

## **AquaChem 3.7**

### **Section Objectives**

- Create a Database in AquaChem (Current session)
- Perform Data input and import (Future session)
- Basic Database Management (Future session)

### **AquaChem licenses managed by Keyserver Software**

- Keyserver License Manager Software administers 15 concurrent AquaChem licenses bought by OSMRE.
- When you double click the icon, one license at OSM is checked out via Key Server.
- Key Server tracks users, use and standing time.
- Don't leave running, close program when not in use to release the license.

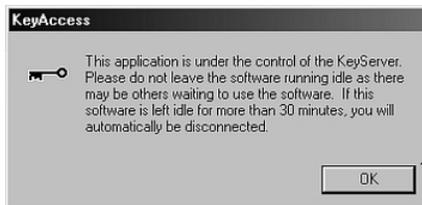
## Starting AquaChem



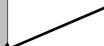
Double click this icon to start AquaChem



## Starting AquaChem

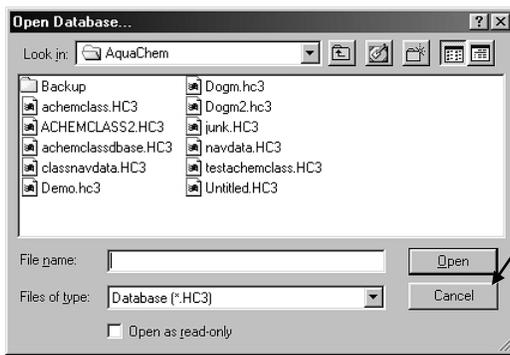


Click **OK** when the Keyserver prompt appears



## Starting AquaChem

You will be prompted to open an existing database.



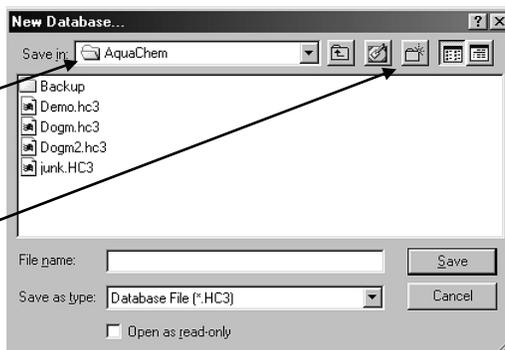
Click **CANCEL**.  
In this exercise we  
will create a new  
project and  
database.

The first step in designing the AquaChem database is to define the parameters and database structure.

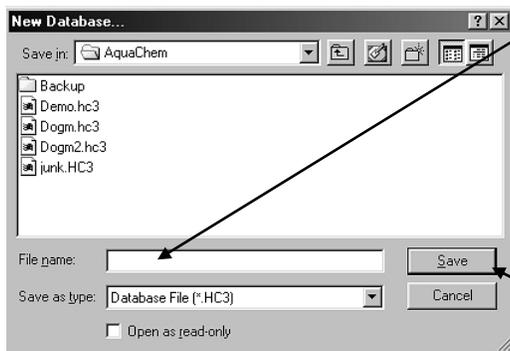
## Creating a new Database

- From Menu, click on **File**, followed by **New**.
- A New database Dialogue box appears.

Navigate to your  
AquaChem Class  
Directory  
or  
Create a new  
directory with a  
name of your  
choice.



### Creating a new Database



•Name your new database file. The extension will default to \*.HC3.

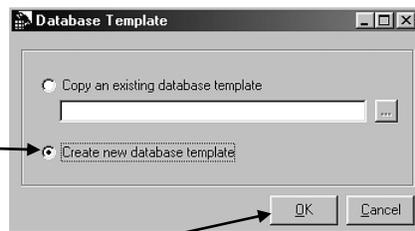
•Click **SAVE** when finished

In this example we used Achemclass.HC3 for the database name.

### Creating a new Database

You will be prompted to use an existing database template or create a new one.

Click the **Create new database template** radio button.

