrow{k2nd} C_2H_4 + 2KBr + KI_3$$

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

Given	Result
Cao = 0.02864_mol/l	f (0.1_h) = 6.03
Cbo = 0.1531_mol/l	f (0.5_h) = 9.78
k2nd = 5.0 x 10^{-3}_l/(mol·s)	f (1_h) = 17.9
a = 1	f (10_h) = 9.5E5

b = 3
t = 0.5_h

x1 = 0
x2 = 10
y = autoscale



Arrhenius Law

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

$$k1 = A\ e^{-\left(Ea / (R \cdot T)\right)}$$

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

Variable	**Description**	**Units**
k1	rate constant at T1	1
k2	rate constant at T2	1
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 10^{-5}_1/s and 3.16 x 10^{-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 10^{-5}
k2 = 3.16 x 10^{-3}
T1 = 189.7_°C
T2 = 251.2_°C

Result

Ea = 159_kJ/mol
A = 1.96 x 10^{13}

Fractional Life

The time necessary for a given fraction of a reagent to react will depend on the initial concentrations of reactants and the rate expression for the reaction. The following equations calculate the time necessary for the reactant to reach to a fraction of its original concentration.

$$\text{if } no \neq 1, \text{ then } tfract = \frac{\left(\frac{1}{1-f}\right)^{no-1} - 1}{(no-1) \cdot a \cdot kgen \cdot Cao^{no-1}}$$

$$\text{if } no = 1, \text{ then } tfract = \frac{-LN(1-f)}{kgen}$$

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

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

Given	Result
no = 2	tfract = 1.94 E7_s 10%
kgen = 1.03×10^{-3}_1/h	tfract = 5.82 E7_s 25%
Cao = 0.01	tfract = 17.5 E7_s 50%
a = 2	tfract = 52.4 E7_s 75%
f = 0.10	

Notes:

Chapter 3

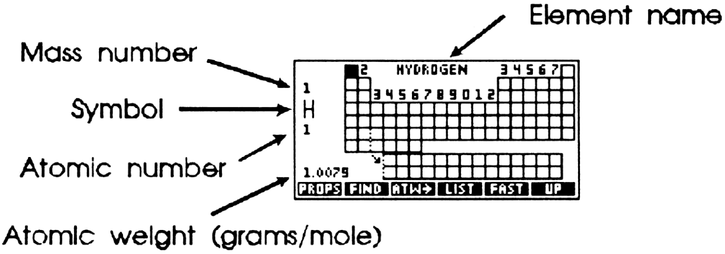
Periodic Table

In This Chapter

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

Using the Periodic Table

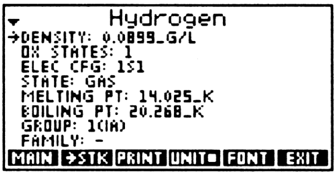
The Periodic Table screen displays after selecting this topic at the main menu. The figure below illustrates the information given on the screen for each element:



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

Properties of Each Element

Press **PROPS** or ENTER to view a list of properties for the current element:



```
▼         Hydrogen
→DENSITY: 0.0899_G/L
 OX STATES: 1
 ELEC CFG: 1S1
 STATE: GAS
 MELTING PT: 14.025_K
 BOILING PT: 20.268_K
 GROUP: 1(IA)
 FAMILY: -
MAIN →STK PRINT UNIT■ FONT EXIT
```

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:

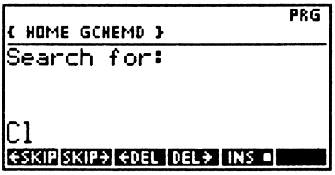
- ☐ Atomic Number (Table)
- ☐ Atomic Weight (Table)
- ☐ Oxidation State
- ☐ Physical State
- ☐ Atomic Radii
- ☐ First Ionization Potential
- ☐ Group and Family
- ☐ Mass Number (Table)
- ☐ Density
- ☐ Electron Configuration
- ☐ Electronegativity (Pauling's)
- ☐ Covalent Radii
- ☐ Boiling Point
- ☐ Melting Point

Moving Around the Periodic Table

Use the cursor keys (▼, ►, ◄, ▲) to move the pointer to any element. Pressing the ↰ key with a cursor key moves the cursor to the beginning or end of the current row or column. Pressing **FAST** eliminates the element information from the screen and allows you to quickly move from element to element using the cursor keys. Press **FAST** again to retrieve the screen information.

