Chemventory™ 1.1

I. Introduction

What it does: This is a Hypercard stack that I wrote to keep track of the chemical inventory in my research labs. Various kinds of information can be entered for each chemical and the inventory cards may be sorted and searched with ease.

System Requirements: Chemventory can run on any Mac running Hypercard 2.2 or greater. I put some really cool features in this stack; alas, this makes the stack inoperable on earlier versions of Hypercard. If you really want to use Chemventory, but don't have Hypercard 2.2, the stack can be converted into a standalone application (it is rather fat; 950 K because it includes the Hypercard engine) using Hypercard 2.2. For the latest version of Chemventory or to find a standalone version, ~~see our web site at http://www.chem.uky.edu/software/welcome.html~~. Contact me at info@ilpi.com

The basic concept: This stack consists of a series of cards, one for each chemical in your inventory. Here's an example of a card you might find in a research laboratory:

There are several different places to fill in information. See the section, **Filling in Information**.

Notice that in the upper right corner, there is a line stating "Card x of y". This always indicates how many chemicals are in your inventory and which one you're looking at.

II. Navigation Controls

These are found at the bottom of the card. Here we can make or delete cards, perform a search, create a report etc. Let's go through each of them...

New Card Click on this to create a new inventory card. All information fields will be blank, waiting for your input and the cursor will appear in the **Mol. Formula** field. There is a short time delay from the time you press this until you can enter information, so be patient.

Delete Card This removes a chemical from the inventory. You will be prompted to confirm the delete command in case you hit this button by accident.

> All chemicals that are deleted are placed into a tab delimited text file called "Removed From Inventory" that resides in the same folder as Hypercard. The date of the deletion is also stored in that file. I put this feature in just in case an OSHA inspector wants to know when something was officially removed from inventory. The file can be opened in Microsoft Excel™ or an equivalent program for easy manipulation.

Search This presents you with options for searching. You can search for virtually anything; more details can be found in the section titled **Searching**

Sort Cards This features a popup menu that lets you arrange your cards by any of the following choices:
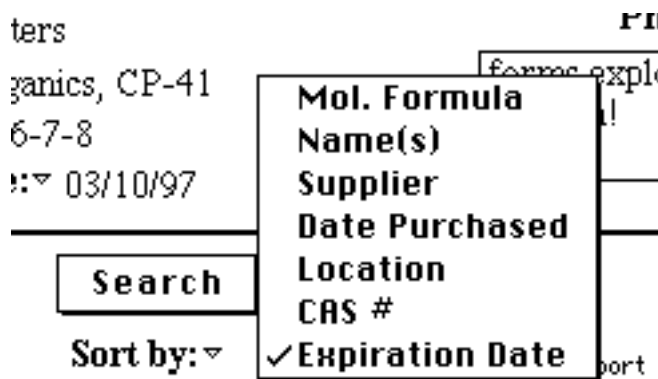
> Most chemists like to sort their cards by molecular formula. The usual protocol is to list them in alphabetical order with one oddity: C and H are listed before any of the other elements. Hence, $C_2H_4Br_2$ is preferred over $Br_2C_2H_4$. This stack automatically does that for you.

> When you sort in the name field, any preceding numbers, dashes or common chemical prefixes (i.e. *cis*, *exo* etc.) are ignored. Hence, *cis*-2-pentene comes after pentane, not calcium.

Whichever field you choose to sort, you will then be prompted like this:

You will then be presented with a second dialog box that permits you to sort in ascending or descending (A to Z versus Z to A) order. After that, the sorting begins.

In practice, sorting takes very little time at all. Hypercard is very good at fast sorting, but I have not yet tried to sort a 10,000 card stack....if you ever do let me know how long it takes.

Quit When you click here you will be asked if you really want to quit. After that you will be asked if you really want to quit Hypercard™ . If you choose "No" for the latter then you will go to a place called the Home Card (but if you are running a standalone version of this stack then you simply go to the first card of this stack....)

Help (i.e. the big question mark) Will display an on-line help screen that has short summaries of what you are reading here. It is also where I put the **Preferences** button....See **Preferences** for more info. You can also get Help by pressing the Help key on your keyboard (if it has one).