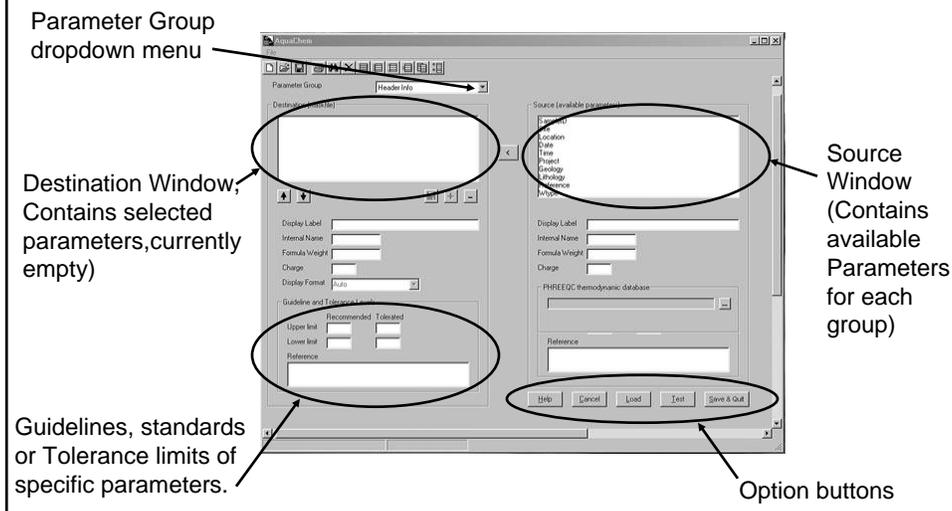


Select OK when finished.

*TIP: If you are repeating the same database structure as a previously created database, it can be specified during the data import process. This will save you from having to build the database structure all over again.*

## Specifying the Database Design Use the Data Structure Tab

Click on FILE, PREFERENCES, Data Structure tab.  
You will be presented with a dialogue box for creating a new database template.



## About Parameter Groups

AquaChem uses the following Parameter Groups

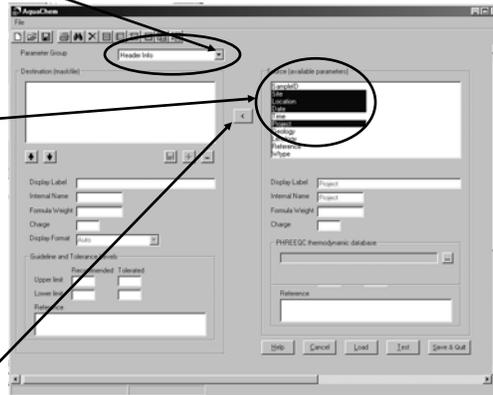
- Header Info** (Site, date, time, project, geology, etc.)
- Physical Data** (Field data, x,y,z coords, TDS, Cond.)
- Cations** (+ charged constituents, Ca, Mg, Na, K, etc.)
- Anions** (- charged constituents, Cl, SO<sub>4</sub>, HCO<sub>3</sub>, CO<sub>3</sub>)
- Uncharged Compounds** (SiO<sub>2</sub>, H<sub>2</sub>S, CH<sub>4</sub>, etc.)
- Varia** (Isotopes, Coliforms, Noble gases)

Available but not covered in this course

- PHREEQC Description**
- PHREEQC Minerals**
- PHREEQC Activities**

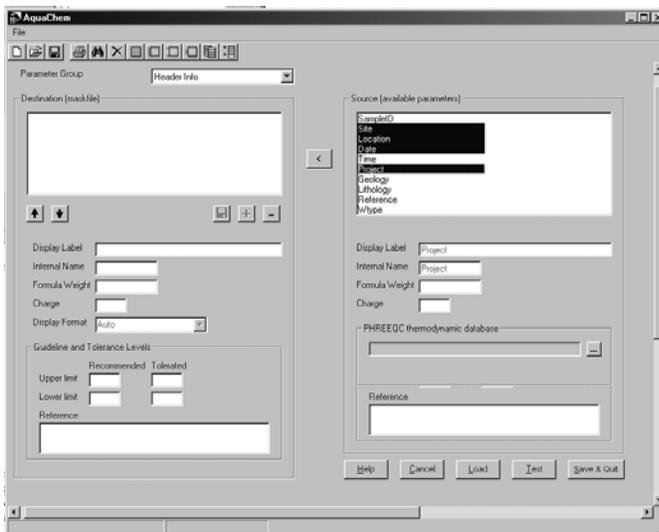
## Selecting Parameters

- Click on the Parameter Group Dropdown Menu to view the various parameter groups. In this class we will work with the first five parameter groups.
- In the Source window are the available parameters for each group. Notice that Site, Location, Date and Project are selected and highlighted in blue.
- Parameters of interest are moved to the Destination Window by selecting them and copying using the “<” button to move it.