Using Search and List Utilities

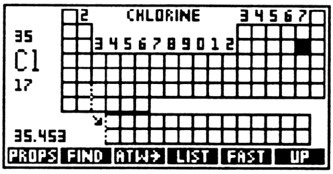
To search for a particular element press the **FIND** softkey. At the prompt, type in the symbol or atomic number of the element you want to search for, as shown:



PRG
{ HOME GCHEMD }
Search for:

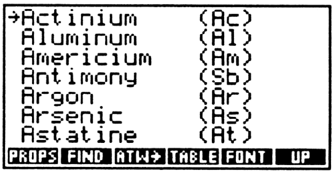
Cl

If you are entering an element's symbol, the second letter must be lower case. Lower case entries are made by pressing ↰ before typing in the letter. Press ENTER to move to the Periodic Table screen containing the element you were searching for, in this case, chlorine:



List of Element Names and Symbols

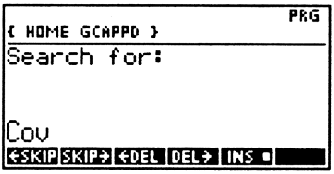
Pressing **LIST** displays the names and symbols of all the elements in the Periodic Table, in alphabetical order:



```
→Actinium      (Ac)
 Aluminum      (Al)
 Americium     (Am)
 Antimony      (Sb)
 Argon         (Ar)
 Arsenic       (As)
 Astatine      (At)
```

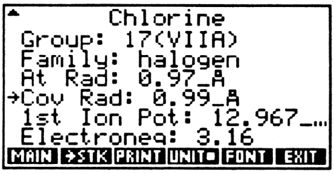
Searching for a Property

To search for particular property, press α 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:



```
                         PRG
{ HOME GCAPPD }
Search for:


Cov
```

Then press ENTER to initiate the search. The following screen displays:



```
▲       Chlorine
 Group: 17(VIIA)
 Family: halogen
 At Rad: 0.97_Å
→Cov Rad: 0.99_Å
 1st Ion Pot: 12.967_…
 Electroneg: 3.16
```

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 48SX and allow you to edit the search string. Their functions are summarized below:

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

Using the Print Function

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

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

Summary of Softkeys

MAIN	Returns to the main menu.
→STK	Copies selected entry to calculator stack.
PRINT	Sends selected data to an IR printer.
UNITS	Toggles units on and off. When off, all variables are assumed to be SI.
UNIT■	Indicates that units are on.
EXIT	Exits to the Periodic Table or list of elements
FONT	Toggles the display font between large and small.
TABLE	Returns to the Periodic Table display from the element list.
PROPS	Displays a list of various properties for each element.
FIND	Initiates a search for an element name, number, symbol or property.
LIST	Displays an alphabetical listing of elements and symbols.
FAST	Toggles fast display mode on and off.
FAST■	Indicates that fast mode is on.
ATW→	Places the atomic weight of the current element on the stack as a tagged object

Notes:

Chapter 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

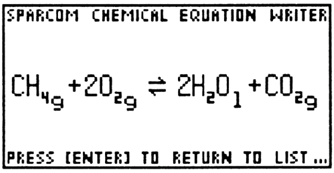
The stoichiometry function is designed for you to enter, name, and store your own chemical reactions in the calculator's memory. The software checks for mass and charge balance and allows you to easily calculate theoretical yields and limiting reagents. Two chemical reactions, methane combustion and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

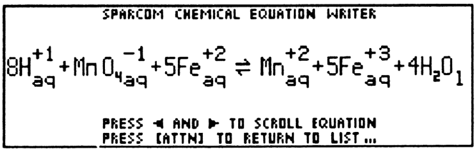


SPARCOM CHEMICAL EQUATION WRITER

$$CH_{4_g} + 2O_{2_g} \rightleftharpoons 2H_2O_l + CO_{2_g}$$

PRESS [ENTER] TO RETURN TO LIST ...

