

The PocketProfessional®

Chemistry Reference Pac

Owner's Manual

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Table of Contents

1	Getting Started	1
	Welcome	1
	Installing and Removing the Pocket Professional	1
	To Install the Card	1
	To Remove the Card	2
	To Access the Reference Pac	2
	Using the Main Menu	3
	Moving Around the Screen	4
	Viewing Items Too Wide for the Display	5
	Changing the Font Size	5
	Example: Using the Reference Pac	5
	Multiple stack entries	6
	Managing Units	7
	Using the Search Mode	7
	Null Entries	8
	Summary of Functions	8
2	Reference Library	9
	Constants Library	9
	Fundamental	10
	Derived Atomic Constants	11
	Universal Constants	11
	General Constants	12
	Solids/Liquids	12
	Linear Expansion	12
	Cubical Expansion	12
	Cubic Structures	13
	Ebullioscopic Constants	13
	Cryoscopic Constants	13
	Boiling Points at 760 mm Hg	13
	Gases	13
	Vapor Pressure	14
	Van Der Waals	15
	Cryogenic Gases	16
	Density of Hg	16
	Vapor Pressure of Hg	16
	Acids and Bases	17
	Indicators	17
	Inorganic Acids/Bases	17
	Organic Acids/Bases	17

Common Acids/Bases	18
Thermodynamics	19
Elements and Oxides	19
Group 1 through 0	19
Complexes	20
Solubilities	20
Gases, 100g (water)	21
Inert Gases, 1ml (water)	21
Air Solubility, (1ml water)	21
Compounds in Water	21
Solubility Products	21
Electrochemistry	21
Reduction Potentials	22
Liquid Conductivities	22
Electrolytes	22
Water	22
Bonds	22
Bond Calculations	23
Bond Energies	24
Bond Lengths	24
Bond Structures	24
3 Periodic Table	25
Using the Periodic Table	25
Properties of Each Element	26
Moving around the Periodic Table	26
Using Search and List Utilities	26
List of Elements and Symbols	27
Searching for a Property	27
Summary of Softkeys	27
4 Molecular Weight	
Using Molecular Weight Function	29
Entering Molecular Formulas	29
Appendix A Warranty and Service	31
PocketProfessional Support	31
Limited One Year Warranty	31
What is covered	31
What is not Covered	31
If the Card Requires Service	32
Service Charge	32

Shipping Instructions	32
Environmental Limits	32
Appendix B References	33
Appendix C Questions and Answers	34
Commonly Asked Questions	34
Index	35

1 Getting Started

In This Chapter

- Welcome
- Installing and Removing the Pocket Professional
- Using the Main Menu
- Using the Reference Library
- Summary of Functions

Welcome

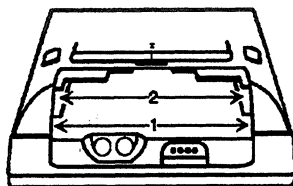
Da Vinci Technology Group's Pocket Professional software is the first of its kind, developed to provide speed, efficiency and portability to students and professionals in the technical fields. The PocketProfessional™ Chemistry Reference Pac instantly transforms the HP 48GX calculator into an electronic handbook, containing over 100 tables of data commonly used by chemists and chemical engineers. The information is organized in a menu tree with topics and sub-topics displayed in an easy-to-use "browser" menu format.

Installing, Removing the Pocket Professional

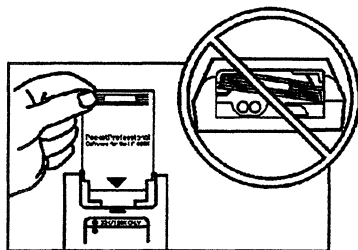
The HP 48GX has two ports for installing plug-in cards. You can install this card in either port. Be sure to **turn off the calculator** while installing or removing the card. Otherwise, user memory may be erased.

To Install the 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 PocketProfessional card.

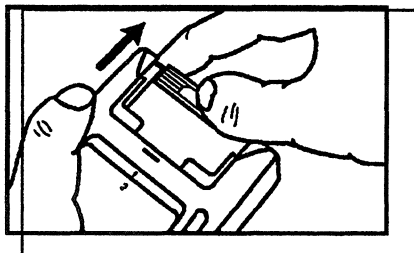


- Position the card just outside the slot. Point the triangular arrow on the card toward the calculator port opening, as shown below.
- Slide the card firmly into the slot. After you first feel resistance, push the card about 1/4 inch further, until it is fully seated.
- Replace the port cover.



To Remove the Card

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

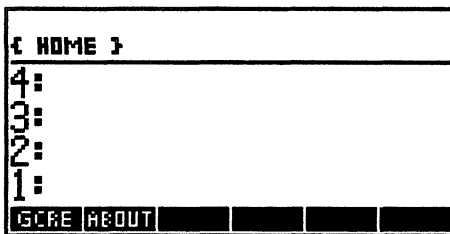


To Access the Reference Pac

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

First Method:

Press **→** **LIBRARY** to display all libraries available to the HP 48GX. Press the **GCRC**, "softkey" (the corresponding blank menu key on the top row of the HP 48GX keyboard) to start the Chemistry Reference



Pac.

Second Method:

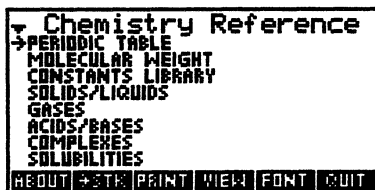
Type in the letters GCREF (using alpha entry mode, as described in the *HP 48GX Owner's Manual*) and press **ENTER**.

Third Method:

Add the command GCREF to the **CST**. After the command has been added, press **CST**, then press **GCRE** to start the Chemistry Reference application.

Using the Main Menu

After you start the Pac, the main menu screen appears. The main menu lists the main categories available in the Pac in a “browser” menu format. The term “Browser” refers to the ability to use the cursor



keys **▼** and **▲** to move the pointer to the menu item desired and access it by pressing **ENTER**. The row of “softkeys” along the bottom of the screen may give you options that relate to the information displayed on any given screen.

Because the size of the calculator screen is limited, the names of constants and properties are usually abbreviated throughout the reference Pac. This manual includes “translations” of these abbreviations where appropriate.