Create Report This will take the information that is on the card (with the exception of any pictures) and create a new tab-delimited text file. You will be asked for a file name and destination (the default name is "Inventory.txt"). This new file then can be opened by a program such as Microsoft Excel™ where it can be manipulated and printed.

You may also *import* data if it is in a tab-delimited text file. The text file must have the same format as one output by Chemventory, but these are trivial to create in something such as Microsoft Excel™ . A proper input file has no blank lines and has 11 input fields per line (corresponding to Mol. Formula through Chemical Properties in Chemventory). To import data select **Import Data...** from the **Edit** menu. You will be prompted if there is a problem in reading in your data.

ChemDraw Chemdraw™ is Cambridge Scientific Computing's chemical structural drawing package. By placing an alias named "Chemdraw" in the same folder as this stack, it will automatically open Chemdraw™ for you so you can draw a pretty picture of your chemical and then paste it into this stack. Of course, you don't have to draw pictures for all of your chemicals...

You can easily change the name of the drawing program -- see **Preferences** below. You can also use Hypercard's onboard drawing tools if you don't want to use another program or don't have one that is suitable.

See **Drawing Structures** (below) for more info.

Left/Right Pointing Hands Clicking on the right hand will take you to the next card in the stack and clicking on the left hand will take you to the previous card in the stack.

Holding down the Shift or Option key while you click will make you move more than one card at a time and holding down both makes you move even faster.

You may also move forward one card or backward one card by using the arrow keys on the keyboard.

If you have done a successful **Search** then the arrow keys and these icons will move you to the next card that matches your search criteria. You will know this is the case because the button that says **Browse All** (see next item) will be enabled and a message like "5 matches" will appear above it.

Target is that funny bull's-eye between the **pointing hands**. If you click on it you can go directly to a card number that you type in. If you are browsing a subset of cards from a search and that card is not included, you are asked whether you still want to go there.

Browse All This button becomes enabled when you do a search and have found at least one match. Until you perform another search or click this button, you will only be looking at cards that match your search criteria. Click here to restore normal navigation controls (see the previous two items).

III. Filling In Information

If you have just created a new card, then you will see the following:

Notice that we start with the molecular formula.

To switch between the fields of information on this card we can either click on the field we are interested in, use the up or down arrow keys or hit the Tab, Return or Enter key.

Note: if you are in the Names or Physical Properties field, then all the arrow keys and Return work normally. To go to the next/previous field hit the down/up arrow while holding down the command key. Or hit Tab to go to the next field.

Let's examine each of these fields and what they are all about:

Mol. Formula This field contains the molecular formula of the chemical. That is, something in the form of C_4H_9Cl instead of BuCl etc.

Most chemists like to sort their cards by molecular formula. The usual protocol is to list them by alphabetical order with one oddity: C and H are listed before any of the

other elements. Hence, $C_2H_4Br_2$ is preferred over $Br_2C_2H_4$. This stack automatically does this for you.

When you type information in this field it is not subscripted. That's because Hypercard does not support subscripts in text fields. However, this stack fakes it pretty well. When you hit Enter or Tab or click somewhere else on the card, the following happens:

- The elements you entered are double checked to see if they are actually elements (I only went as high as Lr; even this is ridiculous). Me, Et etc. are *not* allowed. Maybe in future release.

- Duplicates are combined. If you entered $C_2H_4C_6$ the stack rearranges this to C_8H_4.

- The stack is alphabetized as described above.

- The elements are properly subscripted. You may have numbers as large as 999,999 and up to three decimal places in each number.

Note: proper capitalization of elements is mandatory. Hence "C6H6" is a fine entry, but "c6h6" will not be accepted. FYI: Hypercard does not recognize case sensitivity without an incredible amount of footwork, that's why there is a short time lag from when you hit Enter until the subscripted formula appears.

You automatically go to the next field, **Names(s)**.

Name(s) This is where you can enter the name of the chemical. The field is a scrolling field so if the name is particularly long or you want to enter other common names you have all the room in the world to do that.