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 the display to the right or to the left. The figure below illustrates what a long reaction (in this case, the permanganate reaction) would look like if the screen were wide enough to display all the data at once.



SPARCOM CHEMICAL EQUATION WRITER

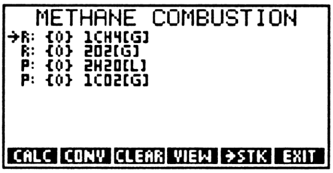
$$8H^{+1}_{aq} + MnO^{-1}_{4_{aq}} + 5Fe^{+2}_{aq} \rightleftharpoons Mn^{+2}_{aq} + 5Fe^{+3}_{aq} + 4H_2O_l$$

PRESS ◄ AND ► TO SCROLL EQUATION
PRESS [ATTN] TO RETURN TO LIST ...

Press [ATTN] to return to the STOICHIOMETRY menu screen.

Calculating Theoretical Yields

Suppose you want to calculate the mass of O_2 required to react with 1_g of CH_4 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:

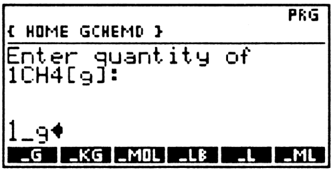


```
  METHANE COMBUSTION
→R: {0} 1CH4[G]
 R: {0} 2O2[G]
 P: {0} 2H2O[L]
 P: {0} 1CO2[G]
```

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.

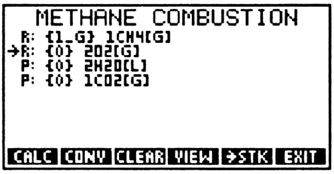
Entering a Quantity of a Reactant

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:



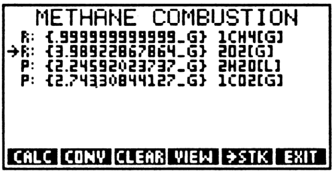
```
                        PRG
{ HOME GCHEMD }
Enter quantity of
1CH4[g]:

1_g◆
```

Press ENTER to store 1_g as the quantity of CH_4:



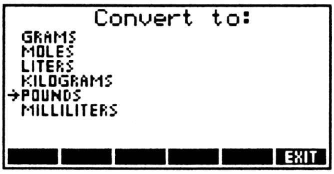
```
  METHANE COMBUSTION
 R: {1_G} 1CH4[G]
→R: {0} 2O2[G]
 P: {0} 2H2O[L]
 P: {0} 1CO2[G]
```

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.



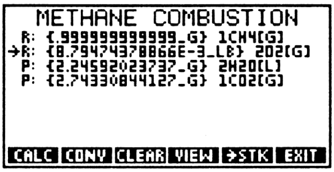
```
  METHANE COMBUSTION
 R: {.999999999999_G} 1CH4[G]
→R: {3.98922867864_G} 2O2[G]
 P: {2.24592023737_G} 2H2O[L]
 P: {2.74330844127_G} 1CO2[G]
```

To convert the mass of oxygen (or any reactant or product) into units other than grams, move the pointer to the reactant or product you want to covert (in this case, O_2) and press **CONV**. This displays a list of available units:



```
      Convert to:
 GRAMS
 MOLES
 LITERS
 KILOGRAMS
→POUNDS
 MILLILITERS
```

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

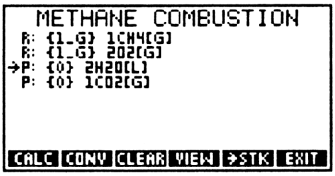


```
   METHANE COMBUSTION
 R: {.999999999999_G} 1CH4[G]
→R: {8.79474378866E-3_LB} 2O2[G]
 P: {2.24592023737_G} 2H2O[L]
 P: {2.74330844127_G} 1CO2[G]
```

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

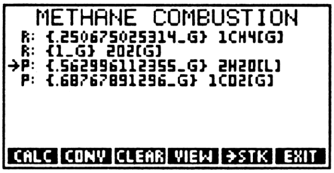
Limiting Reagents

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



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

Press **CALC** to start the calculation. The result is shown below:

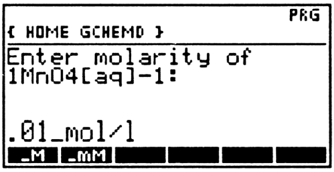


```
   METHANE COMBUSTION
 R: {.25067502531 4_G} 1CH4[G]
 R: {1_G} 2O2[G]
→P: {.562996112355_G} 2H2O[L]
 P: {.68767891296_G} 1CO2[G]
```

This shows that all the O_2 is consumed in the reaction (it's the limiting reagent) whereas only 0.25_g of CH_4 was consumed. Limiting reagent calculations may be performed with any number of reactants and products specified.

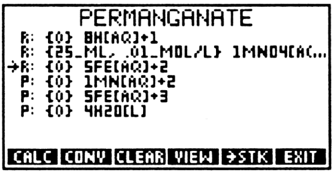
Stoichiometry with Solutions

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



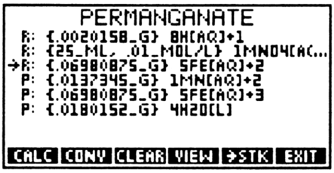
```
                      PRG
{ HOME GCHEMD }
Enter molarity of
1MnO4[aq]-1:

.01_mol/l
```

Press ENTER to place the volume and concentration onto the stoichiometry list for permanganate, as shown:



```
      PERMANGANATE
 R: {0} 8H[AQ]+1
 R: {25_ML, .01_MOL/L} 1MNO4[AC...
→R: {0} 5FE[AQ]+2
 P: {0} 1MN[AQ]+2
 P: {0} 5FE[AQ]+3
 P: {0} 4H2O[L]
```

Press **CALC** to initiate the theoretical yield calculation for this reaction. The result is shown below:



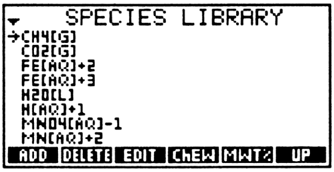
```
        PERMANGANATE
 R: {.0020158_G} 8H[AQ]+1
 R: {25_ML, .01_MOL/L} 1MNO4[AC...
→R: {.06980875_G} 5FE[AQ]+2
 P: {.0137345_G} 1MN[AQ]+2
 P: {.06980875_G} 5FE[AQ]+3
 P: {.0180152_G} 4H2O[L]
```

Using the Species Library

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

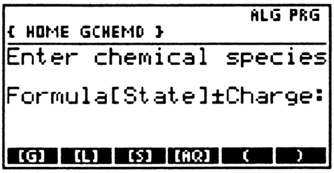
$CH_{4(g)}$ $CO_{2(g)}$
$Fe^{+2}_{(aq)}$ $Fe^{+3}_{(aq)}$
$H_2O_{(l)}$ $H^{+1}_{(aq)}$
$MnO_4^{-1}{}_{(aq)}$ $Mn^{+2}_{(aq)}$
$O_{2(g)}$ $OH^{-1}{}_{(aq)}$

To view these chemical species, select SPECIES LIBRARY at the main menu:



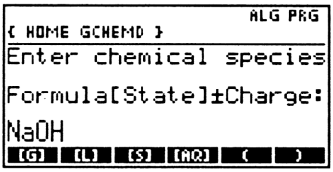
```
▾    SPECIES LIBRARY
→CH4[G]
 CO2[G]
 FE[AQ]+2
 FE[AQ]+3
 H2O[L]
 H[AQ]+1
 MNO4[AQ]-1
 MN[AQ]+2
```

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:



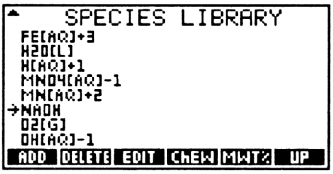
```
                    ALG PRG
{ HOME GCHEMD }
Enter chemical species
Formula[State]±Charge:
```

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



```
                     ALG PRG
{ HOME GCHEMD }
Enter chemical species
Formula[State]±Charge:
NaOH
```

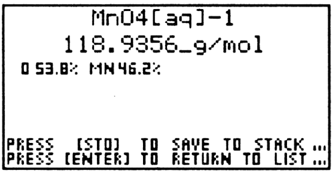
Press ENTER to place NaOH into the Species Library:



```
▲    SPECIES LIBRARY
  FE[AQ]+3
  H2O[L]
  H[AQ]+1
  MNO4[AQ]-1
  MN[AQ]+2
→NAOH
  O2[G]
  OH[AQ]-1
```

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.

