# How to analyze complex NMR signals through spin simulation/iteration

**1. Introduction** When a NMR signal's multiplicity exceeds the common doublet, triplet, quartet or doublet of doublet structure, analysis of the coupling pattern can be difficult. The difficulty may or may not be due to higher order effects. Just the presence of many couplings, even if all are first order, can make the analysis challenging.

There are commercial programs and a multitude of freeware programs available to do what is known as **spin simulation and iteration**. The theory of NMR is complicated but well known and the phenomena of chemical shift and spin-spin couplings can be described mathematically. This makes it possible to calculate a theoretical spectrum based on input of chemical shifts and coupling constants. The theoretical spectrum is then compared to the experimental spectrum and further optimization can be obtained through iterative processes.

This how-to manual describes the process based on the spin-simulation software called **SpinWorks 2.5.5**. which is installed on all NMR data stations. If desired, SpinWorks can be downloaded free of charge to your own computer from the website *www.umanitoba.ca/chemistry/nmr/spinworks.*

All 1D spectra, including 1D-TOCSY, can be simulated using these instructions. Prior to making any attempt at spin simulation, the spectrum has to be processed correctly. It is very helpful to have narrow line shapes (sharp lines) in order to distinguish and assign as many lines as possible.

Correct phasing of the spectrum is best done in VNMRJ, but further optimization of the phase can also be done in SpinWorks. **Resolution enhancement has to be done in SpinWorks** (see step 5).

To demonstrate a spin simulation with SpinWorks, an **ABX** system is simulated initially and then expanded to an **ABXYZP** to reproduce the experimental spectrum more adequately. The molecular structure of the molecule used throughout these notes is shown in Figure 1, including the labeling of the spin system:

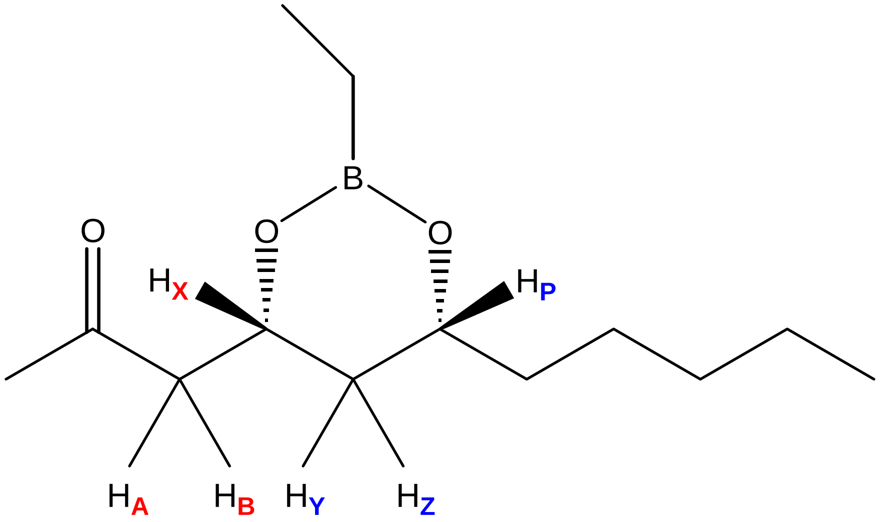


Figure 1: Chemical structure with labeled spin system

(molecule courtesy of Dr. Hall's research group)

**2. Starting SpinWorks 2.5.5** Either type *spinworks* on the VNMRJ command line or click on the button *Spin Simulation* on the EZ NMR P+P panel.

**3. Open a well-phased 1D spectrum** by using *File: Open...*. Some navigation in the file system is likely needed to find the folder where the data are stored. This is done in the same way as on PCs. Open the *filename.fid* folder of your choice then open *fid*. If opening the fid of a 1D-TOCSY, click on NO when SpinWorks asks "This appears to be 2D data, change to 2D mode?", then click OK.

The fid is displayed in blue and black colors (both the real and the complex component are shown).

Figure 2: The real and complex part of the fid

To Fourier transform the fid, open the command line with the cmd icon and type ***wft*** then click on APPLY (Figure 3) and your spectrum will be displayed as shown in Figure 4. Alternatively, go directly to **step 5** by opening the Process window with the Proc button, followed by adjustments to the processing parameters and by clicking on the Process button at the bottom of the Process window.