When you sort the cards of this stack by name, common chemical prefixes such as *cis*, *iso* etc. are ignored. So feel free to enter them as they really are. Also note that this alphabetic sort by name will only use the text from the first line as a sorting criterion; other names are ignored.

Functionalities This one is really special! I included this field because I often find myself asking "Do I have any amino-olefins?" or similar questions. By putting this info in when I put a chemical in the inventory I save myself much trouble.

Even better, this field doesn't require typing! Instead, if you click inside the text box you are taken to a card that looks like this:

chemical inventory

Which functionalities does this chemical contain??

○ Alkane	○ Amine	○ Phosphine	○ Alkali Metal	○ Sulfide
○ Alkene	○ Ammonium	○ Phosphite	○ Alk. Earth	○ Selenide
○ Alkyne	○ Amide	○ Phosphonium	○ Main Group	○ Telluride
● Aryl	○ Pyridine	○ Phosphate	○ Trans. Metal	● Halide
○ Alkyl	○ Pyrrole	○ Thiol	○ Lanthanide	○ Fluoride
○ Silyl	○ Pyrazine	○ Sulfide	○ Ether	● Chloride
○ Alcohol	○ Lactam	○ Disulfide	○ Epoxide	○ Bromide
○ Phenol	○ Nitro	○ Sulfonate	○ Peroxide	○ Iodide
○ Acid	○ Nitrate	○ Sulfate	○ Spare	
○ Ester	○ Nitrite	○ Carbonyl	○ Spare	**Finished**
○ Aldehyde	○ Nitrosyl	○ Carbonate	○ Spare	
○ Ketone	○ Azo	○ Fullerene	○ Spare	**Clear**
○ Lactone	○ Cyano	○ Hydride	○ Chalcogen	**?** Help **Rename**
○ Enol	○ Isocyanate	○ Hydrate	○ Oxide	

All you have to do is click on the functionalities that this chemical has! When you are done simply click on **Finished** and you'll return to your new card; any choices that you have selected automatically go into the functionality field! Clicking on **Clear** turns all of these radio buttons to off.

The **Rename** button is enabled if you have permitted the renaming of functionalities in your **Preferences**. The 64 functionalities you see above are some of the ones I commonly run into, but if there are some that you don't use (or you want to change the order of), you can do so at will:

Click on **Rename**. The header on the screen will state "Click on the functionality that you wish to alter". Click on the button you wish to rename. You will then be asked for a new name. That's it!

Note that if I renamed the "Ketone" button, it does not affect any of the cards that already have "Ketone" on them unless you click on the Functionality field of that card. For consistency's sake, it is a good idea to disable the **Rename** feature once you have a good idea of the functionalities that you commonly use.

You can't rename the halide or chalcogen buttons...

Also notice that if you click "Chloride" then "Halide" is automatically enabled, too. Suppose I was looking for an aryl chloride, but didn't find it. I could look for any of the aryl halide combinations without having to try four different possibilities!

You can have two buttons with the same name (in case you are in the midst of renaming and rearranging etc.), but you will be warned about this if you try it.

Supplier Here is where you enter the name of the chemical manufacturer. Since I usually use Aldrich, that is my default. You can type in any name you want or, easier yet, you can simply use the popup menu by clicking on the word "Supplier"

Adding and removing companies from this popup list are two of the options on the list!

When you put in a new company or remove an old one the list is automatically alphabetized.

The first name in the list is the automatic default. If you want to put a company into the first line, but the alphabetic ordering doesn't permit it, then simply put a space before the company name!