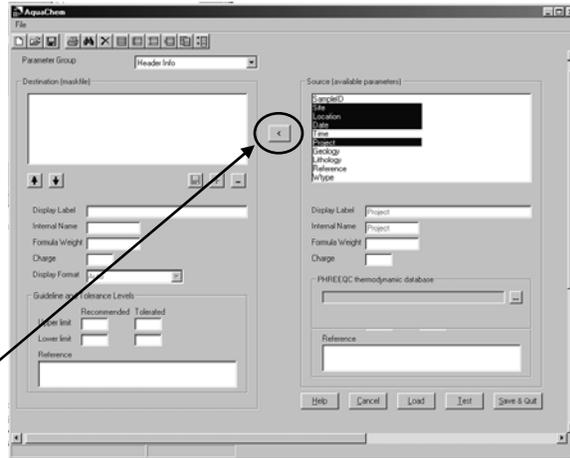
## Selecting Header Info

- Click on **Site** in the source window.
- Hold down the Ctrl key, and click **Location**, **Date**, & **Project**.



## Header Info

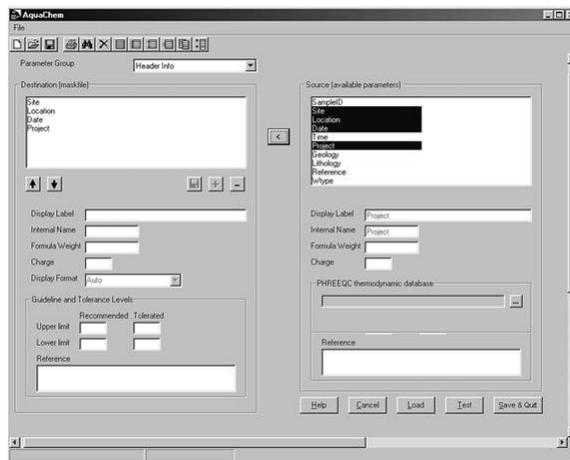
You should see the Header Group parameters highlighted.



Click on the “<” button to move highlighted items into the Destination list.

## Database Field Names

The Destination List will be used to define and save the database field names, This information is contained in the Mask file with an extension \*.MSK.

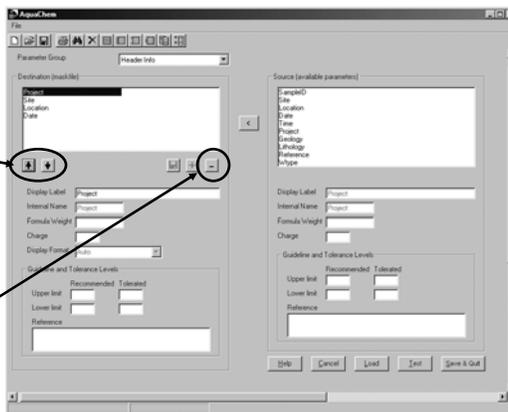


You should now see the Site, Location, Date and Project in the “Header Info” Destination window as shown above.

## Parameter Re-arrangement

Parameters in each Group can be Rearranged using the ↑ and ↓ icons directly below the destination window.

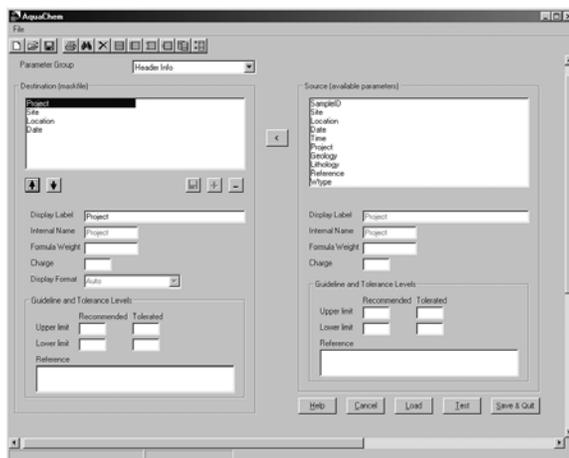
- Click on the parameter you want to re-order and move it up or down using the ↑ and ↓ arrows directly below the destination window.
- Selected parameters can also be removed from the list using the “-” (minus) key at the bottom right of the Destination window.



Re order Project to the top of the list as shown above. Click on Project, then click the ↑ 3 times. Your Destination Window should display as shown above.

## Parameter Re-arrangement

The Header Info group should now appear as shown below.

