

# Using Spectral Math

This tutorial explains how to use the Spectral Math command in the Process menu of your OMNIC software to perform arithmetic and other math operations on spectra.

Click the buttons at the left to view the lessons. The Overview introduces you to the features of the Spectral Math window. The other lessons are examples that take you through ..

- Ratioing two spectra:  $A/B$
- Creating a synthetic spectrum using a factor:  $A + k \cdot B$

## Overview

You can use Spectral Math to perform math operations on one or two spectra. You specify the operations by typing or selecting a sequence of symbols and numbers. The software displays the result of the operations as a spectrum that you can move to a spectral window.

When you choose the command, the Spectral Math window appears showing the selected spectrum or spectra, a default operation and the result spectrum. You can see an example on the next page. The symbol "k" in the example is a factor you can adjust using the scroll bar at the left side.

You can perform operations such as these:

- Add or subtract a constant from a spectrum.
- Add two spectra together.
- Subtract a spectrum from another.
- Multiply a spectrum by a number.
- Divide a spectrum by a number.

Select an operation from the Operation drop-down list box or type an operation in the text box.

Click the Calculate button to perform the operation.

To move the result to a spectral window, select an option from the window selection box and choose Add.

The upper pane or panes show the spectra on which you are performing the operation. The lower pane shows the result spectrum.

Click the upper button to expand the Y scale of the result spectrum. Click the lower button to contract the Y scale.

Use the view finder to display a different spectral region.

Choose Help for complete information about the Spectral Math command.

Use the scroll bar to specify the value of the factor k. You can click the Coarser button to double the range of the scroll bar; click the Finer button to reduce the range by one-half. Click the Factor button if you want to type a value.

## Ratioing spectra

Imagine you have the spectra of two computer hard disks, one coated with lubricant and one uncoated. You need to find the thickness of the lubricant by examining the peak heights, but the spectrum of the lubricated disk has a broad background that interferes.

You can eliminate the problem by ratioing the spectrum of the lubed disk against the other spectrum and then measuring the peak heights in the result. to find the relative thickness.

## How to ratio two spectra

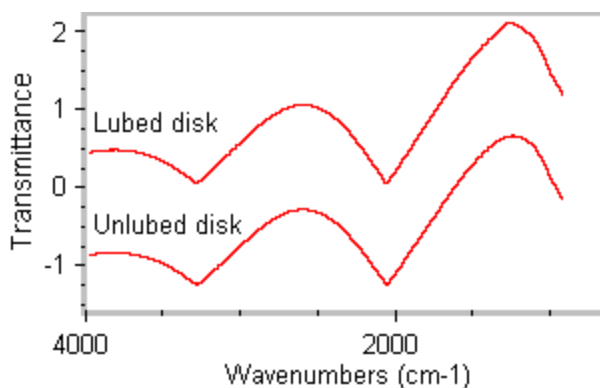
1. Select the spectrum

In this example the filenames of the spectra are LUBED.SPA and UNLUBED.SPA, normally found in the SPECTRA directory within the OMNIC directory. If the spectra are not in a spectral window, open them using Open in the File menu.

First select the spectrum of the lubricated disk by clicking it. This spectrum will be the numerator in the ratio  $A/B$ . Then hold down the Control key and select the second spectrum.

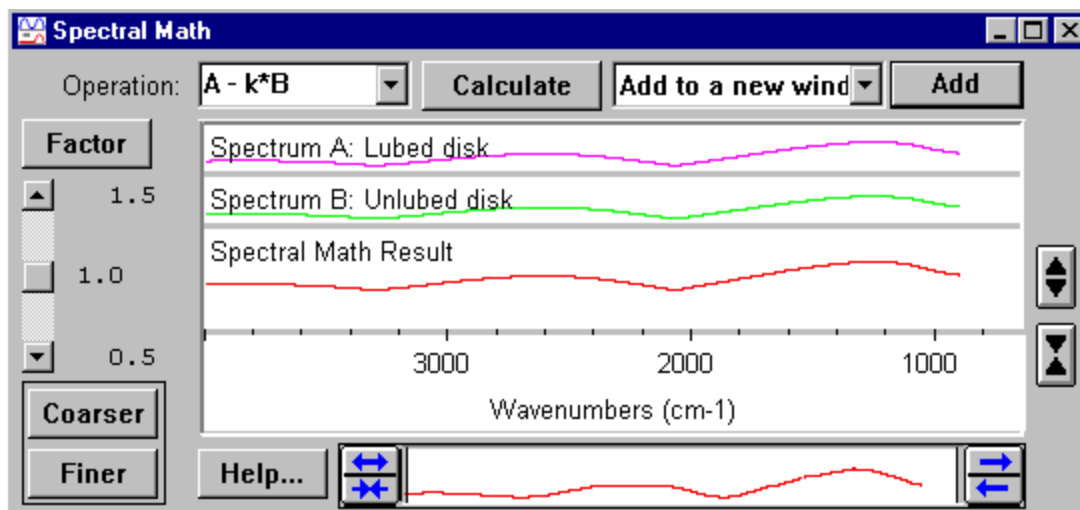
Note These spectra are actual examples collected using the PM-IRRAS technique. The lubricated disk had a monolayer of perfluoroalkyl ether lubricant. The unusual baseline (bessel function) is normal for the technique. For more information call Thermo Fisher Scientific and request information about this technique.