The items in the main menu are outlined in the Table below:











Periodic Table	Displays selected properties for each element of the Periodic Table
Molecular Weight	Allows for molecular weight and percent composition calculations
Constants Library	Thirty nine constants commonly used by chemists and chemical engineers
Solids/Liquids	Linear, cubic coefficients of expansion

	of materials; cubical cell characteristics for selected materials; physical properties of selective inorganic and organic fluids.
Gases	Vapor pressure, Van der Waals constants for selected gases
Acids/Bases	Dissociation constants for selected inorganic, organic acids, bases and indicators
Complexes	Formation constants of transition metals with common ligands
Solubilities	Solubility products and aqueous solubilities of organic and inorganic compounds
Bonds	Tables of bond lengths, energies; structures of common compounds
Water	Sixteen properties of water and their variation with pressure and temperature
Electrochemistry	Reduction potentials of selected half reactions, and conductivity of pure liquids & common electrolytes.
Thermodynamics	Selected thermodynamic data of inorganic and organic compounds
ABOUT	Displays screen showing information about this software
>STK	Places a single or all browser entries on the calculator stack
PRINT	Allows you to print one or all data entries in a particular field
VIEW	Allows you to view entries that are too wide to be displayed
FONT	Toggles between small and medium size display font size
QUIT	Exits the Chemistry Reference Pac. Pressing CANCEL performs the same function.



Each main category of the reference pac contains several topics and sub-topics. They are described in detail in Chapter 2. The information

contained in each topic from a variety of sources. Values given in the here may vary slightly from values listed by sources not documented in this manual.



Moving Around the Screen

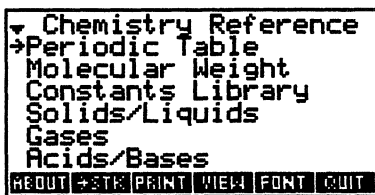
Use the  and  keys to move the pointer up and down in the menu list. Pressing   moves the pointer to the bottom of the screen, or pages down if the pointer is already at the bottom of the screen. Pressing   moves to the top of the screen or pages up if the pointer is already at the top of the screen.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

Viewing Items Too Wide for the Display

If the text of a topic or subtopic is too wide to fit within the display, an ellipsis (...) appears at the end of the line. Press the softkey  to display the rest of the text. To return the previous display, press  key.






Changing the Font Size

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



Example: Using the Reference Pac

Suppose you need to know the second dissociation constant of Chromic acid (K_a for HCrO_4^{-1}). At the main menu, move the pointer to

Acids/Bases and press . Move the pointer to Inorganic Acids/Bases and press . In the new screen, move the pointer to H_2CrO_4 and again press . The screen now shows $\text{p}K_a$ of Chromic acid, and use the pointer to select $\text{p}K_2$ and press  . The calculator prompts you for where the data should be sent as shown in the screen shown. Pressing

ONE will transfer pK2 to the stack. Now press **CANCEL** at the previous screen to exit the Pac. The resulting display is also shown in the series of displays listed here.

```

Acids/Bases
→INDICATORS
INORGANIC ACID/BASES
ORGANIC ACIDS/BASES
COMMON ACIDS/BASES
MAIN →STK PRINT VIEW FONT UP
  
```

```

Inorganic Acid/Bases
→CO2
H2CO3
H2O
H2SO4
H3PO4
H2B4O7
H2CR04
H2NCL02
MAIN →STK PRINT VIEW FONT UP
  
```

```

H2CrO4
→PK1: -.88
PK2: 6.50
PK3: -
MAIN →STK PRINT VIEW FONT UP
  
```

```

Send what data?
ONE ALL
  
```

```

{ HOME }
4:
3:
2:
1: PK2: 6.5
GCRC REOUT
  
```

```

{ HOME }
4:
3:
2:
1: 3.16227766017E-7
OBJ+ +ARR +LIST +STR +TAG +UNIT
  
```

To get K_a from from pKa, (change the sign using the **+/-**) and press **←** **y^x**. This yields the value shown in the last display screen shown above. You can now proceed with other calculations possible in the Pac.

Multiple Stack Entries

Suppose for example, you're interested in retrieving all the three pKas of phosphoric acid instead of just one as shown in the example above. At the prompt simply press **->STK ALL** and notice the following screen when you exit the Pac.

```

{ HOME }
3:
2:
1: { :pK1: 2.15 :pK2:
7.2 :pK3: 12.38 }
GCRC REOUT
  
```

To extract data from the list, press **PRG TYPE OBJ->**. This results in all the three values on successive levels of the stack along with total

```

[ HOME ]
3:
2:
1: { :PK1: 2.15 :PK2:
      7.2 :PK3: 12.38 }
[SCRE] [R0UT]

```

```

[ HOME ]
4: PK1: 2.15
3: PK2: 7.2
2: PK3: 12.38
1:
[DEJ+] [ARR] [LIST] [STR] [TMS] [UNIT]

```

number of stack entries (in this case 3) as shown in the display screens above.

Managing Units

You can choose whether you want the Pac to display units on the screen or not by pressing the **UNITS** softkey. This softkey toggles between the unit and non-unit modes. **UNIT** indicates that units will be displayed with all entries. When units are displayed, pressing **ENTER** places the entry onto the stack **with** units. When units are not displayed on the screen, units are not included when **ENTER** is pressed. Note that values in the constants library will be displayed with units whether units are toggled on or off. The Pocket Professional uses standard international units, customarily used in electrical engineering. **Be aware that using units usually increases the processing time for display.**

Using the Search Mode

When data lists are long, it may be faster to locate an item using the search mode. To initiate a search, press the



key. The screen displayed is shown to the right. The calculator is now in **alpha** entry mode, as

```

PRG
[ HOME ]
Search for:
[SKIP] [SKIP+] [DEL] [DEL+] [INS]

```

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. 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. The search mode softkeys **<-SKIP**

< - DEL **INS** along the bottom of the screen are command line editing keys which allow you to edit the search string. Their functions are summarized at the end of this chapter.

Null Entries

When a menu displays only a minus sign (-) after its name, it means that the item is being used as a placeholder in the database. The minus sign is not an indication of a minus or zero value.