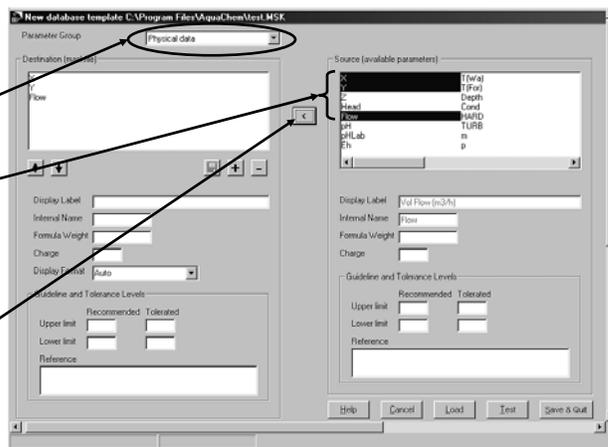


Each of the other Parameter Groups is defined by selecting the parameters in the same manner and re-ordering them as desired.

## Physical Data

Now add Physical Data parameters to the Destination Window and Mask file.

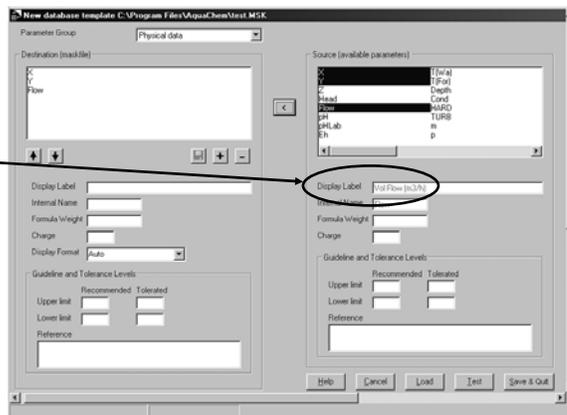
- Select “Physical Data” in the Parameter Group dropdown menu.
- Select X, Y, & Flow from the Source list.
- Transfer these parameters to the Destination Window using the < button.



## Physical Data

The Physical Data parameters have been selected and moved to the Destination Window.

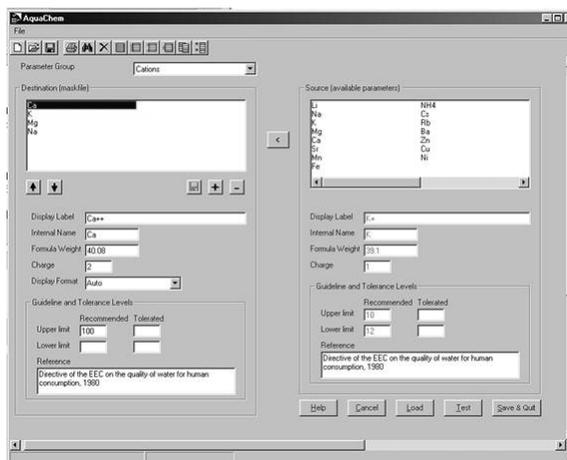
Notice the units for Flow are m<sup>3</sup>/hr. Change these to read: Vol Flow (GPM) in the Display Label window.



## Cations

Cation parameters are selected in the same manner.

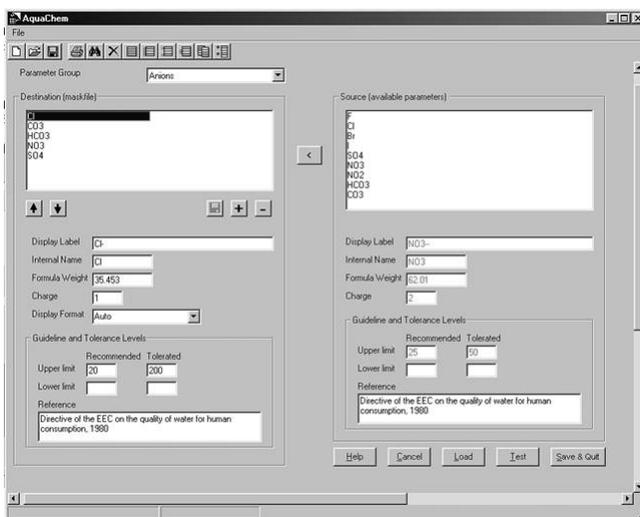
- To select multiple parameters, hold down the 'Ctrl' key and click on Na, K, Mg, Ca from the source list.
- Use the < button to transfer these parameters to the destination window and re-order them alphabetically to produce the above screen.



## Anions

Anion parameters are selected the same way.