wft

Figure 3: SpinWorks command line

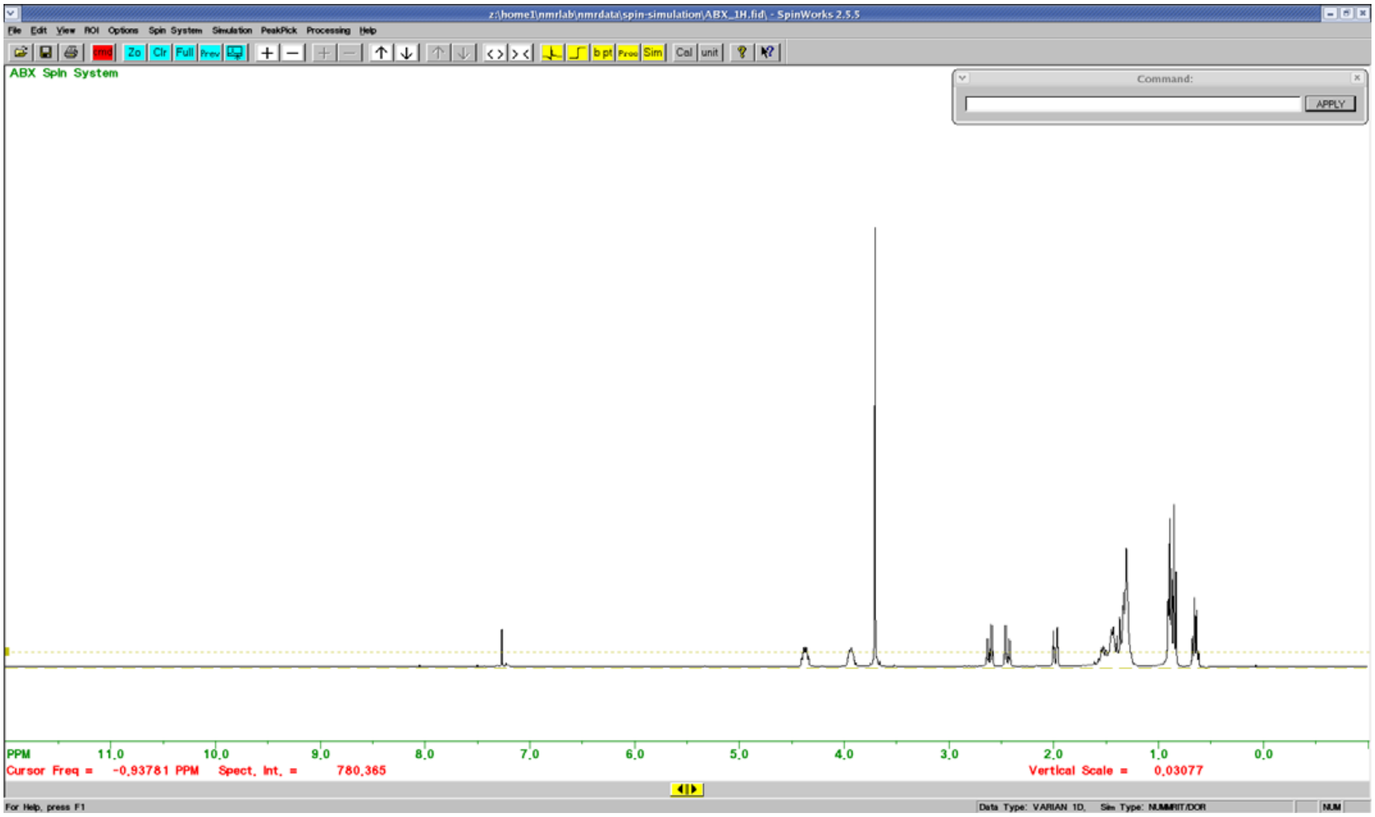


Figure 4: The spectrum display after typing *wft* on the command line

**4. Expand the peak(s) of interest** by left clicking on either side of the peak(s), then use the Zo icon to zoom in. The following buttons control the appearance and position of the spectrum:

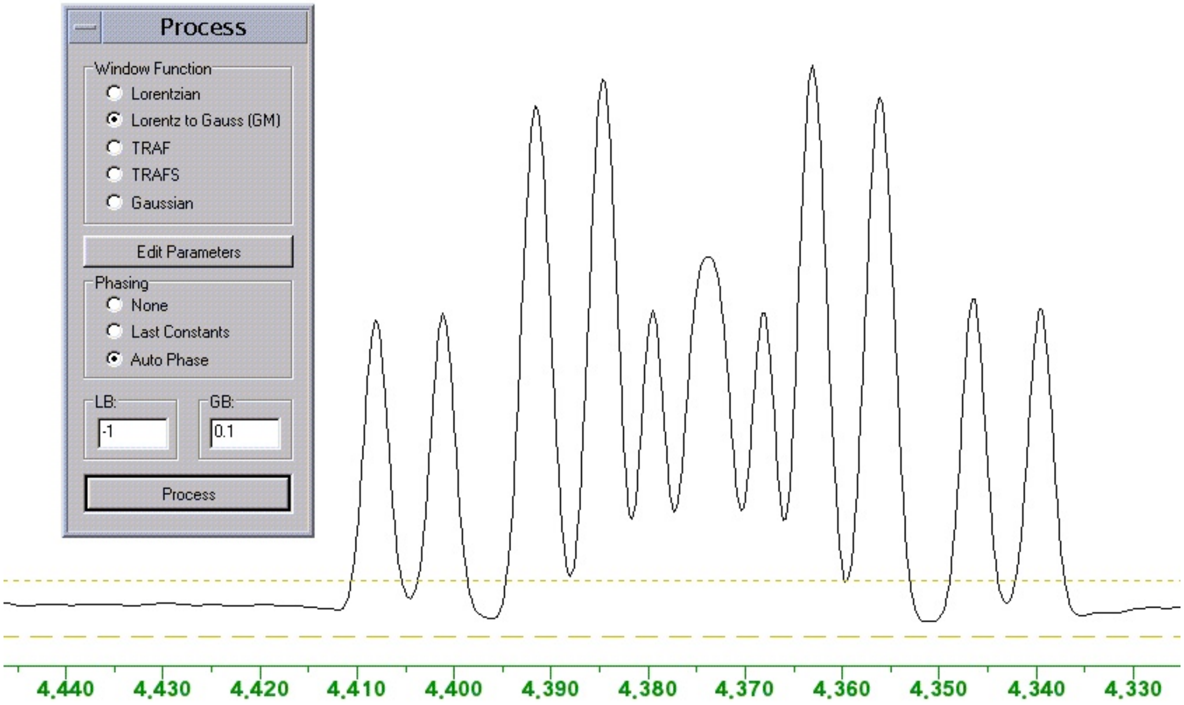
| | |
|---|---|
| increase/decrease **vertical scale** of the peaks | ↑ ↓ |
| increase/decrease **vertical position** of the spectrum | + − |
| increase/decrease **horizontal scale** (zoom in/out ) | <> >< |
| view **full** spectrum | Full |
| return to previously **expanded** region | Prev |
| adjust **peak threshold** (click and hold the small yellow rectangle and move it up or down) | ▮ - - - - |
| **phasing** | ⊥ |
| change **scale** (ppm *vs.* Hz) | unit |

Adjust vertical scale, vertical position and horizontal scale of the spectrum by using the buttons described above. If necessary open the Interactive Phasing window to phase the spectrum. Usually only coarse and fine phasing of ph0 is needed. If not, then adjust ph1 in the same way as ph0. Phase constants are adjusted via sliders in the Interactive Phasing window. When the spectrum is phased as desired, select **Apply and Exit**. The scale can be changed from ppm to Hz. This might be useful because spin simulations work in Hz only, i.e. the chemical shifts of the peaks must be entered in Hz. But it is not essential as most information is taken from cursors and those work in Hz only.

**5. Open the Process window** Proc (see inserts in Figures 5 to 7). Adjust Line Broadening (LB) and Gaussian Broadening (GB) to resolution-enhance the spectrum. To do this set LB to a negative value (start with -1) and GB to a number between 0 and 1. Make sure *Lorentz to Gauss (GM)* and *Auto Phase* are selected (see inserts Figure 5 to 7), then click on **Process**. After processing, the vertical scale has to be increased substantially.

Figures 5 to 7 are examples of a complicated multiplet (spin X, Figure 1) processed with various levels of resolution enhancement. For spin simulations the resolution enhancement shown in Figures 6 or 7 is needed. Some experimenting is required to find optimum LB and GB values and, despite Auto Phase, some manual re-phasing is likely needed (see 4). LB = -1 and GB = 0.33 (Figure 6) is used in this how-to manual.

>> Refer to pages 14-17 of the electronic manual for further explanations [Help: View Manual(pdf)] <<