You can also edit the whole list of suppliers by choosing **Suppliers...** from the Edit menu (if the Preferences permit it). This will take you to a screen where you can edit the whole list at once!
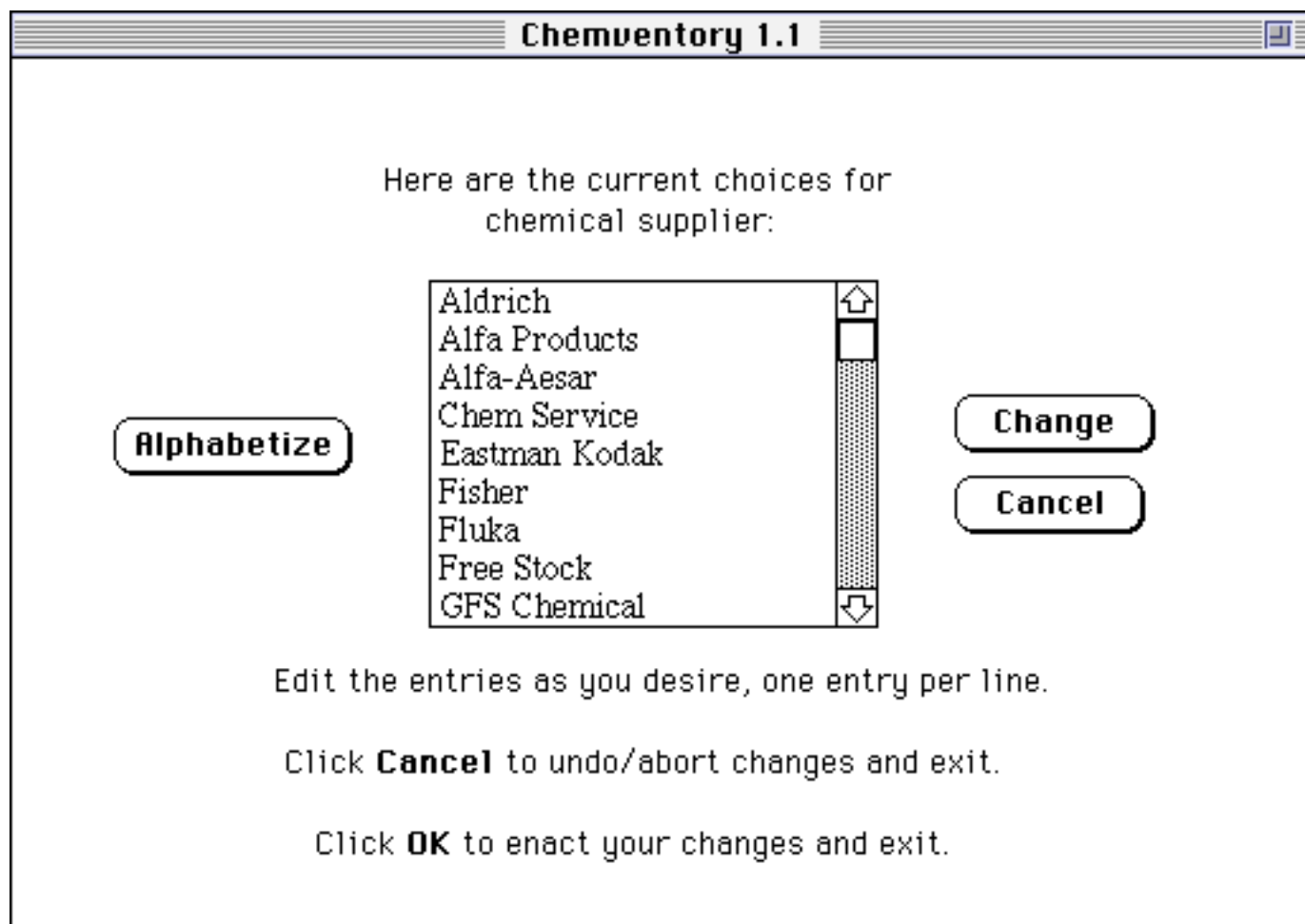
If you click the **Alphabetize** button, your list will be alphabetized A to Z or Z to A, whichever you specify.

When you click **Change**, you will be returned to your original card. Any empty lines in the list will be eliminated automatically.

Once you pick a company etc. you go to the next field:

Date Purchased This will default to today's date (Or what your Mac thinks today's date is). You can also type in whatever date you wish. If you ever wish to change a date to today's date all you have to do is click on the word "Date" and a popup menu will offer that selection.