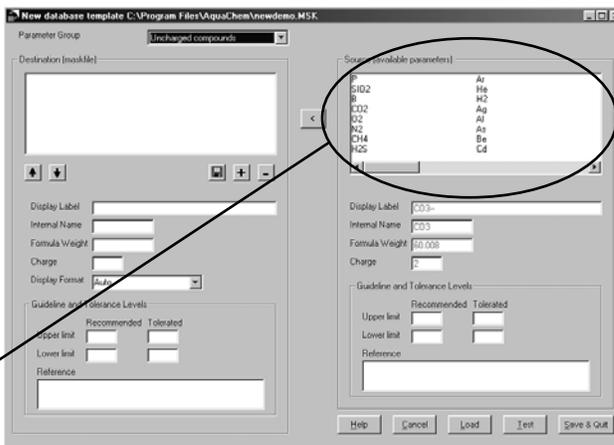
- Select and add the following Anions: Cl, SO4, HCO3, NO3, CO3.
- Re-ordering these parameters alphabetically produces the screen shown at right.



## Uncharged Compounds

AquaChem has the capacity to add uncharged compounds to the database in addition to Cations and Anions.

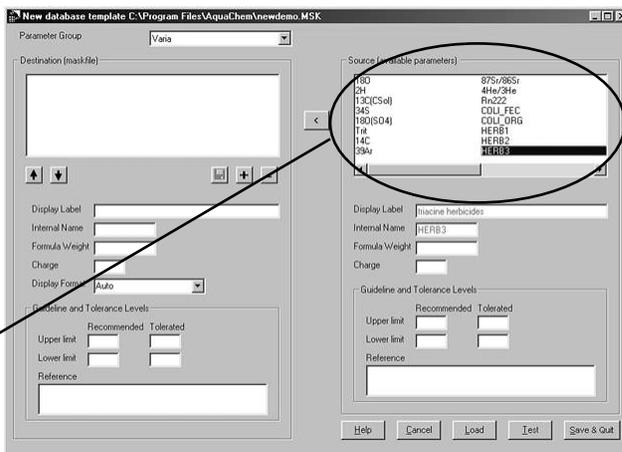
- The default database includes a number of constituents such as Al that are not always uncharged.
- Switch to the Uncharged compounds list using the Parameter Group dropdown menu.
- Scroll right and look at the various parameters included in this group.



## Varia

AquaChem has the capacity to add other compounds and constituents to the database.

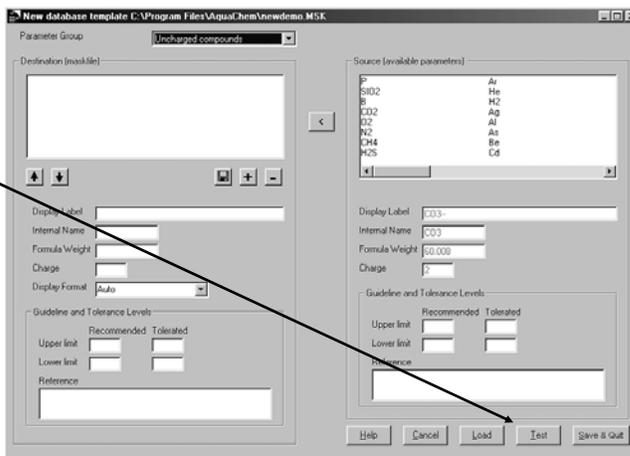
- The Parameter Group Varia contains miscellaneous parameters such as Fecal Coliforms, radio isotopes, herbicides and Noble gases.
- Click on the Varia Parameter Group dropdown menu.
- Look at the various parameters included in this group.



## Testing your Database

Use the Test button at the bottom of the screen to preview the data input form

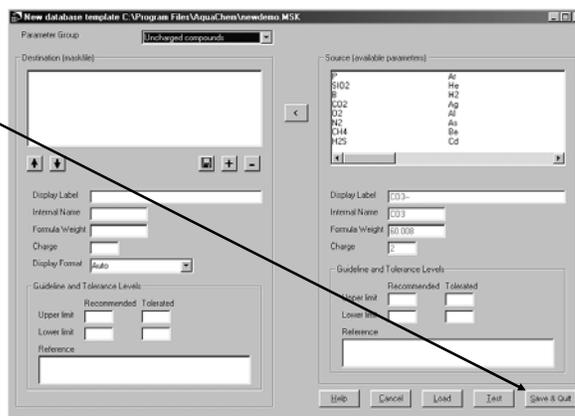
- You can test your database structure at any time by pressing the **“Test”** button.
- This loads a sample data input form based on the design you’ve selected.
- If the design is suitable, click Close.



## Saving Your Database

Use the Save & Quit button at the bottom of the screen to save your design and quit the Data Structure Tab

- Click **“Save & Quit”** to save the structure you have created so far.
- When prompted, click **“Yes”** to confirm the save.
- An empty database Active Record list will be displayed similar to the following screen.