To evaluate the molecular weight of any species in the list, for example $MnO_4^{-1}{}_{(aq)}$, 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:



```
        MnO4[aq]-1
      118.9356_g/mol
 O 53.8% MN 46.2%



PRESS  [STO]  TO SAVE TO STACK ...
PRESS [ENTER] TO RETURN TO LIST ...
```

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

Creating a Chemical Reaction

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

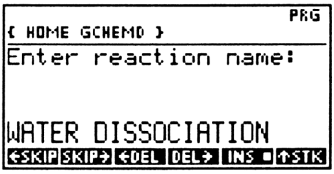
Upon entering the STOICHIOMETRY function of the General Chemistry Application Pac, all stored reactions are listed on the screen, as shown:


STOICHIOMETRY
→METHANE COMBUSTION
PERMANGANATE

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

$$H_20_{[l]} \rightarrow H^{+}_{[aq]} + OH^{-}_{[aq]}$$

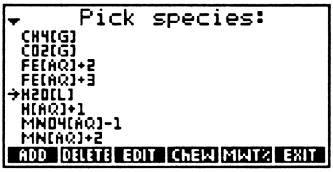
Press the ADD softkey. At the prompt, type in the name of the reaction:


PRG
{ HOME GCHEMD }
Enter reaction name:
WATER DISSOCIATION

(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:

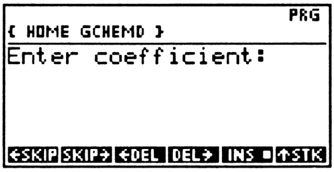

WATER DISSOCIATION
→PRESS ADD

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



```
▾     Pick species:
  CH4[G]
  CO2[G]
  FE[AQ]+2
  FE[AQ]+3
→H2O[L]
  H[AQ]+1
  MNO4[AQ]-1
  MN[AQ]+2
```

The prompt then asks for the stoichiometric coefficient, which in this case is 1. Type 1 at the prompt and press ENTER:

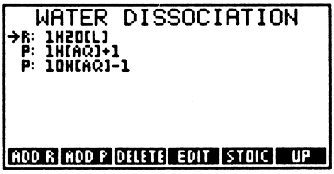


```
                              PRG
{ HOME GCHEMD }
Enter coefficient:
```

This places H_2O on the reaction list, labeled R for reactant. The coefficient 1 preceeds the species entry on the list.

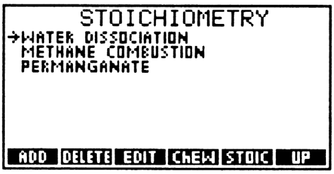
```
  WATER DISSOCIATION
→R: 1H2O[L]
```

Press **ADD P** to add a product species. Once again, scroll down the list until you find OH[aq]-1 and press ENTER. Repeat this procedure to add H^+ to the reaction list as a product (look for H[aq] + 1). If you make a mistake, press **DELETE** to delete a reactant. Pressing **EDIT** allows you to enter a replacement species and new stoichiometric coefficient. This results in the complete reaction listing for the WATER DISSOCIATION reaction, as shown:



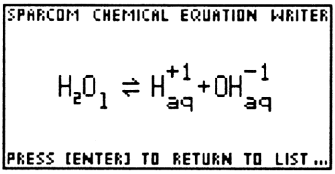
```
  WATER DISSOCIATION
→R: 1H2O[L]
 P: 1H[AQ]+1
 P: 1OH[AQ]-1
```

Press **STOIC** to peform 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:



STOICHIOMETRY
→WATER DISSOCIATION
METHANE COMBUSTION
PERMANGANATE

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



SPARCOM CHEMICAL EQUATION WRITER

$$H_2O_l \rightleftharpoons H^{+1}_{aq} + OH^{-1}_{aq}$$

PRESS [ENTER] TO RETURN TO LIST...