> You can type the date in any format you desire, but Hypercard will convert it to whatever format your Mac is set for. The date is displayed in mm/dd/yyyy format to avoid ambiguities with the turn of the century and the "Year 2000" bug.

Catalog # Is where you can enter the catalog #. Pretty self-explanatory

Quantity Is for the size of the container. You can always type whatever you want, but if you click on the word "Quantity" you will get a popup menu with the most common sizes (mass as well as volume). As with **Supplier**, you can edit the entries in this menu by selecting **Quantities...** from the Edit menu (if the Preferences permit this).

Location Is where you store your chemical. This, too, comes with a popup menu for your favorite locations. I have installed my some of my most common locations and made one of them default; you can change these by selecting **Chemical Locations...** from the Edit menu (if the Preferences permit this).

> As with any field except Functionalities, you can also just type in a location manually.

CAS # Is also self-explanatory. It is worth filling this in because you might be searching for the name "methylene chloride" when the name really is "dichloromethane". CAS numbers are unique to each chemical and avoid this kind of common vs. trivial name confusion.

Expiration Date Is the date that a chemical is "too old" and should be removed from the inventory. For compounds such as ethers this is a good idea, but I know someone who was required to dispose of NaCl because it "expired".   Go figure.

> In the popup menu for Expiration Date are "1 year, 5 years" etc. If you select one of these, then that time will be added to the date displayed in the **Date Purchased** field and put into the Expiration Date.   You can also type in a number by hand or choose "Never".

> You can type the date in any format you desire, but Hypercard will convert it to whatever format your Mac is set for. The date is displayed in mm/dd/yyyy format to avoid ambiguities with the turn of the century and the "Year 2000" bug.

> If you would like to edit the information in the Expiration Date popup menu, simply select **Expiration Dates...** from the Edit menu (if the Preferences permit this). **Note:** the software is expecting any number on a line to be an integer year.

Physical Properties Is where you can store any info that you wish, especially things that I didn't make fields for. You might want to put lot numbers, flash points, hazards etc. in here. I commonly put mp, bp and any unusual hazards.

Structural Formula You can make or paste a drawing of your compound (in case it has a really long name or common name that is not obvious). See the next section, **Drawing Structures**, for more info on how to do this.

IV. Drawing Structures

Most chemists I know use ChemDraw for drawing structures, but you can use whatever you wish. To set the default drawing program of your choice, see the pertinent information in the section, **Preferences**.

You have two options for drawing a structure: use an external program then cut and paste **or** you can use Hypercard's drawing tools. I find the former much easier.

Using an external program:

- Click on the **ChemDraw** icon (or whatever you have renamed it) on your inventory card. Assuming that you have an alias of that program in the same folder as the inventory stack, it will automatically open Chemdraw. If not, then you will be prompted for the location.

- Draw your picture then copy it to the Clipboard.

- Click on the Hypercard window (or use the menu in the upper right of your screen to get back).

- Hit command-v (or pull down Paste Picture from the Edit menu).

- Your picture will appear inside a box. A message will appear over the words "Structural Formula" that says: Press "\" when you are done being artistic...

- Position your graphic where you wish by clicking and dragging on it. When you have it where you wish then type "\" and you'll be done.

  WARNING: If you click outside of the box, the graphic will be placed. If this is not where you wanted it you will have to immediately select "Undo" from the Edit menu (or hit command-z). If you mess this up, you can still erase it using Hypercard's drawing tools, found under the "Tools" menu.

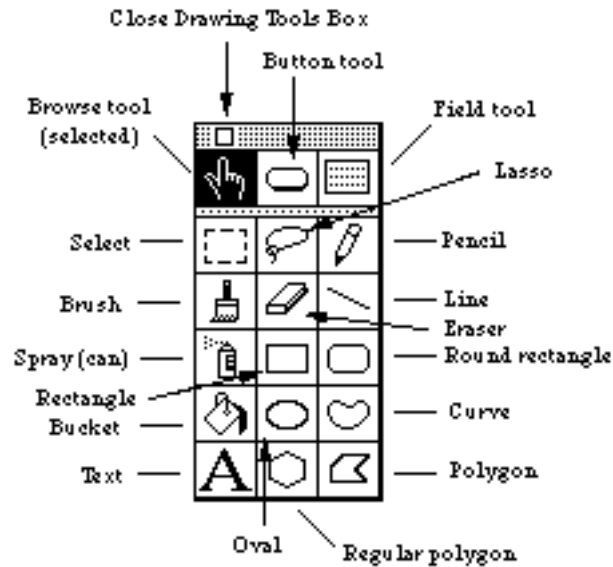Using Hypercard's drawing tools:

  You can set the default drawing program as the Hypercard palette in **Preferences**.

  There are three ways to make the Tools Palette appear:

  - From the "Tools" menu (unless you have disabled SuperUser).

    The Tools Palette (as it is called), is actually a tear-off palette -- if you click on it and drag it away from the menu bar rapidly then you'll be able to move it around the screen as a separate window!

  - By clicking on the ChemDraw icon after you have reset the default program to "Palette" in **Preferences**.

  - Option-Clicking the ChemDraw icon, regardless of what name it currently has. This makes the Palette accessible even if the menu bar is hidden (SuperUser is off).

  Here are the functions of the Tools Palette. I won't go into details on how to use them.

Close Drawing Tools Box
Button tool
Browse tool (selected)
Field tool
Lasso
Select — Pencil
Brush — Line
Eraser
Spray (can) — Round rectangle
Rectangle
Bucket — Curve
Text — Polygon
Oval — Regular polygon

Double clicking on some of these icons gives you added features. Explore!

V. Searching

When you press the **Search** button at the bottom of you inventory card, you will go to this screen. If **Text** is not selected, then the 12 buttons under it will not be visible. Likewise, if either **Received** or **Purchased** is not selected, you won't see the popup menus or date entry fields:

Card Search

○ **Text** alk

○ Mol. Formula   ○ Quantity
◉ Name(s)   ○ Location
◉ Functionalities   ○ CAS #
○ Supplier   ○ Expiration Date
○ Date Purchased   ◉ Physical Properties
○ Catalog #   ○ Everywhere

◉ Expiration   [Before ▼] 03/13/2002   [Search now]
◉ Received   [After ▼] 03/05/1997   [Cancel]

[?]
Help

Right now, the **Text** button is on so this search will look for the letters "alk" in the **Name(s)**, **Functionalities** and **Physical Properties** fields.

If you wish to change the text, simply click on it and change it. Text searches are NOT case sensitive. That's Hypercard's doing, not mine.

If you want to change the fields to search for this text, simply click on those as well. If you pick "Everywhere" then all information in the database will be searched, including the date fields.

• If you click on the button **Functionalities** then you will be taken to the **Functionalities** screen, just as you are when you edit the **Functionalities** field. When you hit "Finished" on that screen, the chosen functionalities will appear in your search string.

If you put any spaces in between the words in your text string, they will be treated in a Boolean AND manner. Thus, typing "Lithium Pent" will find all cards that have "Lithium" and "Pent" on them, including "Neopentyl Lithium" and "Lithium, suspension in pentane".

When you activate the **Expiration** button, you can specify searching for chemicals that have no expiration dates or ones with expiration dates equal/before/after the date you enter at the left:

The **Received** button works similarly, but there is no "none" option for it.

When you are ready to perform the search hit the button **Search Now**. Things to note:

- Text, Expiration and Received work in a Boolean AND manner. Therefore, the search screen shown in our example will find chemicals with "Alk" in their name only if they were received after 3/5/97 and expire before 3/13/02. Very powerful!

    This is also a good way to find chemicals that may be expiring soon...

- If no matches are found, you will be informed of this.

- If any matches are found you will automatically go to the first card that matches your search criteria. At this point three important changes occur:

    1) The left/right arrows and icons now take you to the next *matching* card, not the necessarily the next card in the inventory

    2) The **Browse All** button becomes enabled.