Here are our two spectra, displayed offset in a spectral window:



2. Choose Spectral Math from the Process menu.

The Spectral Math window appears, with the spectrum of the lubricated disk (A) at the top and the spectrum of the other disk (B) below it.



A number of math operations are provided for your selection in the Operation drop-down list box. Click the down arrow button to see them.

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The symbol "A" represents the first spectrum you selected (the spectrum of the lubricated disk). The second spectrum is represented by "B."

You can also type the desired operation directly in the Operation text box.

3. Select A / B from the Operation drop-down list box, or type A / B in the text box.

This operation will divide the Y value of every data point in spectrum A by the Y value of the corresponding data point in spectrum B.

When you type operations in the text box, type them just as you would any equation, except do not include an equals sign.

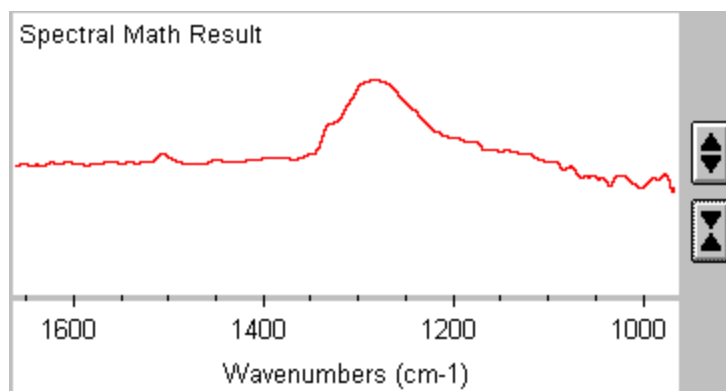
The software uses the standard order of priority for operations:

Multiplication and division before addition or subtraction, and operations to the left before those to the right when they have the same priority. You can use parentheses just as in a normal equation.

4. Click the Calculate button to perform the operation.

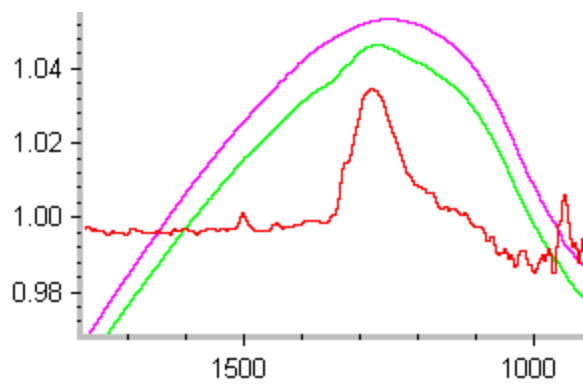
The result spectrum appears in the bottom pane. You can expand or contract the Y scale of the spectrum to see greater detail by clicking the buttons to the right of the pane. You can also adjust the spectral region displayed in the pane by using the view finder below it.

Here we have adjusted the display to get a better view of a peak of interest.



5. To move the result into a spectral window, select an option from the window selection box and then click the Add button.

Here is our result spectrum (in red) in a spectral window, along with the original spectra. The display limits have been adjusted for better viewing.



## Creating a synthetic spectrum

Suppose you have a liquid sample that is a mixture of two compounds. When you collect a spectrum of the sample and search it against a spectral library, the best match is cyclohexane. After examining the sample peaks, you suspect that the other compound is toluene. You can verify this by creating a synthetic spectrum from reference spectra of cyclohexane and diphenylmethane and then comparing it with the unknown.

To perform the steps in OMNIC as you follow along, open the spectra whose filenames are SUBREF.SPA and FINDPEAK.SPA in the SPECTRA directory within the OMNIC directory and then select both spectra.

## How to create a synthetic spectrum

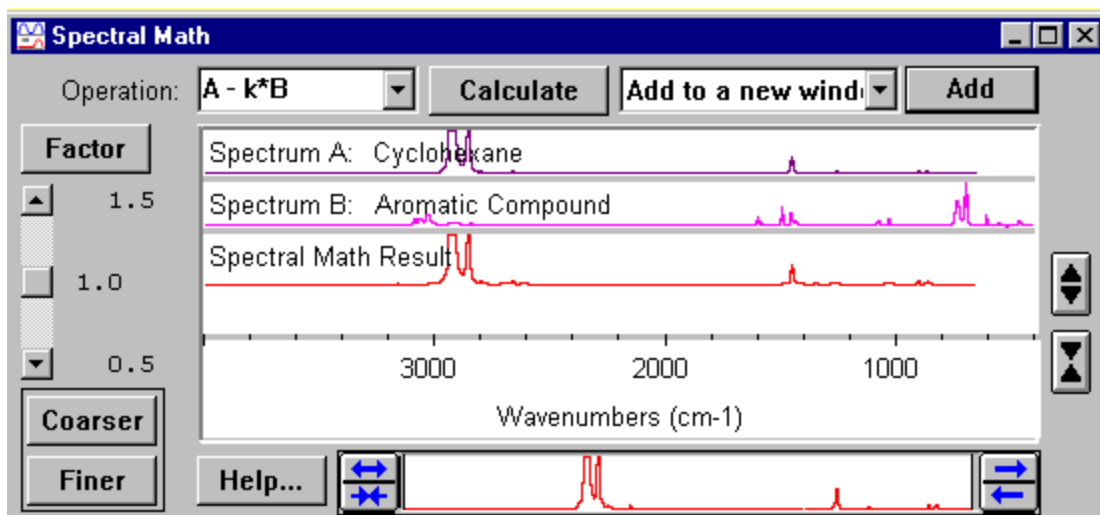
1. Select the reference spectrum.