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 α and pressing the appropriate softkey. Charges must be preceded by the sign (either + or -). Parentheses may be entered by either pressing ⬅ ÷ or the two softkeys shown in the display. (Note that ⬅ ÷ does not require unlocking alpha-entry mode.)

Some examples of acceptable chemical formulas are:

Compound	**Input**
HCl	HC ⬅L
HNO_3	HNO3
$Ca(NO_3)_2$	C ⬅A ⬅ ÷ NO3 α ▶2
$H^+[aq]$	H α [aq]+1
$C(CH_3)_3{}^+$	C ⬅ ÷ C H 3 α ▶3+1
$Ca(OH)_2 \cdot 6H_2O$	C ⬅A ⬅ ÷ OH α ▶2 ⬅ ÷ H2O α ▶6

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

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

R-COOH + Rz-OH -> Products.

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

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

Summary of Softkeys

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

Stoichiometry Softkeys

ADD	Adds a new chemical reaction to the list.
ADD R	Adds a reactant from the Species Library and a stoichiometric coefficient to the selected chemical reaction.
ADD P	Adds a product from the Species Library and a stoichiometric coefficient to the selected chemical reaction.
CALC	Utilizes the current species quantities to perform theoretical yield or limiting reagent calculations.

ChEW	Displays a chemical reaction on the screen in the Sparcom Chemical Equation Writer format.
CLEAR	Clears all quantities in the stoichiometry function.
CONV	Converts a quantity to a different unit.
DELETE	Deletes a chemical reaction or a reactant or product from a chemical reaction.
EDIT	Edits a chemical reaction or a reactant or a product.
ENTER	Allows you to specify the quantity of a reactant or product.
EXIT	Exits the Stoichiometry solving screen.
→STK	Copies selected entry to calculator stack.
STOIC	Enters the stoichiometry solving screen after the selected chemical reaction is mass and charge balanced.
UP	Moves up one level in the menu structure.
VIEW	Displays entries too wide to fit on the screen. It is not functional if the line does fit on the screen. ADD

Species Library Softkeys

ADD	Adds a new chemical species to the Species Library.
ChEW	Displays a chemical species on the screen in the Sparcom 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.

Chapter 5

Constants Library

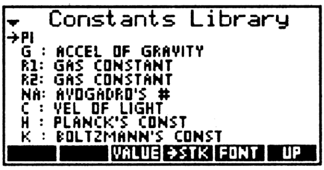
In This Chapter

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:



```
▼   Constants Library
→PI
  G : ACCEL OF GRAVITY
  R1: GAS CONSTANT
  R2: GAS CONSTANT
  NA: AVOGADRO'S #
  C : VEL OF LIGHT
  H : PLANCK'S CONST
  K : BOLTZMANN'S CONST
```

The Constants Library menu lists 29 constants and their symbols, listed below:

pi	π
g	Acceleration of gravity
R1	Universal gas constant - J/(mol*K)
R2	Gas constant - l*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

εo	Permittivity of vacuum
me	Electron mass
re	Classical electron radius
mp	Proton rest mass
R∞	Rydberg's constant
α	Fine structure constant
ao	Bohr radius
μB	Bohr magneton
λ	Wavelength for 1 eV
λc	Compton's wavelength
σ	Stefan-Boltzmann
c1	First radiation constant
c2	Second radiation constant
Vt	Thermal voltage at 300 K
μo	Permeability of free space
φo	Magnetic flux quantum
F	Faraday constant
μe	Electron magnetic moment
μp	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 [α] [↰] [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)' EVAL to call for the speed of light.

Stack Method

Type '$c' into level 1 of the stack and press the **GCON** library softkey or type the letters GCON and press [ENTER].