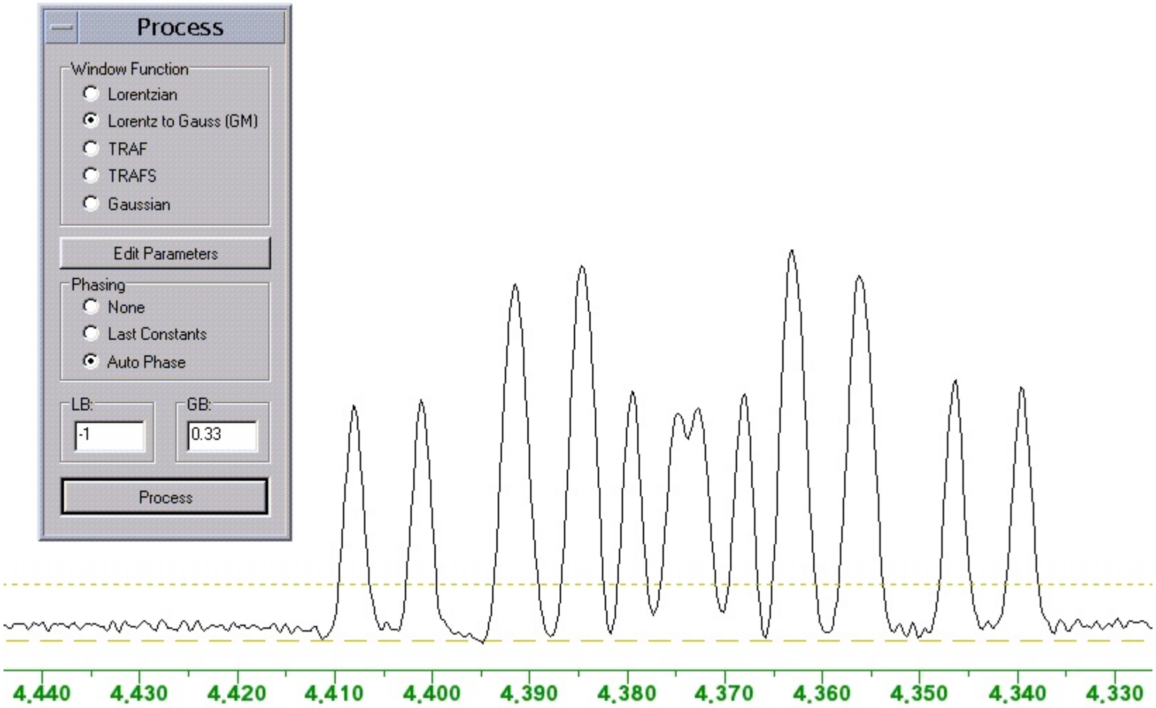
Window Function
○ Lorentzian
● Lorentz to Gauss (GM)
○ TRAF
○ TRAFS
○ Gaussian

Phasing
○ None
○ Last Constants
● Auto Phase

LB: -1
GB: 0.1

Figure 5: H(**X**) multiplet processed with LB = -1 and GB = 0.1.

The Edit Parameters button in the Process window is best left alone at this point. More damage than good can be done unless the user is well aware about what the changes imply.