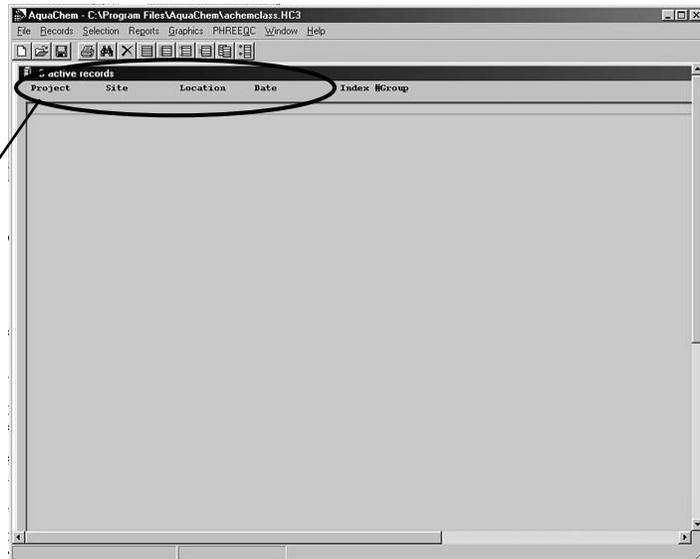


## The Active Record List

The empty Active Records Display is shown at right.

Notice that the items in the "Header Info" group are listed across the top.

The order of these headers can be modified using the Startup Defaults Tab.



## Adjusting the Active Record List Display

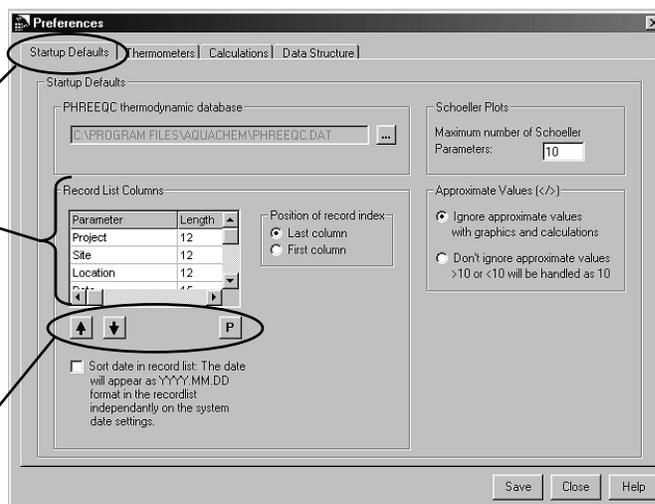
The Headers in the Active Records List Can Be Modified in the Startup Defaults

- Click **File**, followed by **Preferences**.

- The Preferences dialogue window opens in the **Startup Defaults Tab**.

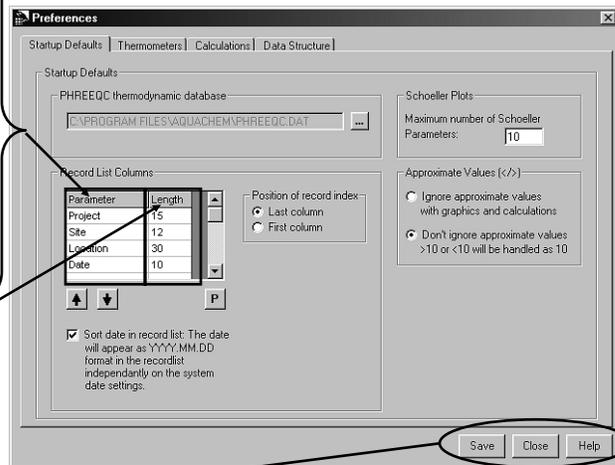
- The Record List Columns are used to define the order and width of the database headers that appear on the Active Records List.

- Parameters may be reordered, added, or column widths modified.



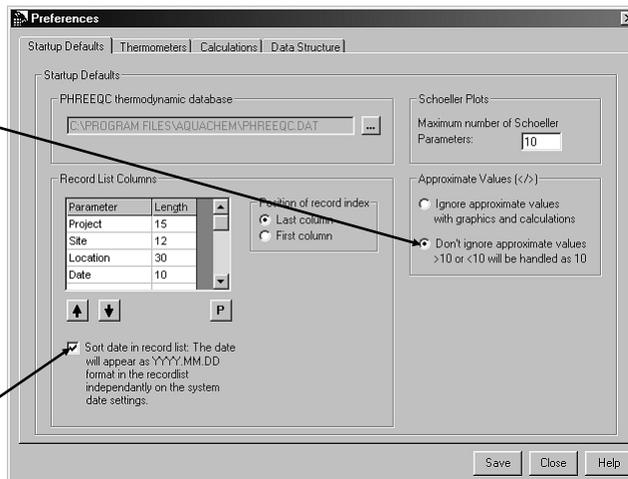
## Adjusting the Active Record List Display