Summary of Functions

FONT	Toggles the display font between condensed and large sizes.
QUIT	Exits the Electrical Engineering Reference Pac.
UP	Moves up one level in the menus.
MAIN	Moves to the main menu of the Electrical Engineering Reference Pac.
PICT	In a few cases, a picture is available to help explain the data item. Pressing this softkey displays the figure on the screen
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 between unit and non-unit modes. The Pocket Professional uses standard international (SI) units customarily used in electrical engineering.
< - SKIP	Moves the SKIP>cursor from its current position to the beginning of the word (left).
SKIP - >	Moves the cursor to the beginning of the next word (right).
< - DEL	Deletes all the characters from the cursor's position to the beginning of the word (left).
DEL - >	Delete all the characters from the cursor's position to the first character of the next word (right).
INS	Toggles between insert and typeover modes
VIEW	Displays remaining data (a screen width at a time) on the screen for entries too wide for the screen. If the topic is too long to fit within the display, an ellipsis (...) is displayed on the right of the screen.
ENTER	Moves to the category, topic, or sub-topic indicated by the pointer.
CANCEL	Exits the Electrical Engineering Reference Pac.



Initiates a case sensitive search for a specific entry.



Moves to the bottom of the screen or pages down



Moves to the top of the screen or pages up.



Moves the pointer to the bottom of the list



Moves to the top of the screen or pages up.

2 Reference Library

In This Chapter

The General Chemistry Reference Library consists of reference data commonly used by chemists and chemical engineers. All entries are listed under the ten categories below. Within each category are several topics and sub-topics.

- Constants Library
- Solids/Liquids
- Gases
- Acids/Bases
- Thermodynamics
- Complexes
- Solubilities
- Electrochemistry
- Water
- Bonds

Please note that when chemical formulas are displayed on the screen they are shown without subscripts and superscripts as is normally found in chemistry.

Constants Library

The constants Library offers you immediate access to 39 constants commonly used in general chemistry. Constants are listed under the four categories below:

Fundamental Constants

1.660566 X 10 ⁻²⁷	Atomic mass unit
6.022045 X 10 ²³ mol ⁻¹	Avogadro's number
1.380662 X 10 ⁻²³ J/K	Boltzmann's constant
1.054589 X 10 ⁻²³ J · s	Dirac's constant ($\hbar/2\pi$)
1.602189 X 10 ⁻¹⁹ C	Electron charge
9.284832 X 10 ⁻²⁴ J/T	Electron magnetic moment
0.910953 X 10 ⁻³⁰ Kg	Electron mass
2.675199 X 10 ⁸ T ⁻¹ · s ⁻¹	Gyromagnetic ratio
4.490474 X 10 ⁻²³ J/T	Muon magnetic moment
1.883566 X 10 ⁻²⁸	Muon mass

1.674954 X 10⁻²⁷ Kg
1.410617 X 10⁻²⁶ J/T
1.672649 X 10⁻²⁷ Kg
4π X 10⁻⁷ H·m⁻¹
6.626176 X 10⁻³⁴ J·s
1.09737318 X 10⁷ m⁻¹
2.99792458 X 10⁸ m/s
0.28978 cm·K

Derived Atomic Constants

3.74183 X 10⁻¹⁶ W/m²
1.438786 X 10⁻² m·K
9.274078 X 10⁻²⁴ J/T
0.52917706 X 10⁻¹⁰ m
2.426309 X 10⁻¹² m
1.319591 X 10⁻¹⁵ m
1.321410 X 10⁻¹⁵ m
1.00002564
1.758805 X 10¹¹ C/Kg
1.001159657
2.817938 X 10⁻¹⁵ m
0.007297351
7.727389 X 10⁻⁴ J·s/Kg
4.835939 X 10¹⁴ Hz/V
8.617347 X 10⁻⁵ J K⁻¹ C⁻¹
2.067851 X 10⁻¹⁵ Wb
1836.15
5.050824 X 10⁻²⁷ J/T
8.85418782 X 10⁻¹² F/m
4.135701 X 10⁻¹⁵ J/Hz·C
5.6703 X 10⁻⁸ W/(m²·K⁴)
6.652448 X 10⁻²⁹ m²
658.210697872

Universal Constants

9.648456 X 10⁴ C/mol
8.31441 J⁻¹·mol⁻¹·K⁻¹
1.98719 cal mol⁻¹·K⁻¹
82.0568 cm³·atm·mol⁻¹·K⁻¹
6.672 X 10⁻¹¹ N·m²·Kg⁻²
9.80665 m/s²
0.0224138 m³/mol

Neutron mass
Proton magnetic moment
Proton mass
Permeability of vacuum
Planck's constant
Rydberg's constant
Speed of light
Wien's displacement constant

1st radiation constant
2nd radiation constant
Bohr magneton
Bohr radius
Compton's electron wavelength
Compton's neutron wavelength
Compton's proton wavelength
Diamagnetic shield of H₂O
Electron charge to mass ratio
Electron g-factor
Classical electron radius
Fine structure constant
h to electron mass ratio
Josephson's frequency to voltage ratio
k/q ratio
Magnetic flux quantum
proton to electron mass ratio
Nuclear magneton
Permittivity of vacuum
Quantum of circulation
Stefan-Boltzmann constant
Thompson's Cross section
μ_e/μ_p ratio

Faraday's constant
Gas constant
Gas constant
Gas constant
Gravitational constant
Acceleration of gravity
Molar volume

General Constants

-459.67 °F

11.9

3.9

13.53362 g/cm³

273.15 K

1 atm

Absolute zero in F

Dielectric constant of Si

Dielectric constant of SiO₂

Density of Hg at 25 °C

Standard temperature

Standard pressure

Solids/Liquids

The solids/liquids category includes reference data on the following topics:

- Linear Expansion
- Cubical Expansion
- Simple Cubic
- Body Centered Cubic
- Face-centered cubic
- Ebullioscopic Constants
- Cryoscopic Constants
- Boiling Points

Linear Expansion Coefficient

In this table, coefficients of linear expansion of various solids are given. The coefficient of expansion is defined by:

$$l_t = l_0 \cdot (1 + \alpha \cdot t)$$

where l_0 is the length of the material, l_t is the length at t °C, and α is the linear coefficient of expansion. The valid temperature range where the coefficient of expansion is included.