    3) A message saying "x matches" appears above the **Browse All** button:
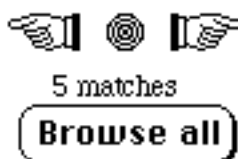
    To see all of your inventory cards again, click the **Browse All** button. The "x matches" message will disappear, the Browse All button will become disabled, and the arrows will work as they normally do.

VI. Preferences

You can set the preferences by clicking on the **Help** icon at the bottom of the inventory card. Not only will Help information be displayed, but a button marked **Preferences** will appear. Press it to get to the Preferences screen.

Note that you can password protect the Preferences screen. If the password is enabled, then you will be asked to supply it. If you can't then you will return to your inventory.

If the password is not on or you have entered it correctly, you will see the Preferences screen:

Preferences

☒ Play intro sound
☐ Enable ability to rename the functionalities
☐ Require password to change preferences
☒ Enable SuperUser status (menubar etc)
☒ Scan for expired chemicals on startup

Drawing program name: ChemDraw

○ Use onboard tools for drawing

[Delete all cards]   [Change Password]

(Done)   [?]
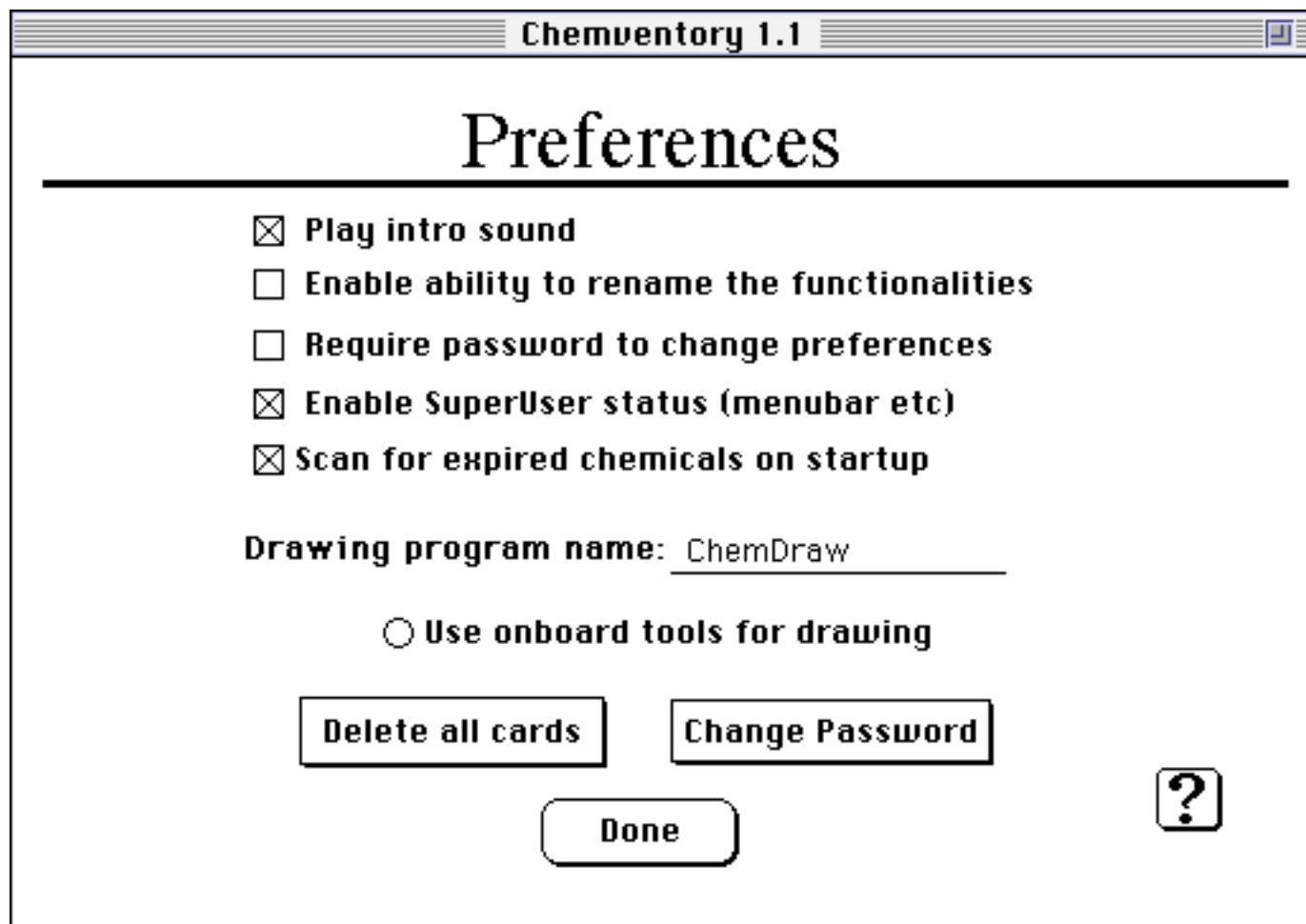
There are many things you can do here!

