Using a single file for frequency domain fitting of intensity and anisotropy decay

It is possible to combine the intensity and the anisotropy decay in a single file so that one doesn’t need to change files when fitting the lifetime and the rotations.

To combine files, you must load the pair of files (first the lifetime and then the anisotropy decay) in the input screen. Files can have any format for frequency domain. The lifetime and the anisotropy formats can be different.

Once the files have been loaded in pairs, the lifetime file first followed by the anisotropy file, in the file menu select “combine F-Domain files”. Pairs of files are combined. The filename of the combined file is the file name of the intensity decay with the word “combined” appended.

The combined files use the D format and record #2.

The following example shows the structure of the combined files and how to use them.

The ACSII file of the combination is shown below

```
FREQUENCY DOMAIN INTENSITY DECAY
25.0000, 18.2200, 0.8949, 0.1360, 0.0006
29.0030, 20.3500, 0.8690, 0.0890, 0.0007
33.6470, 22.6500, 0.8453, 0.1360, 0.0006
39.0350, 25.1800, 0.8173, 0.1260, 0.0005
45.2860, 27.4300, 0.7918, 0.1220, 0.0005
52.5370, 30.1700, 0.7591, 0.1130, 0.0005
60.9500, 33.0300, 0.7250, 0.1390, 0.0005
70.7100, 36.0900, 0.6875, 0.1180, 0.0004
82.0330, 39.3500, 0.6480, 0.1380, 0.0004
95.1690, 42.6100, 0.6089, 0.1390, 0.0003
110.4000, 45.7900, 0.5658, 0.1390, 0.0003
128.0800, 49.0300, 0.5197, 0.1400, 0.0003
148.5900, 52.5200, 0.4763, 0.1400, 0.0003
172.3900, 55.0700, 0.4306, 0.1400, 0.0003
200.0000, 58.6500, 0.3896, 0.1410, 0.0002
ENDDATA
*
FREQUENCY DOMAIN ANISOTROPY DECAY
3.0000, 0.3002, 0.5367, 0.0921, 0.0005
4.1146, 0.5559, 0.5367, 0.0386, 0.0005
5.6432, 0.6046, 0.5348, 0.0838, 0.0004
7.7397, 0.9575, 0.5345, 0.0941, 0.0006
10.6152, 1.0347, 0.5340, 0.0694, 0.0009
14.5590, 1.3382, 0.5313, 0.0258, 0.0004
19.9678, 1.5228, 0.5298, 0.0423, 0.0005
```
All the words and separators are added automatically. When record 2 is used for this file, the intensity or the anisotropy decay part of the file will be used depending on the selection in the minimization screen page shown in the red highlighted part below.

Note that in this screen there is also a button for fixing the values of all variables.

First, choose the model for the intensity decay and perform the fit using the fit intensity decay only selection. When the fit is satisfactory, press the “fix all” button. Then select the anisotropy decay model for your system. Set the selection to fit the anisotropy decay only. At this point you can fit the anisotropy using the same combined file.

If you want to go back to the fit of the lifetime, you must

- select fit intensity decay only
2. manually change the variables that have been fixed
3. change the model to the lifetime model
4. perform the fit
5. Then you can add again the anisotropy model.

Globals will remember the previous values so that you will not need to enter new initial guesses for the rotational model unless you modify the anisotropy decay model.

After you use the combined file a couple of time, you will find this addition to Globals very useful.

Have fun