- Any parameter can be deleted by clicking on it and hitting the **Delete** key on the keyboard.
- To add a parameter **Double click** in the Parameter column of the row where you want the parameter placed. A drop down menu appears from which parameters can be selected.
- To redefine a column's width, **click** in the second column of any row to change. Enter the new column width over the old.
- When finished, Click **Save, OK, & Close**.



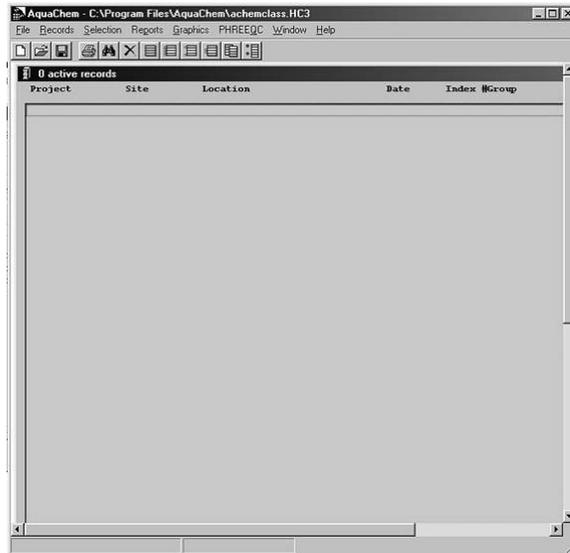
## More on Records List Display

- Select the radio button: **“Don't ignore approximate values”**  
This allows AquaChem to handle less than detection values. The other selection ignores “<” or “>” values.
- Select the check box: **“Sort date in record list”** to list samples chronologically.



## Active Records Display

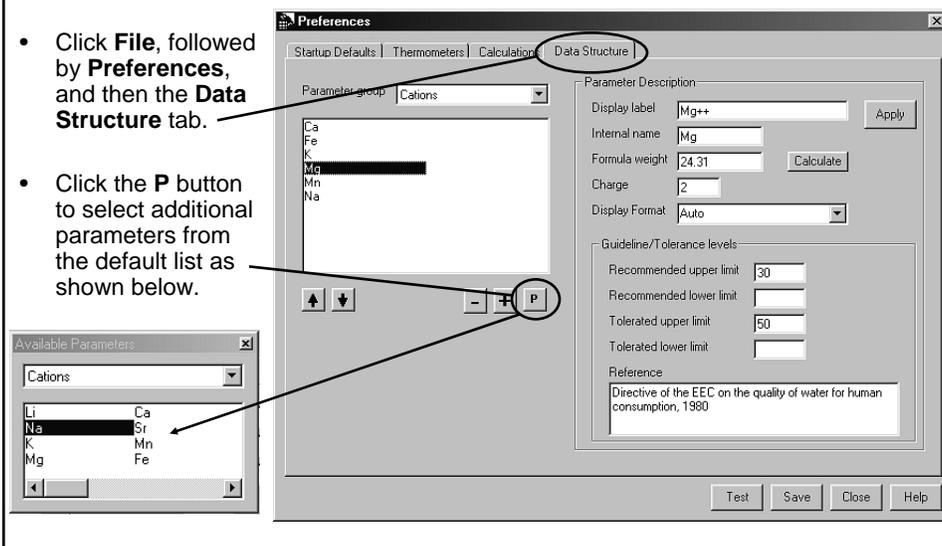
Your **Active Records Display** should appear as shown in the figure at right. Notice the new column widths are displayed.



## Adding Parameters From List

Users may add or delete any fields from each Parameter Group using the Selection Box of Available Parameters.

- Click **File**, followed by **Preferences**, and then the **Data Structure** tab.
- Click the **P** button to select additional parameters from the default list as shown below.