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

Constants Library Softkeys

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

Notes:

Chapter 6

Reference Library

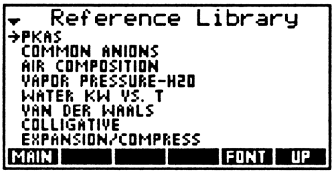
In This Chapter

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:



```
▾  Reference Library
→PKAS
 COMMON ANIONS
 AIR COMPOSITION
 VAPOR PRESSURE-H2O
 WATER KW VS. T
 VAN DER WAALS
 COLLIGATIVE
 EXPANSION/COMPRESS
```

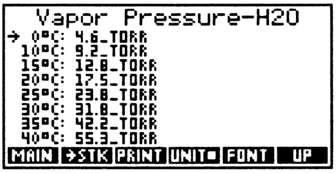
The Reference Library application, accessed from the main menu, consists of 10 topics. To access a given topic, move the pointer to the desired topic and press ENTER. The 10 Reference Library topics are described below:

PKas	The dissociation constants of selected weak acids.
Common anions	Names and formulas of common anions.
Air composition	Percent composition (by volume) of air at sea level.
Vapor pressure - H_2O	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 for common bonds.

Example Using the Reference Library

Suppose you need the vapor pressure of water at 25_°C for a gas law calculation you're working on in the calculator stack. Use the cursor keys to move the pointer to the VAPOR PRESSURE - H2O menu item. Press ENTER to display the following screen:



```
   Vapor Pressure-H2O
→  0°C: 4.6_TORR
  10°C: 9.2_TORR
  15°C: 12.8_TORR
  20°C: 17.5_TORR
  25°C: 23.8_TORR
  30°C: 31.8_TORR
  35°C: 42.2_TORR
  40°C: 55.3_TORR
```

Move the pointer to 25_°C and press ENTER. This copies the value 23.8_torr onto the calculator stack. You need to exit the Pac to continue your calculation on the stack.

Summary of Softkeys

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

Appendix A

Warranty and Service

Pocket Professional Support

You can get answers to your questions about using your Pocket Professional card from Sparcom. If you don't find the information in this manual or in the HP 48SX *Owner's Manual*, contact us in writing, at :

Sparcom Corporation
Attn: Technical Support Dept.
897 NW Grant Avenue, Corvallis, OR 97330, U.S.A. (503) 757-8416

or send E-mail:

from **Internet:** support@sparcom.com
from **Compuserve:** >Internet:support@sparcom.com
from **FidoNet:** To:support@sparcom.com

Limited One-Year Warranty

What Is Covered

The Pocket Professional is warranted by Sparcom Corporation against defects in material and workmanship for one year from the date of original purchase. If you sell your card or give it 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 Sparcom.

What Is Not Covered

This warranty does not apply if the product has been damaged by accident or misuse or as the result of service or modification by any entity other than Sparcom Corporation.

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 SPARCOM CORP. BE LIABLE FOR CONSEQUENTIAL DAMAGES. Products are sold on the basis of specifications applicable at the time of manufacture. Sparcom shall have no obligation to modify or update products, once sold.

If the Card Requires Service

Sparcom 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 based on time and material.

Shipping Instructions

If your card requires service, ship it to Sparcom Corporation, 897 NW Grant Avenue, Corvallis, OR 97330, U.S.A.

- Include your return address and a description of the problem.
- Include proof-of-purchase date if the warranty has not expired.
- Include a purchase order, along with a check, or credit card number and expiration date (VISA or MasterCard) to cover the standard repair charge.
- Ship your card, postage prepaid, in adequate protective packaging to prevent damage. Shipping damage is not covered by the warranty, so insuring the shipment is recommended.

Cards are usually serviced and reshipped within five working days.

Environmental Limits

The reliability of the Pocket Professional depends upon the following temperature and humidity limits:

- 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% relative humidity at 40 °C (104 °F) maximum.

Notes:

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:

a. Check to make sure that the card is properly seated in the calculator port.

b. Turn the calculator off and on.

c. 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. What do three dots (...) mean at the end of a display line?

A. The three dots indicate that the object is too long to show on one line. To view the complete object, use the cursor keys to move the arrow to the object and press ↱ VISIT. Pressing ENTER or ATTN returns you to the browser.

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

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

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

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

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

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

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

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

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

Appendix C
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Index

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