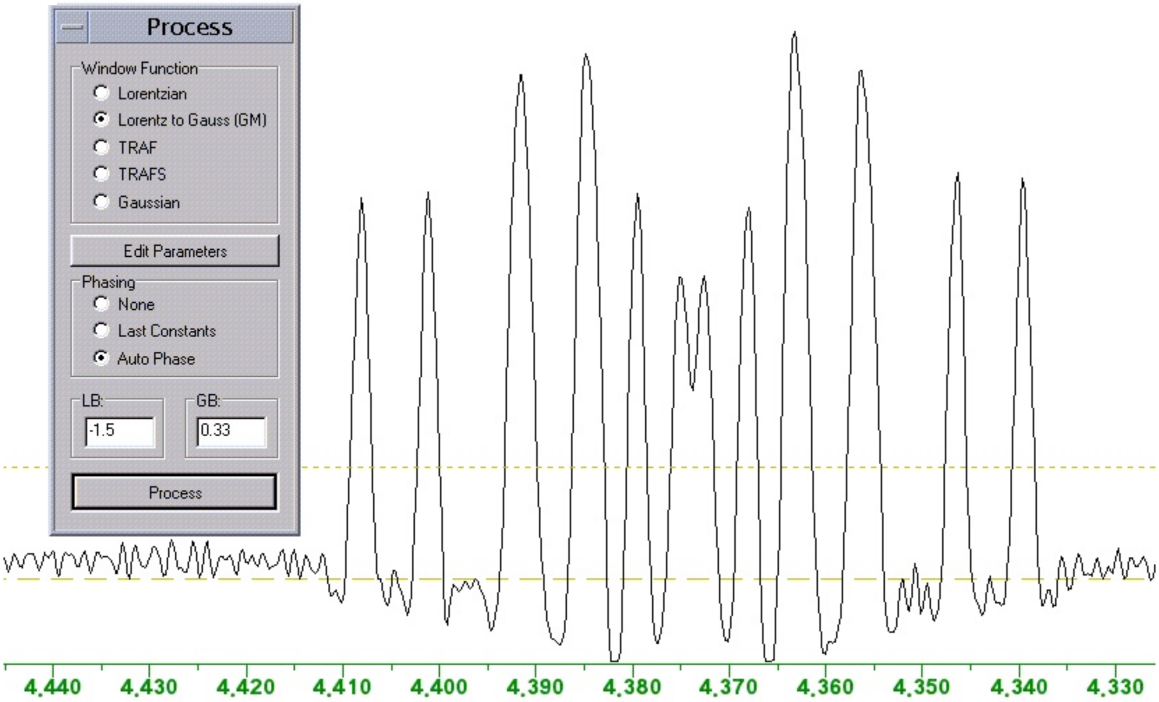
Process

Window Function
○ Lorentzian
● Lorentz to Gauss (GM)
○ TRAF
○ TRAFS
○ Gaussian

Phasing
○ None
○ Last Constants
● Auto Phase

LB: -1
GB: 0.33

Figure 6: H(**X**) multiplet processed with LB = -1 and GB = 0.33.



Process

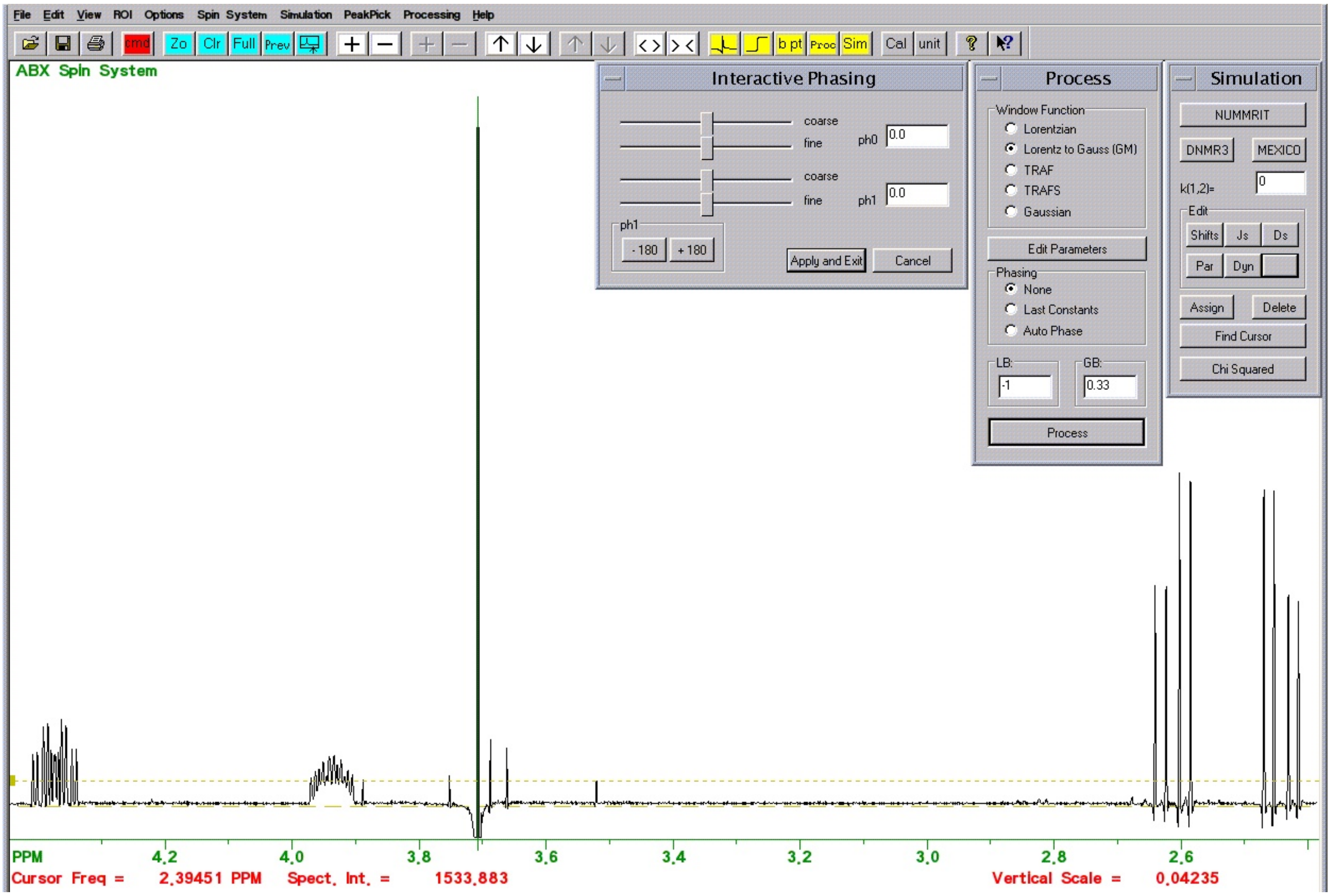
Window Function
○ Lorentzian
● Lorentz to Gauss (GM)
○ TRAF
○ TRAFS
○ Gaussian

Phasing
○ None
○ Last Constants
● Auto Phase

LB: -1.5
GB: 0.33

Figure 7: H(**X**) multiplet processed with LB = -1.5 and GB = 0.33.

