

Lesson 6: Modifying Templates

The **RawITC**, **DeltaH**, and **ITCFinal** plot windows (and all other plot windows in Origin) are created from **template files** (*.OTP file extension). A template file is a file that contains all of the attributes of a plot window (or a worksheet) except the data. The important thing about template files is that you can change a plot window, and then save the changes into the template file for that window. The next time you open the window it will include your changes. Thus template files let you customize plot windows to meet your specifications.

You can change any of Origin's template files. In this lesson we will edit both the **DeltaH** and **ITCFinal** plot windows, then save the changes into the corresponding template file. Though the changes we make will be minor, you can actually change any property of a template. For more information about customizing templates, refer to the **Origin User's Manual** or press the F1 key for **Online Help**.

Caution: In this lesson you will be modifying plot window templates that are basic to Origin's operation. In the unlikely event that you make a mistake you are unable to correct, simply copy the original template file from the Custom folder of the installation CD-ROM. This will correct any problem that may arise.

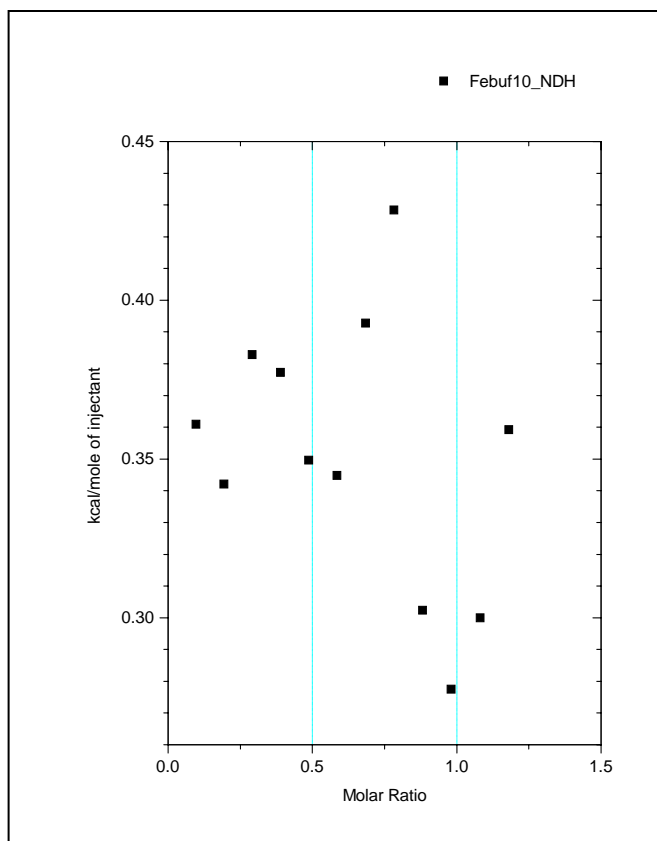
Modifying the DeltaH Template

The **DeltaH** template shows units of kilocalories/mole of injectant along the left Y axis. The scale for this axis is actually defined in terms of calories/mole of injectant, but the axis is factored by 1000 to yield units of kilocalories/mole.

The right Y axis labels for the **DeltaH** template are hidden from view. In the following example we will modify the template so that the right Y axis labels are visible. We will then factor the labels by 1000, so they will be identical to the left Y axis labels, and then save these changes into the **DeltaH** template file.