Cubical Expansion

The coefficient of cubical expansion is defined as the increase in volume per unit volume per degree C rise in temperature. In this table, cubical expansion coefficients of various crystalline solids are given along with their valid temperature range.

$$V = V_0 \cdot (1 + \alpha' \cdot t)$$

Cubic Structures

Cubic structures (simple, body-centered, and face-centered) contain lattice parameters of the three simplest unit cell structures. The information contained for each cubic structure is:

- Lattice points/cell
- Atomic radius
- Number of nearest neighbor
- Packing fraction
- Nearest neighbor distance

Ebullioscopic Constants

The ebullioscopic constant K_b gives the increase of the boiling point, ΔT (in $^{\circ}\text{C}$), produced when one mole of solute is dissolved in 1000g of a solvent. Note that molecular weights can be determined with the relation

$$M = K_b \cdot \frac{1000 \cdot w_2}{w_1 \cdot \Delta T_b}$$

where ΔT_b is the elevation of the boiling point brought about by the addition of w_2 grams of solute to w_1 grams of solvent and K_b is the ebullioscopic constant. The normal boiling point is listed for each solvent.

Cryoscopic Constants

The cryoscopic constant K_f gives the depression of the melting point, ΔT (in $^{\circ}\text{C}$), produced when one mole of solute is dissolved in 1000g of a solvent. Once again this equation may be used to determine molecular weight with the following relation

$$M = K_f \cdot \frac{1000 \cdot w_2}{w_1 \cdot \Delta T_b}$$

In this table, the cryoscopic constant and normal freezing point of each solvent is listed.

Boiling Points

This table contains 72 solvents arranged in order of increasing boiling point.

Gases

This section concentrates on the vapor pressure of various substances,

including mercury. It also includes Vander Waals constants and properties of selected cryogenic gases:

- Vapor Pressure
- Van der Waals
- Cryogenic Gases
- Density of Hg
- Vapor Pressure of Hg

Vapor Pressure

There are several mathematical relationships between the temperature of a condensed phase and its equilibrium vapor pressure. The Antoine equation (Eq 1) correlates well with experimental values. Equation 2 is simpler and is often accurate over limited temperature ranges.

$$\log p = A - \frac{B}{t + C} \quad (\text{Eq.1}) \qquad \log p = A - \frac{B}{t} \quad (\text{Eq.2})$$

In these equations, p is the vapor pressure of the compound in mm Hg (torr) t is the temperature in ° Celsius, and T is the temperature in Kelvin.

In this table, the constants A,B, and C are listed for various organic compounds along with the temperature range for which they are valid. To obtain the vapor pressure at any temperature, press the **SOLVE** softkey . You may then enter the temperature and the vapor pressure will be calculated automatically using the proper equation.

Note: Calculations are only valid in the suggested temperature range. However, if you compute outside the range, the result should be treated as an estimate.

Example - To obtain the vapor pressure of benzene at 50 °C, highlight

```

Benzene
→LOW T (°C): 8_°C
HIGH T (°C): 103_°C
A: 6.90565
B: 1211.033
C: 220.79
MAIN  ←STP PRINT SOLVE FONT UP
  
```

```

PRG
{ HOME GCHEMD }
Enter temperature from
8 to 103_°C:
<temp>
50_°C
_°C  _K  _°F  _°R
  
```

benzene with the pointer and press **ENTER** to display the screen shown .

This shows the constants A, B, C for benzene and that the valid temperature range for these constants is 8 to 103 °C. Press **SOLVE** to enter temperature. You may append any unit onto your entered value of temperature by pressing the appropriate softkey. In this case, the temperature of 50 °C has been entered. Press **ENTER** and the vapor pressure of benzene at 50 °C is calculated. Press the **STO** key to store the vapor pressure on the calculator stack or **ENTER** to return to the list.

```

Result:
:VP: '271.286375311.MMHG'

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

Van der Waals

The Van der Waals equation offers empirical corrections to the ideal gas law by assuming a finite particle volume and molecular interactions. This equation has the form:

$$\left(P + \frac{n^2 \cdot a}{V^2}\right) \cdot (V - n \cdot b) = n \cdot R \cdot T$$

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

$$V_c = 3 \cdot n \cdot b$$

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

where a and b are constants, R is the universal gas constant, n is the number of moles of gas, V is the gas volume, P is the pressure, and T_c , V_c , and P_c are the critical temperature, volume, and pressure respectively.

This table contains a and b for 61 gases. To obtain the pressure of a gas at any given temperature, volume, and quantity, press the **SOLVE** key.

```

CH4
→A: 2.253LL^2KATM/MOL^2
B: .0427B.L/MOL

MAIN  ←STP  PRINT  SOLVE  FONT  UP
  
```

You may then enter T, n and V and the pressure will be calculated

automatically. For example, suppose your interested in calculating the pressure of required to confine 1 mol of methane to a volume of 0.248 liters at a temperature of 298 K. Position the pointer to CH4 (use the search mode to find CH4 or move the pointer down 29 times) and

press **ENTER** . This displays the a and b constants for CH4, as shown:

Press **SOLVE** and enter the number of moles, the temperature, and

```
PRG
{ HOME GCHEMD }
Enter moles, volume,
and temperature:
<moles> <vol> <temp>
1 .248_1 298_K
_L _ML _°C _K _°F _°R
```