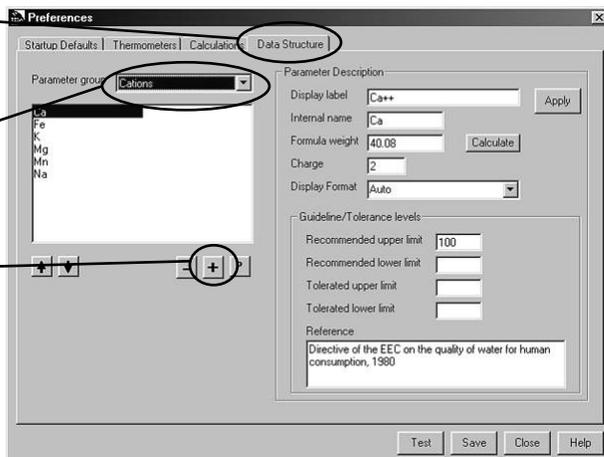
## Adding New Parameters

New parameters may be created using the "+" button.

- Click **File, Preferences, & Data Structure Tab.**

- Select Cations from the Parameter Group dropdown menu.

- Click the "+" under the Destination Window. A new parameter is created as shown on next slide.



## Adding New Parameters

Once a new Parameter is generated, Parameter information must be entered.

Fill in the Dialogue boxes for Parameter Description as follows:

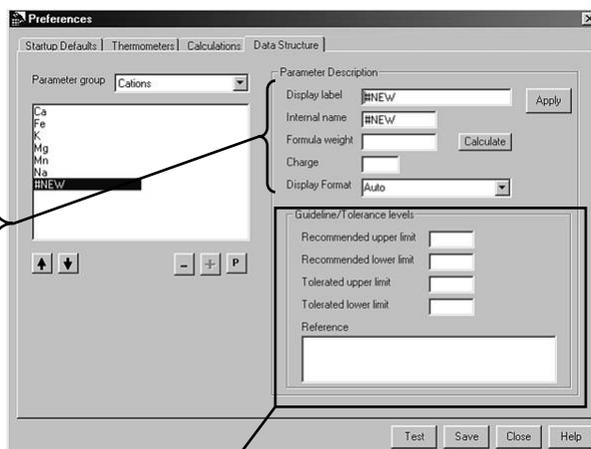
- **Display Label** = Label used in the data input windows.

- **Internal name:** Name used by AquaChem to locate data from fields for internal calculations.

- **Formula Weight:** is the numeric value of the molecular weight where applicable. Click the **[Calculate]** button to automatically calculate the molecular weight.

- **Charge:** Numeric value for the valence state (where applicable) Always Positive.

- Click **Apply** to update the information.



Guidelines, Standards, and Tolerance levels for specific parameters may be entered here.

### Index Number & #Group

- The Index is a unique database index number that AquaChem internally assigns to each database record.

- The #Group column is used to assign unique symbols to groups of records (IE: a unique symbol for each sample at one location.)

Project	Site	Location	Date	Index	#Group
CASTLE GATE	B-20	Price River	08/17/1983	0002	(01)
CASTLE GATE	B-20	Price River	08/27/1981	0014	(01)
CASTLE GATE	B-20	Price River	10/07/1982	0007	(01)
CASTLE GATE	B-20	Price River	10/11/1978	0026	(01)
CASTLE GATE	B-20	Price River	10/18/1983	0001	(01)
CASTLE GATE	B-20	Price River	10/28/1980	0019	(01)
CASTLE GATE	B-20	Price River	10/29/1981	0013	(01)
CASTLE GATE	B-20	Price River	12/03/1981	0012	(01)
CASTLE GATE	B-20	Price River	12/13/1978	0025	(01)
CASTLE GATE	B-20	Price River	12/21/1982	0006	(01)
CASTLE GATE	B-20	Price River	12/29/1980	0018	(01)
CASTLE GATE	B-5	Price River	01/11/1978	0088	(02)
CASTLE GATE	B-5	Price River	02/04/1981	0072	(02)
CASTLE GATE	B-5	Price River	02/08/1978	0087	(02)
CASTLE GATE	B-5	Price River	02/13/1980	0078	(02)
CASTLE GATE	B-5	Price River	02/15/1979	0079	(02)
CASTLE GATE	B-5	Price River	02/15/1982	0066	(02)
CASTLE GATE	B-5	Price River	02/24/1983	0060	(02)
CASTLE GATE	B-5	Price River	03/04/1992	0047	(02)
CASTLE GATE	B-5	Price River	03/08/1978	0086	(02)
CASTLE GATE	B-5	Price River	03/13/1991	0051	(02)
CASTLE GATE	B-5	Price River	03/13/1995	0036	(02)

- In the Active Record Display shown at left:

BC-1 has been assigned to Group (01)

BC-2 has been assigned to Group (02)

Records are sorted using the first column of the Active Records Window. In this case, the **Project** name was used to sort the database followed by **Site**.

This Completes the Process of Assigning the Database Field Names & Specifications.