Play Intro Sound If this box is checked, then Mr. Burns from The Simpsons™ will make a complaint about people spending money whenever this stack starts up. It is cute the first 20 or so times, but after that you may want to turn it off.

Enable Ability to rename the functionalities If this is checked, then on the screen where you choose the functionalities for your cards or searches the user will have the ability to rename the functionalities buttons on that card (see **Functionalities** under **Filling in Information**).

> Once you have a good idea what kinds of functionalities you want on your cards, it is best to DISABLE this feature. That way things will stay consistent in your stack.

Require password to change preferences This lets you lock out this Preferences screen. It is recommended that you use the **Change Password** button to set the password before enabling this feature.

> It is probably best to enable the password protection so that nobody is tempted to diddle with your preferences.

> Warning: do not forget your password. It can be bypassed by an experienced Hypercard user (such as the author), but it is nontrivial to figure out otherwise.

> The best part is that nobody except you can **Delete all cards** from your inventory.

Enable Superuser status (menubar etc.) If SuperUser is turned on, then the menubar and all Hypercard commands will be available to the user.

Unless the users of the stack are very Hypercard literate, <u>it is probably best to leave this feature disabled</u>. In that case, the menubar will not appear, so nothing can be accidentally deleted or reordered and none of the buttons (or their scripts) can be irreversibly changed. In addition, most keyboard shortcuts are disabled, so no accidental navigation or deletion can occur.

Scan for expired chemicals on startup When this is turned on, Hypercard will compare the expiration dates on all your chemicals to the current date. If an expired chemical is found, you will be alerted and given the card number of the first expired chemical. If no expired chemicals are found, you will also be told.

This is a slow process, so you may not want to leave it on all the time. If you are alerted to the presence of an expired chemical you should probably do a search or sort by expiration date to find others that may also have expired.

Drawing Program Name Here you can type in the name of your default drawing program or its alias. So if you really want to use ChemInTosh™ or MacPaint™ 1.0 (shudder) for your default drawing program you can do so. The name under the ChemDraw icon will change accordingly.

Simply click on the program name to change it.

Use Onboard Tools for Drawing If you select this, the Drawing Program Name will change to Palette. When the user clicks on the ChemDraw icon, the Hypercard tools menu will appear for their use. See **Drawing Structures** (above) for how to use these tools.

Delete all cards Will delete all the cards in your inventory except the first one. The only time you want to use it is the first time that you use this stack and start building you own inventory. Therefore, it is a good idea to use a password (see above and below) for your Preferences!

You will be asked to confirm that you really want to delete all cards if you click this button.

Change Password Click on this and you can enter a new password. Bullets (•) will appear in place of whatever you are actually typing. You will be asked to confirm the password by typing it again. See **Require password to change preferences** above.

Done click here or hit Return or Enter when you are done setting your preferences.

VII. Legal Stuff

Chemventory™ is ©1993-1997 by Robert Toreki. It is freeware for all academic or nonprofit entities, but I ask that any corporations etc. that use it send a $25 shareware fee. This program may be freely distributed and copied AS LONG AS NO FEE IS CHARGED FOR THE DISTRIBUTION OR COPYING and no changes are made to the programming elements. This particularly applies to for profit companies (like EduCorp) and exempts nonprofit groups (such as user groups).

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