**6. After processing the spectrum** should be saved with *File: Save Processed Data*. To retrieve the processed spectrum at a later date open first the *fid* as described in Step 3 then *File: Load Processed Data*.



ABX Spin System

ph0 0.0

ph1 0.0

Window Function: ○ Lorentzian ● Lorentz to Gauss (GM) ○ TRAF ○ TRAFS ○ Gaussian

Phasing: ● None ○ Last Constants ○ Auto Phase

LB: -1

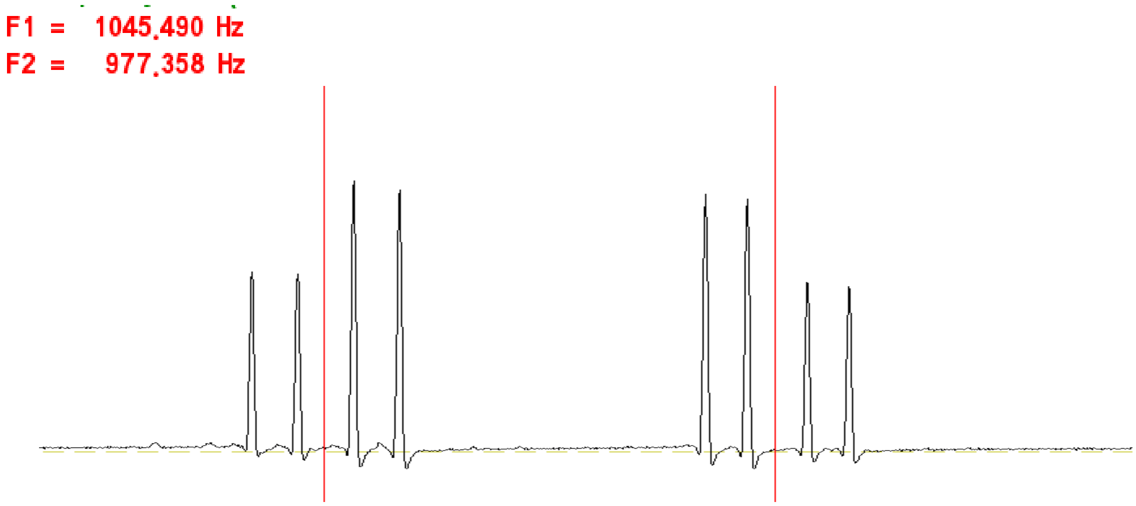
GB: 0.33

k(1,2)= 0

Cursor Freq = 2.39451 PPM   Spect. Int. = 1533.883   Vertical Scale = 0.04235

Figure 8: An expansion of the ABX spin system of interest, with the Interactive Phasing, Process and Simulation windows inserted.

**7. Obtain chemical shifts for A, B and X** spins by placing the cursor in the center of multiplets of each spin. The chemical shifts are displayed in red in the top left corner of the screen as shown in Figure 9.