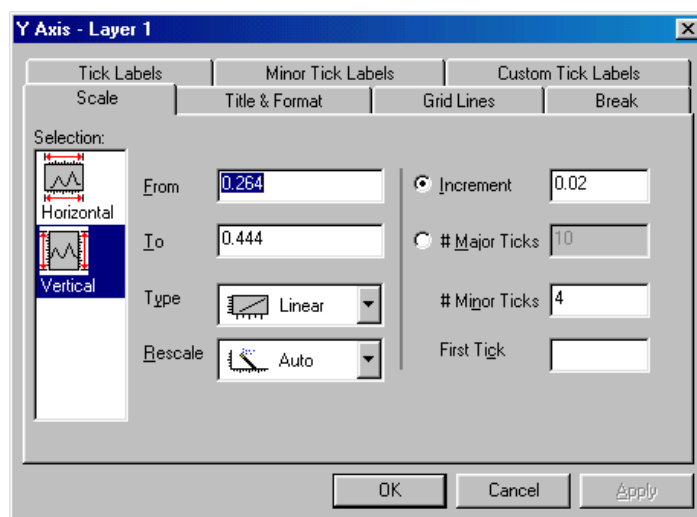
To open the DeltaH plot window

- If you are continuing from a previous lesson click on the New Project button from the Standard toolbar or select **Project** from the **New** sub-menu under the **File** menu to create a new project.
- Click on the **Read Data..** button in the **RawITC** window
The **File Open** dialog box opens, with the **ITC Data (*.ITC)** file extension selected.
- Navigate to the **C:\Origin70\Samples** folder and open any ITC data file (for example, FEBUF10.ITC). The **DeltaH** template opens to show the normalized area data.

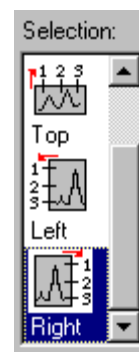


To show the right Y axis units

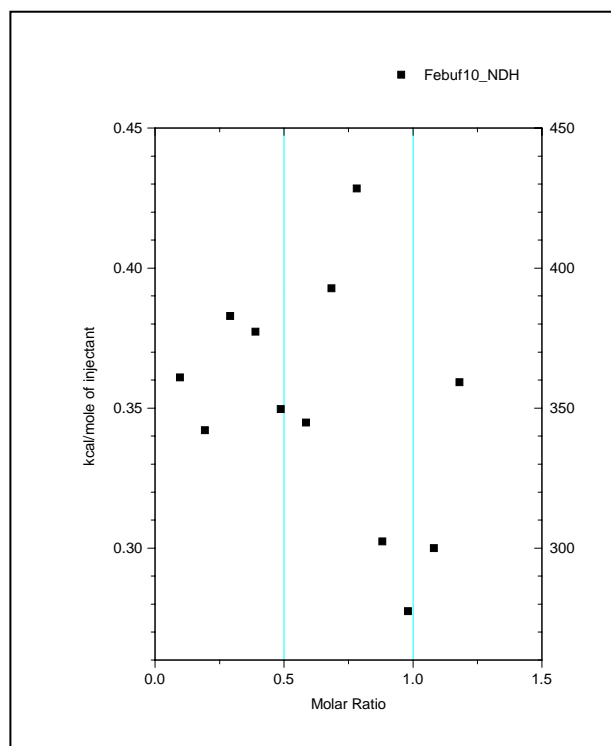
- Double-click on the right Y axis in the DeltaH window. Alternatively, select **Format:Axis:Y Axis**. The **Y Axes** dialog box opens.



- Click on the **Tick Labels Tab**.
- Select **Right** from the Selection List Box.
- Click the **Show Major Labels** check box to insert a check mark.
- Click **OK**.

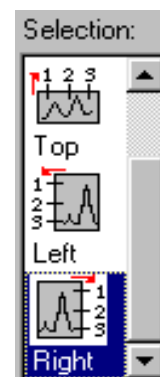


The dialog box closes. The **DeltaH** window redraws to show tick labels along the right Y axis. The right axis labels are in units of calories/mole of injectant, while the left axis labels are in kcal/mole of injectant.



To factor the axis label values by 1000

- Double-click on the right Y axis tick labels or select **Format:Axis:Y Axis**. The **Y Axis** dialog box opens.
- Click on the Tick Labels Tab.
- Select Right from the Selection List Box.
- Enter 1000 in the Divide by Factor text box.
- Click **OK** to close the dialog box.



Note : Now both axes plot in kcal since both are factored by 1000.

To save the changes into the DeltaH template file



*Shortcut:
Click on the **Save
Template** icon from
the Standard toolbar.*

- Select **File:SaveTemplate As...**
Origin opens a dialog box asking if you want to save the file as **DELTAH.OTP** (the **DeltaH** template file).
- Click **Cancel** at this point if you *do not* want to change the original **DeltaH** template. If you click **OK**, Origin will save the modified **DeltaH** window as **DELTAH.OTP**.

If you saved the modified template and now select the **File:Read Data..** button the modified **DeltaH** window will appear. Note that plotted data cannot be saved to a template file, so there is no need to delete the plotted area data before saving the **DeltaH** window.