```
Result:
:P: '82.5229306862_ATM'
:Tc: '190.16564365_K'
:Vc: '.12834_1'
:PC: '45.5948579588_ATM'
PRESS [STO] TO SAVE TO STACK ...
PRESS [ENTER] TO RETURN TO LIST ...
```

volume all on one line, separated by spaces as shown: Then press **ENTER**. The pressure and critical temperature, volume, and pressure are calculated. Note that all units of temperature and milliliters and liters are supported by the softkeys. Press **STO** to store the pressure and critical parameters on the calculator stack or **ENTER** to return to the list.

Note: It is possible for you to enter values for T, V, U which would result in a non-realizable negative pressure.

Cryogenic Gases

This topic lists the following properties for a wide variety of gases used in low temperature applications.

- Density of liquid
- Boiling point
- Melting point
- Heat of vaporization
- Heat of fusion
- Heat capacity
- Heat capacity ratio (Cp/Cv)
- Critical temperature
- Critical Pressure
- Vapor density at boiling point

Density - Hg

This table lists the density of mercury versus temperature over the temperature range from 10 to 30 °C. To obtain the density of mercury at other temperatures, press the **SOLVE**. You may then enter temperature and the density will be calculated automatically.

Vapor Pressure- Hg

This table lists the vapor pressure of mercury versus temperature over the temperature range from 10 to 30 °C.

Acids and Bases

The reference data included for acids and bases covers four tables:

- Indicators
- Organic Substances
- Inorganic Substances
- Common Acids/Bases

Indicators

This table lists the pH range, the pKa, and the expected color change for selected pH indicators. The pH range or transition interval may vary appreciably from one observer to another and is affected by ionic strength, temperature, and light source. The values listed refer to solutions of low ionic strength and room temperature. The pKa (= -log Ka) is offered in some cases. The abbreviations used to describe color change are shown below:

- B Blue
- G Green
- P Purple
- V Violet
- Br Brown
- C Colorless
- O Orange
- R Red
- Y Yellow

Inorganic Acids/Bases

The table lists the pKa (= - log Ka) for the dissociation of inorganic acids at 25 °C defined for the general reaction: $HB \leftrightarrow H^+ + B$. The acid dissociation constant is formulated as follows:

$$K_a = \frac{[H^+][B]}{[HB]}$$

where the brackets (ie [H+]) refer to concentrations in moles/liter.

Organic Acids/Bases

The table lists the pKa (= - log Ka) for the dissociation of organic materials at 25 °C defined for the general reaction: $HB \leftrightarrow H^+ + B$. The acid dissociation constant is formulated as follows:

$$K_a = \frac{[H^+][B]}{[HB]}$$

where the brackets (ie [H+]) refer to concentrations in moles/liter. Ionic strengths are assumed to be zero unless otherwise noted. Protonated cations are designated (+1), (+2), etc after the pKa value. Neutral species

are designated by (0) unless obvious, and negatively charged species by (-1), (-2), etc.

Common Acids/Bases

This table lists typical densities, weight percents, and molarities of commercial concentrated acids and bases. When bottles of concentrated reagents are freshly opened, they are generally at the concentrations listed in this table. This may not be true of bottles opened for long periods and is especially true of ammonium hydroxide. A concentrated C.P. grade reagent comes with an assay label which states its molecular weight, MWT, density or specific gravity, d , and its percentage assay, p . When such a reagent is used to prepare an aqueous solution of desired molarity M , a convenient formula is:

$$V = \frac{100 \cdot MWT \cdot T}{p \cdot d}$$

where V is the number of milliliters of concentrated reagent required for one liter of dilute solution.

Example: Nitric acid has a molecular weight of 63.01 g/mol. If the concentrated reagent has an assay of 70.0% and a density of 1.41 g/ml, the volume required for 1 liter of a 0.1 molar solution is:

$$V = \frac{100 \cdot 63.01 \cdot 0.1}{70.0 \cdot 1.41} = 6.38 \text{ ml}$$

To perform this calculation for material in this table, press **SOLVE**. Enter the desired molarity and then the weight percent and density (if desired). The volume of acid will be calculated automatically.

Thermodynamics

The reference data for thermodynamics is included in the following nine tables:

- Elements and Oxides
- Group I
- Group II
- Group III
- Group IV
- Group V
- Group VI
- Group VII
- Group 0

Elements and Oxides

Thermodynamic calculations over a wide range of temperatures are generally made with the aid of algebraic equations representing the properties of substances. The most convenient starting point for such calculations is the equation for the heat capacity at constant pressure. From this quantity and a knowledge of the properties of any phase transitions, other thermodynamic properties may be computed.

Empirical heat capacity equations are generally of the form of a power series with absolute temperature as the independent variable, ie:

$$C_p = a + (b \cdot 10^{-3}) \cdot T + (c \cdot 10^{-6}) \cdot T^2 + \frac{d \cdot 10^5}{T^2}$$

where a, b, c and d are constants. The enthalpy H, entropy S, and Free Energy Function, FFN are determined from the heat capacity by a simple integration over temperature. Thus, if 298 K (25 °C) is taken as the reference temperature,

$$\Delta H = H_T - H_{298} = a \cdot T + \frac{1}{2} \cdot (b \cdot 10^{-3}) \cdot T^2 + \frac{1}{3} \cdot (c \cdot 10^{-6}) \cdot T^3 - \frac{d \cdot 10^5}{T} - A$$

$$S_T = a \cdot \ln T + (b \cdot 10^{-3}) \cdot T^2 + \frac{1}{2} (c \cdot 10^{-6}) \cdot T^3 - \frac{d \cdot 10^5}{2 \cdot T} - B$$

$$FFN = \frac{G_T - H_{298}}{T} = -a \cdot \ln T - \frac{1}{2} \cdot (b \cdot 10^{-3}) \cdot T - \frac{1}{6} (c \cdot 10^{-6}) \cdot T^2 - \frac{d \cdot 10^5}{2 \cdot T^2} + (B + a)$$

In this table, the constants a, b, c, d, A, and B are listed for selected elements and their oxides. Units for all constants are cal/mol except for A which has units of kcal/mol.

To calculate C_p , ΔH , S_T or FFN for any substance in the table, you may press **SOLVE**. Enter temperature and these values will be calculated automatically.

Group 1 through 0

The reference data in this section contain values of the enthalpy and Gibbs free energy of formation, entropy, and heat capacity at 298.15_K (25 °C). The physical state of each substance is abbreviated as follows: Crystalline solid (s), liquid (l), gaseous (g). The values of the thermodynamic properties given in this section assume that the substances are pure and

are in the following standard states: A pure solid or liquid is in the condensed phase under a pressure of one atmosphere. Gas is the hypothetical ideal gas at unit fugacity, where the enthalpy is that of the real gas at the same temperature and at zero pressure.

The change in thermodynamic quantity when one gram of the substance is formed isothermally, at the temperature listed and in its standard reference state, is represented by the values of ΔH_f° and ΔG_f° . The standard reference state used for each element is at 25 °C and one atmosphere. The values of S° indicate the "thermal" entropy of the substance in the standard state at 298.15 K, and do not take into account influences from nuclear spins. Also largely omitted are isotope mixing effects.

The values of ΔH_f° and ΔG_f° in the tables are expressed in kilocalories per mole; values of S° and C_p° are expressed in calories per degree per mole.

Complexes

This section included tables of dissociation constants for inorganic complexes with 14 common ligands. All tables are listed under the ligand name and include cation name and charge (if not obvious) and dissociation constants $\log K_1$ through $\log K_6$ as appropriate:

- Ammonia
- Bromine
- Chloride
- Cyanide
- Fluoride
- Hydroxide
- Iodate
- Iodide
- Nitrate
- Pyrophosphate
- Sulfate
- Sulfite
- Thiocyanate
- Thiosulfate

Solubilities

This section lists the solubilities of selected gases, inert gases, and various electrolytes in water at three temperatures. Also contained are the solubility products of selected inorganic precipitates at 25 °C. The reference material in this section is listed under the following four categories.

- Gases, 100g (water)
- Inert Gases, 1ml (water)
- Air Solubility, 1ml (Water)
- Compounds in Water
- Solubility Products

Gases in 100 g water

In this table, solubilities of selected gases are listed at 0 °C, 20 °C, and 80 °C. Solubilities are offered in terms of the weight of gas dissolved in 100 grams of water when the pressure of the gas plus that of the water vapor is 760 mmHg.

Inert Gases (1 ml Water)

In this table, solubilities of inert gases are listed at 0 °C, 20 °C, and 80 °C. Unless noted otherwise, solubilities are offered in terms of the weight of gas dissolved in 100 grams of water when the pressure of the gas plus that of the water vapor is 760 mmHg.

Air Solubility, 1ml Water

In this table, the solubility of Air at 0 °C, 20 °C, and 80 °C are listed.

Compounds in water

In this table, solubilities of compounds are listed at 0 °C, 20 °C and 80°C. Unless noted otherwise, solubilities are offered in terms of the mass dissolved per 100 g of water.

Solubility Products

This table contains solubility products of common precipitates at room temperature. The solubility product of a compound A_nB_m undergoing dissociation by the reaction $A_nB_m \leftrightarrow [A]^n + [B]^m$ is defined by the following equation

$$K_{sp} = [A]^n [B]^m$$

where A and B are in units of mole/liter.

Electrochemistry

This section lists half-reaction reduction potentials, conductivities of pure liquids, and conductivities of electrolytes at various ionic strengths.

- Reduction Potentials
- Liquid Conductivities
- Electrolytes

Reduction Potentials

It is convenient to consider that the total emf of an electrochemical cell is the sum of two “single electrode potentials.” That is,

$$E_{\text{cell}} = E_{\text{ox}} + E_{\text{red}}$$

where E_{ox} is the single electrode potential of the electrode forming the negative pole of the cell, and E_{red} is the single electrode potential of the electrode forming the positive pole of the cell. This table lists the half reaction potentials, E_{red} , when each substance involved in the electrode reaction is at unit “activity.” Values of E_{ox} may be obtained merely by changing the sign of the E_{red} values. If the half-reaction involves H^+ as product or reactant, the solution is acid. Half-reactions involving OH^- , NH_3 , CN^- , CO_3^{2-} , or S^{2-} are reactions occurring in an alkaline solution.

Liquid Conductivities

This table contains the electrical conductivity of various pure liquids. All conductivities are 25 °C unless otherwise noted and have units of $1/(\Omega \cdot \text{cm})$.

Electrolytes

This table contains the electrical conductivity of various electrolytes at 18 °C at concentrations of 0.01, 0.1, and 1 N. All conductivities have units of cm^2/Ω .

Water

This section lists tables for the following properties of water:

- Boiling Point (P)
- Compressibility (P)
- Conductivity (T)
- Density (T)
- Dielectric Constant (T)
- Expansion Coefficient (T)
- Heat Capacity versus (T)
- Ionization (P)
- Ionization constant (T)

- Mass H₂O in Saturated Air (T)
- Refractive Index (T)
- Surface Tension (T)
- Thermodynamic values
- Vapor Pressure (T)
- Viscosity (T)

Note that (T) and (P) in the above list indicates that the property is listed as a function of temperature or pressure. To calculate the expansion coefficient, density, or vapor pressure of water in the table, you may press **SOLVE**. Enter temperature and these values will be calculated automatically.

Bonds

This section gives the bond lengths and energies for a wide variety of chemical bonds. Also included are molecular shapes and characteristics for 12 compounds along with a separate section on bond calculations.

Bond Calculations

To access the bond character between a pair of atoms it is useful to calculate the following:

$$\Delta\text{Electronegativity} = |EA - EB|$$

$$\text{DegreeIonicCharacter} = 0.46 \cdot |EA - EB| - 0.035 \cdot (EA - EB)^2$$

For example, to examine the bonding between Cesium and Iodine, select “Bond Calculations” with the pointer and press **ENTER**. In the screen

