UVU200 VVM-23Sep04CD

Manipulation of Multiple Spectra

One of the most common data manipulations requires the user to take spectra acquired separately, that is, one at a time, and compare them. Examples would be a dynamic dataset, where each spectrum was acquired at a different temperature, or a kinetic dataset, where an arrayed dataset was acquired for the first two hours of a reaction, but an additional group of spectra were acquired individually at well-spaced times in order to monitor the reaction. In each case, analysis and graphical display of the data is easier if all the data can be formed into one "arrayed" dataset. The advantage is that all the intensities can be compared, automated integration can be employed, data analysis can be simplified.

The requirement is that all data must be acquired with the same sweep width (sw), acquisition time (at), number of points (np), lock solvent, and same frequency. If the S/N of each spectrum is comparable, the comparison will be more meaningful, but this is not always possible.

For example, consider five spectra, test1.fid, test2.fid, test3.fid, test4.fid, and test5.fid.

On the SUNDS, to combine into one arrayed dataset:

jexp1 <>	join experiment 1
LC Main Menu	activate main menu display
LC File Menu	activate file menu
LC test1.fid	select test1.fid file
LC 5. Load	load file
clradd <>	clears the exp5 buffer by deleting exp5
add <>	creates exp5 and adds the FID from the current exp (1) to exp5 (the add/subtract buffer)
LC File Menu	activate file menu
LC test2.fid	select test2.fid file
LC 5. Load	load file
add('new') <>	creates a new fid element in exp5; in this case, creates and array of two spectra
Continue until all spectra all loaded:	
LC File Menu	activate file menu
LC test3.fid	select test3.fid file
LC 5. Load	load file
add('new') <>	creates a new fid element in exp5; in this case, creates and array of three spectra
LC File Menu	activate file menu
LC test4.fid	select test4.fid file
LC 5. Load	load file
add('new') <>	creates a new fid element in exp5; in this case, creates and array of four spectra

LC File Menu	activate file menu
LC test5.fid	select test5.fid file
LC 5. Load	load file
add('new') <>	creates a new fid element in exp5; in this case, creates and array of five spectra

When all the spectra have been added to exp5:

jexp5 <>	join exp5
setvalue('arraydim',# spectra,'processed') <>	defines the number of spectra in the new array. In this case # spectra =5, so the command would be setvalue('arraydim',5,'processed') <>
svf('testarray') <>	save arrayed data to a new filename
wft <>	FT the entire dataset
ai <>	absolute intensity; scales all the data to a common scale

Display with:

dssh <>	stacked horizontally
dssa <>	stacked vertically
ds(#) <>	display individual spectra, # = index number

After displaying with dssa, plot:

pl('all') pscale page <>	plots all data, with axis under the first (bottom)

if dssa(2,5), i.e., displaying spectra 2 through 5, then pl(2,5) would plot spectra 2 through 5.

If integrating the entire array,

ds(1) <>	display spectrum 1
Make the integral cuts needed.	
dli <>	display list of integrals
fint <>	finds the integrals for all spectra in the array
cpfint <>	writes data to write text table to; macro will ask for a) instrument name, b) directory name, c) filename, which should be name.txt.