In this example the filenames of the spectra are SUBREF.SPA and FINDPEAK.SPA, normally found in the SPECTRA directory within the OMNIC directory. If the spectra are not in a spectral window, open them using Open in the File menu.

Select the cyclohexane spectrum (SUBREF.SPA) first and the diphenylmethane spectrum (FINDPEAK.SPA) second. The cyclohexane spectrum will be A in our operation.

2. Choose Spectral Math from the Process menu.

The Spectral Math window appears, with the cyclohexane spectrum (A) at the top and the diphenylmethane spectrum (B) below it.

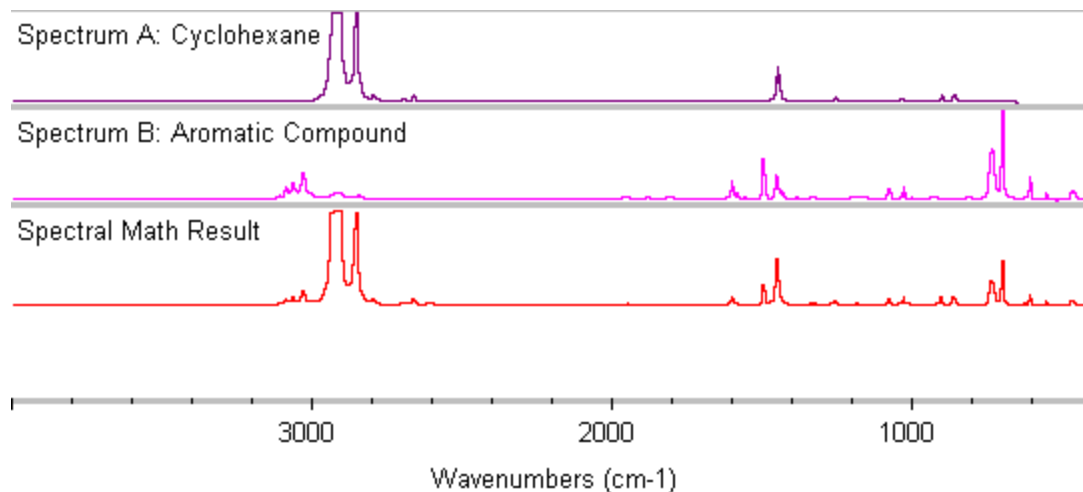


3. Type  $A + k*B$  in the text box.

This operation will multiply the diphenylmethane spectrum by the constant  $k$  and then add it to the cyclohexane spectrum. You will adjust the value of  $k$  later.

4. Click the Calculate button to perform the operation.

The result spectrum appears in the bottom pane. Notice that the result contains peaks from both of the original spectra.



5. While watching the result spectrum, use the scroll bar to adjust the value of  $k$  until you are satisfied with the result.

You can drag the scroll box or click the scroll arrows. To increase the effect of your changes, click the Coarser button; to decrease the effect, click the Finer button.

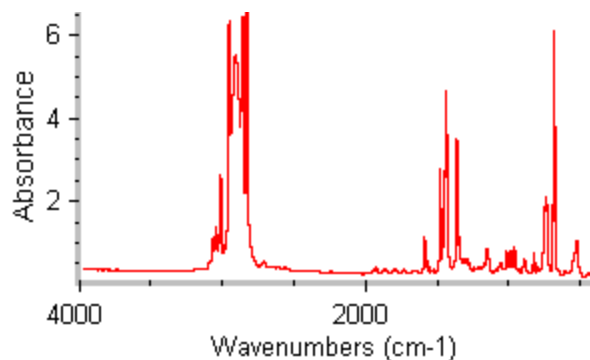
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The relative heights of peaks in the result spectrum change as the value of k changes. Click Next to see an example.

For example, when a factor of 5 is used, the peaks contributed by spectrum 8 become relatively larger, and the peaks contributed by spectrum A become relatively smaller. You can see the change clearly in the region from 3100 to 2800 wavenumbers.

6. To move the result into a spectral window, select an option from the window selection box and then choose Add.

Here is our result spectrum in the pane of a spectral window, ready to be compared with the unknown spectrum.



## For more information

Additional information about the Spectral Math command is available in the OMNIC Help system. Choose OMNIC Help topics from the Help menu, find "spectra" on the Index tab and go to the "Performing arithmetic operations on spectra" topic.