```

PRG
{ HOME GCHEMD }
Enter diatomic species
with a space between
the names of the ions:
Cs I
SKIP SKIP+ DEL DEL+ INS +STR
  
```

```

PRG
{ HOME GCHEMD }
Enter diatomic species
with a space between
the names of the ions:
↓
SKIP SKIP+ DEL DEL+ INS +STR
  
```

```

Result:
:ΔElectroneg: 1.87
:Deg Ionic: .9825915

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

displayed, enter Cs and I with a space in between the elements as shown in the input screen. Press **ENTER** to perform calculations. The resulting calculations are displayed in the screen shown herewith. After viewing the results, you can store them on the stack, or return to list without any further activity.

Bond Energies

This table lists energies for selected bonds. Bond energies are categorized under the following eight elements.

- Bromine
- Carbon
- Chlorine
- Fluorine
- Hydrogen
- Iodine
- Nitrogen
- Oxygen

All bonds listed are in kcal/mole.

Bond Lengths

This table lists lengths for selected bonds. Bond lengths are categorized under the following eight elements.

- Bromine
- Carbon
- Chlorine
- Fluorine
- Hydrogen
- Iodine
- Nitrogen
- Oxygen

All lengths listed are in Angstroms.

Bond Structures

This topic includes molecular structures of 10 compounds. For each of the substances listed below, the formula, structure, bond length, and bond angle(s) are included.