F1 = 1045.490 Hz

F2 = 977.358 Hz

Figure 9: Chemical shifts of the H(**A)** and H(**B)** spins

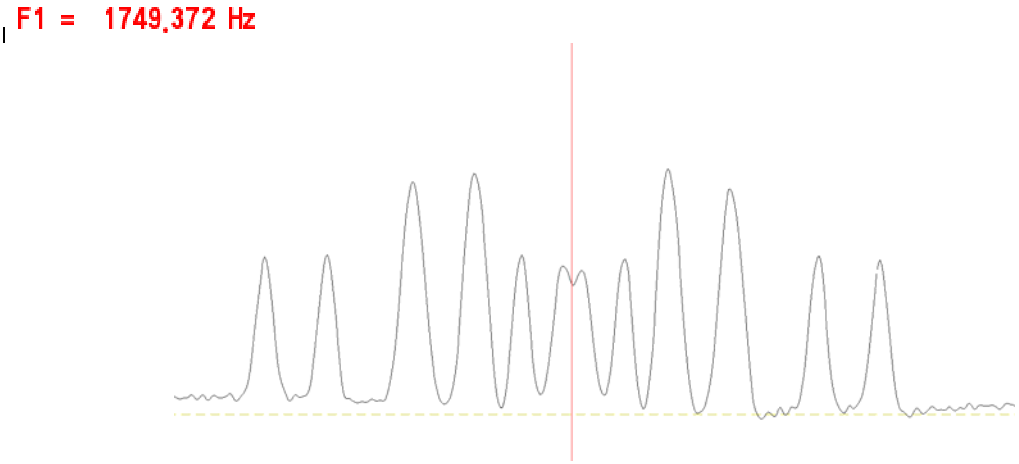
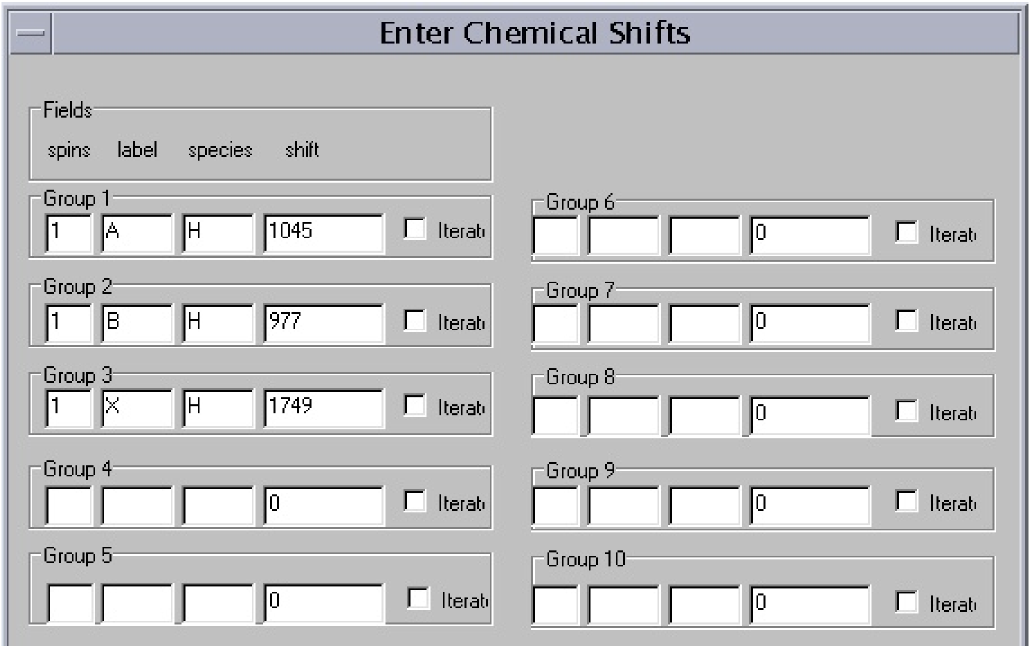


Figure 10: Chemical shifts of the H(**X**) spin

**8. To begin the simulation** open the simulation window with Sim then open the Enter Chemical Shifts window using Shifts (see Figure 11). In the four spaces available enter number of spins, group label, species identifier and chemical shifts (in Hz) for each spin, as obtained in Figures 9 and 10:



Enter Chemical Shifts

Fields: spins label species shift

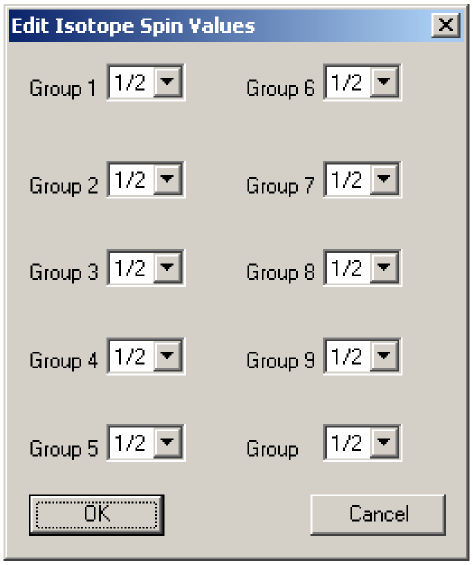
| | spins | label | species | shift | |
|---|---|---|---|---|---|
| Group 1 | 1 | A | H | 1045 | ☐ Iterati |
| Group 2 | 1 | B | H | 977 | ☐ Iterati |
| Group 3 | 1 | X | H | 1749 | ☐ Iterati |
| Group 4 | | | | 0 | ☐ Iterati |
| Group 5 | | | | 0 | ☐ Iterati |
| Group 6 | | | | 0 | ☐ Iterati |
| Group 7 | | | | 0 | ☐ Iterati |
| Group 8 | | | | 0 | ☐ Iterati |
| Group 9 | | | | 0 | ☐ Iterati |
| Group 10 | | | | 0 | ☐ Iterati |

Figure 11: Enter Chemical Shifts window with the parameters appropriate for the ABX spin system.