To revert to the original DeltaH template

If you do decide to modify the **DeltaH** template, it is easy to recreate the original. Simply reverse the steps you used to create the modified template. That is, open the **DeltaH** window, open the Y-Axis dialog box, click on the Tick Labels tab, remove the check mark from the Show Major Labels check box, then select **File: Save Template As...**

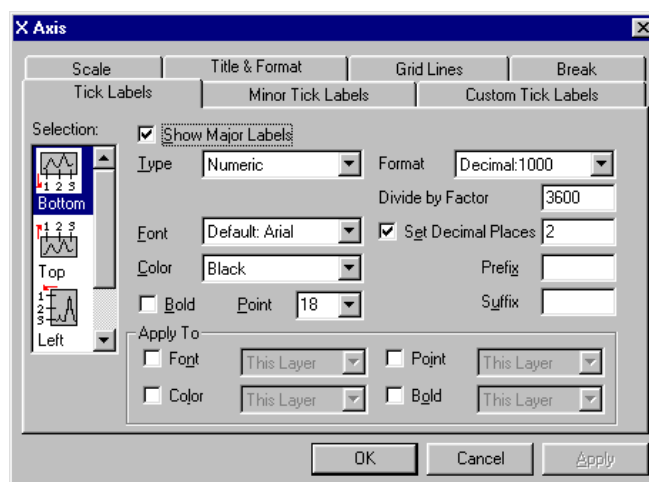
Modifying the RawITC template

The **RawITC** plot window shows bottom X axis tick labels in units of minutes. Let's use what we have just learned about factoring tick labels to change this axis scale so that the tick labels are in units of hours rather than minutes.

To factor the RawITC X axis tick labels by 3600

Shortcut: Right-click on the bottom X-axis tick labels and select Tick Labels from the drop down menu list

- Set the **RawITC** window as the active window (by either pressing and holding the Ctrl key then pressing the Tab key, or selecting **RawITC** from the **Window** menu).
- Double-click on the bottom X axis tick labels or select **Format:Axis:X Axis**. The **X Axis** dialog box opens.
- Click on the Tick Labels Tab.
- Select Bottom from the Selection List Box.
- Enter 3600 in the Divide by Factor text box.
Since the worksheet X values for raw ITC data are in terms of *seconds*, a factor of 3600 gives us axis tick label values in units of *hours* for this axis.
- Set Decimal Places to 2.



- Click **OK** to close the dialog box.
- Finally, double-click on the X axis title (it reads **Time (min)**) to open the Text Control dialog box, and edit the text to read **Time (hrs)**.

To save the changes into the RawITC template file

- Just as we did for the **DeltaH** template, select **File: Save Template As**.
- Click **Cancel** in the **Attention** dialog box if you *do not* want to change the original **RawITC** template. If you click **OK**, Origin will save the modified **RawITC** window as **RawITC.OTP**.

A Note About Units

Raw data in ITC files are stored in terms of $\mu\text{cal}/\text{second}$ versus seconds, as you will see if you open a worksheet containing raw data. The integrated area under the peaks data are stored (in the worksheet column **DH**) in units of μcal per injection. This is apparent if you open a worksheet containing integrated data.

However, for curve fitting and for better publication presentation, both the **DeltaH** and **ITCFinal** plot windows present the integrated heat data as H' (kcal per mole of ligand *injected*) which is more closely related to the fitting parameter H (calories per mole of ligand *bound*). That is, H' will be nearly equal to H (except for the factor of 1000) in early injections when nearly all of the ligand added is bound. The factor of 1000 is achieved by entering that factor to the Y axis tick labels, as discussed earlier in this lesson.

Also, both the **RawITC** plot window and the upper graph in the **ITCFinal** plot window display X axis values in minutes, while the stored values are in seconds. In this case the X axis labels are factored by 60, as we discussed (for the **RawITC** window) earlier in this lesson. If you double-click on the top X axis labels in the **ITCFinal** window, you will notice there is a factor of **60** in the **Divide by Factor** text box, just as there was with the **RawITC** window. Again, this factor setting is saved as part of the **ITCFinal** template.

The Y axis data plotted in the DeltaH and lower ITCFinal templates (i.e., data with .ndh extension) are normalized on moles of injectant. If you ever wish to view the experimental integrated heats in μcal per injection, then double-click on the Layer dialog box, and move the _ndh file out of the Active data and move the _dh file into the Active data. To complete the process, you must double-click on the Y axis tick labels and remove the factor of 1000.