- Ammonia
- Arsine
- Chlorine Dioxide
- Hydrogen Phosphide
- Oxygen Chloride
- Sulfur Dioxide
- Chloroform
- Water
- Carbon Tetrachloride
- Ethane
- Formaldehyde
- Hydrogen Sulfide

3 Periodic Table

In This Chapter

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

Using the Periodic Table

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

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

The screenshot shows a periodic table grid with the element Hydrogen selected. The grid has columns labeled 1 through 7 and rows labeled 1 through 7. The element Hydrogen is located at row 1, column 1. The element name "HYDROGEN" is displayed above the grid. The mass number "1.0079" is displayed below the grid. The element symbol "H" is displayed to the left of the grid. The element atomic number "1" is displayed to the left of the grid. The element molecular weight "1.0079" is displayed below the grid. The bottom of the screen shows a menu with the following options: PROPS, FIND, RTN, LIST, FRT, UP.

Properties of Each Element

Press **PROPS** or **ENTER** to view a list of properties for the current element: Use the cursor keys to scroll down the list to the desired property. Pressing **ENTER** places the data on the calculator stack.






The screenshot shows the element properties screen for Hydrogen. The element name "Hydrogen" is displayed at the top. The properties listed are: DENSITY: 0.090-5.67CM^3, OX STATES: -1,1, ELEC CFG: 1S1, STATE: GAS, MELTING PT: 14.025.K, BOILING PT: 20.268.K, GROUP: 1(A), FAMILY: -. The bottom of the screen shows a menu with the following options: MAIN, SET, PRINT UNIT, FONT, EXIT.

The properties listed for each element (if available) are:


- Atomic Number (Table)
- Mass Number (Table)
- Atomic Weight (Table)
- Density
- Oxidation State
- Electron Configuration

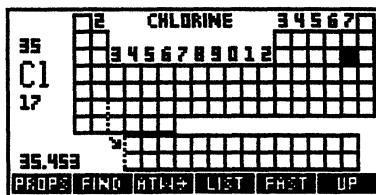
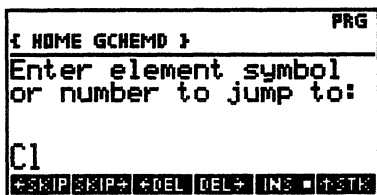
- Physical State
- Selected radioactive isotopes
- Group and family
- Aqueous radii
- Natural occurring isotopes
- Ionic radii
- Electronegativity (Pauling's)
- Atomic Radii
- Covalent Radii
- First Ionization Potential
- Boiling Point
- Group and Family
- Melting Point

Moving Around the Periodic Table

Use the cursor keys , ,  and  to move the points to any element. Pressing  key with a cursor key moves the cursor to the beginning of the current row or column. Pressing **FAST** eliminates element information on 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** key. At the prompt, type in the symbol or atomic number of the element you are searching. The input screen for entering this data is shown here. If you are entering an element's symbol, the second letter must be in lower case. Lower case entries are made by pressing  before typing the letter. Press **ENTER** to move to the Periodic Table screen containing the element you were searching for; in the case shown here, Chlorine.




List of Elements and Symbols



symbol.



Pressing LIST displays the names and symbols of all the elements in the Periodic Table in alphabetical order.; this provides an alternative way to search for an element, if you are unsure of the atomic number or

Searching for a Property

To search for particular property, press  at the list of properties screen. At the “search for” prompt, type in the desired variable, remembering that searches are case sensitive. For example, to search for



the Covalent radii of Chlorine, type in “Cov” at the prompt as shown.

Then Press  to initiate the search. The screen display is shown above. Press  to return to the Periodic Table screen.

Using the Print Function

You can send data from the Periodic Table directly to an infrared (IR) printer compatible with the HP 48 via the infrared port. Follow the printer instructions in the HP 48 documentation.

Summary of Softkeys

- MAIN** Returns to the main menu
- >STK** Copies selected entry or entries to the calculator stack
- PRINT** Send data to an IR printer
- UNITS** Toggles Units On and Off
- UNIT** Indicates that Units are On

EXIT	Exits to the Periodic Table of Elements Screen
FONT	Toggles the display between large and small fonts
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 by name, atomic number or symbol
FAST	Toggles fast display mode
ATW ->	Places the atomic weight of the current element on the stack as a tagged object.

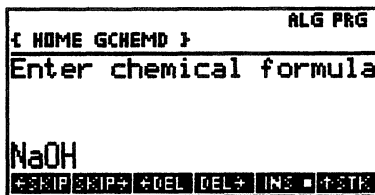
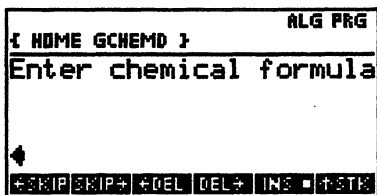
4 Molecular Weight

In This Chapter

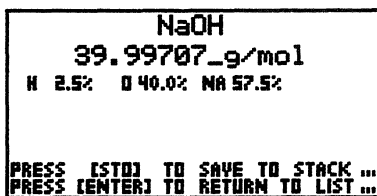
The Molecular Weight function allows you to calculate molecular weights and percent elemental compositions of compounds you enter.

Using the Molecular Weight Function

To calculate molecular weights of chemical compounds, select Molecular Weight from the main menu and press **ENTER**. This yields:
Suppose you want to calculate the molecular weight of sodium hydroxide, NaOH. Type N **☞** A O H at the prompt, as shown:













Press **ENTER** to calculate molecular weight and percent composition:




Press **STO** to store the molecular weight on the calculator stack, or press **ENTER** to return to the main menu.

Entering Molecular Formulas

Chemical 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. Some examples of acceptable chemical formulas are:

Compound	Input
HCl	HC  L
HNO ₃	HNO3
Ca(NO ₃) ₂	C  A   NO3   2
C(CH ₃) ₃	C   CH3   3

After unlocking alpha-entry mode to enter parentheses or to move the cursor, it is necessary to press  once or twice to re-lock alpha-entry mode for subsequent alphabetic entry. For more information on the alpha entry mode of the calculator, see the *HP 48GX Owner's Manual*.

Appendix A

Warranty and Service

PocketProfessional Support

Get answers to your questions about your PocketProfessional card from da Vinci Technologies Group, Inc. If you don't find the information in this manual or in the HP 48GX owner's manual, contact us in writing at:

da Vinci Technologies Group, Inc.
899 NW Grant Avenue
Corvallis, OR 97330
Tel: (541) 757-8416
e-Mail: support@sparcom.com
Website: <http://www.sparcom.com>

Limited One Year Warranty

What is covered

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

What is not Covered

No other warranty is given. Any other implied warranty of merchantability or fitness is limited to the one-year duration of this written warranty. In no event shall da Vinci Technologies Group, Inc., be liable for consequential damages. Products are sold on the basis of specifications applicable at the time of manufacture. Da Vinci

Technologies Group, Inc. has no obligation to modify or update products, once sold.

If the Card Requires Service

Da Vinci Technologies Group will repair a card, or replace it with the same model or one of equal or better functionality. There is a fixed charge for out-of-warranty repairs which 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.

Shipping Instructions

If your card requires service, follow this procedure:

1. Call Da Vinci Technologies Group, Inc. at (541) 757-8416 and obtain authorization by obtaining a RMA number.
2. Ship the card back to Da Vinci Technologies in the following manner:
 - Include your return address, phone number and a brief description of the nature of the problem.
 - Include the RMA number outside the package.
 - If the card is still under warranty, include proof of purchase.
 - Include a check, purchase order, or a credit card number (only VISA, MASTER CARD and DISCOVER cards are honored) and the expiration date to cover the estimated charges.
 - Ship the card, postage prepaid, in protective packing adequate to prevent damage. We strongly recommend that you insure your package. Ship the package to
Da Vinci Technologies Group, Inc.

RMA #: _____

Technical Support

899 NW Grant Avenue
Corvallis, OR 97330 USA

Cards are serviced and reshipped in five business days.

Environmental Limits

Safe temperature and humidity range for PocketProfessional cards is:

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

Appendix B

References


- Handbook of Chemistry and Physics, Chemical Rubber Company, 70th Edition, 1990
- Charles Hill, "Chemical Engineering Kinetics and Reactor Design", John Wiley and Sons
- Sargent-Welsch company, Periodic table of Elements, 1980
- Lang's Handbook of Chemistry, 13th Edition

Appendix C



Commonly Asked Questions

Q. I'm not sure whether the Pocket Professional card is malfunctioning or I'm doing something improperly. How can I verify that the card and the calculator are functioning properly.

A. There are several possibilities for this condition to occur.

- check to make sure that the card is properly seated in the calculator port.
- turn the calculator ON and press  **LIBRARY**. The calculator checks the reference card when it turns on; if “Invalid Card Data or Port Not Available” message is displayed, then the card may require service. If the library menu does not include the reference name shown in Chapter 1, then the card may require service.
- a third possibility occurs when you remove a merged RAM card incorrectly and install the Pocket Professional card. In this case, the calculator display shows “Recovering Memory”.

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

A. The three dots indicate that the object is displayed too long to show on one line. To view the complete object, select the object using the  or the  key by moving the pointing arrow to the object to be displayed, press the softkey **VIEW**. Pressing **ENTER** will return to the browser.

Q. While searching a list of information, I used the alpha key to do the search, but the search did not work. Why?

A. Most likely, the search did not work because of case sensitivity of the alpha search.

Index

- Accessing the PocketProfessional, 2
- Acids/Bases, 17
 - Common Acids/Bases, 18
 - Indicators, 17
 - Inorganic Acids, 17
 - Organic Acids, 17
- Aqueous Radii, 26
- Atomic numbers, 25
- Atomic weight, 25

- Boiling points of elements, 26
- Boiling Points, 26
- Bond lengths, 24
- Bonds, 23
 - Bond calculations, 23
 - Energies, 24
 - Structures, 24

- Coefficients of linear expansion, 12
- Complexes, 20
 - Dissociation constants, 20
- Constants library, 10
 - Derived atomic constants, 11
 - Fundamental constants, 10
 - General constants, 12
 - Universal constants, 11
- Covalent radii, 26
- Cryogenic gases, 16
- Cryoscopic constants, 13
- Cubic expansion coefficients, 12

- Density of elements, 25
- Density of mercury, 16

- Ebullioscopic constants, 13

- Electrochemistry, 21
 - Liquid conductivities, 22
 - of electrolytes, 22
 - Reduction potentials, 22
- Electron configuration, 25
- Electronegativity
 - of Bonds, 24
 - of Elements, 26
- Element Mass number, 25
- Element Physical state, 26
- Environmental limits of the card, 32

- Free energy function (Gibbs), 26

- Gases, 13
 - Cryogenic gases, 16
 - Density of Hg, 16
 - Van der Waals, 15
 - Vapor pressure, 14
 - Vapor pressure of Hg, 26
- Group and family, 26

- Installing an application card, 1
- Ionic Radii, 26
- Ionization potential, 26
- Isotopes, 26
- Key
 - CST (Custom Menu), 2
 - Library, 2
 - ON, 2

- Managing units, 7
- Melting point of elements, 26
- Molecular weight calculations, 29
- Multiple stack entries, 6

Null entries, 8

Oxidation State, 25

Periodic Table, 25
Finding properties, 26
Moving around, 26
Search for a property, 27

pH indicators, 17

Reduction potentials, 26

Removing the card, 2

Service, 32
Service charge, 32
Shipping instructions, 32

Service (if card requires), 32

Softkeys
DEL, 8
SKIP, 7
ABOUT, 2
FAST, 26
FIND, 27
FAST, 28
FONT, 4
GCRE, 2
INS, 8
MAIN, 8
PRINT, 8
PROP, 26
QUIT, 8

UNITS, 7

UP, 8

Solids/Liquids, 12
Boiling points, 13
Cryoscopic constants, 13
Cubic structures, 13
cubical expansion coefficients,
12
Ebullioscopic constants, 13
Face-centered cubic cell, 12
Linear expansion coefficients,
12

Solubilities, 20
of compounds, 21
of Gases, 21
of Inert Gases, 21

Solubility products, 21

Summary of functions, 8
Periodic Table, 27

Thermodynamics, 18
Elements and Oxides, 19
Group 1-0, 19

Using the main menu, 3
Using the reference Pac, 5
Using the search mode, 7

Vapor pressure of Hg, 16

Water, 22