In Group 1, spins “1” indicates that the signal at chemical shift 1045 Hz is the result of one H (called “A”). This could also be 2, 3 in case of CH2 or CH3 groups with identical chemical shifts. *Species* could be C in simulations involving C13 spectra.

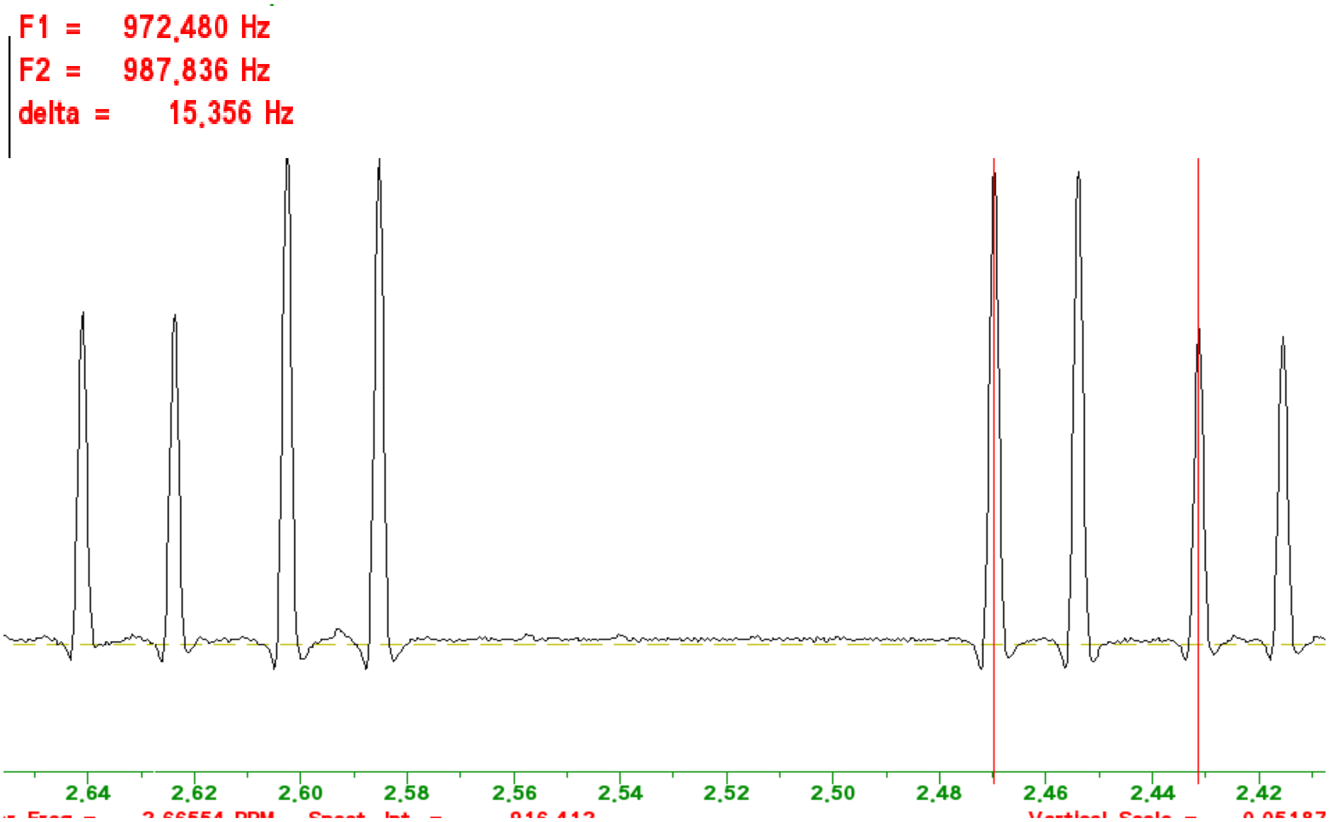
**9. Spin values of each group** can be changed with *Spin System: Edit Species Spin Values...* In this example there are only protons, i.e. the default of ½ is appropriate for all groups. If the spectrum involved spins coupled to nuclei such as deuterium the value would be 1 for the group containing the D instead of ½.

**10. To find the AB, AX and BX coupling constants**, place cursors on the AB multiplets as shown in Figures 13 to 15. First click: the first cursor appears with its position displayed as F1 in the top left corner. Second click: the second cursor appears with its position displayed as F2. The difference between the two cursors is shown as **delta (the coupling constant)**. The sign of delta is irrelevant and thus can be ignored (it depends on the sequence of clicks, left *vs.* right side first). Third click: clear values, i.e. ready for next coupling constant measurement.



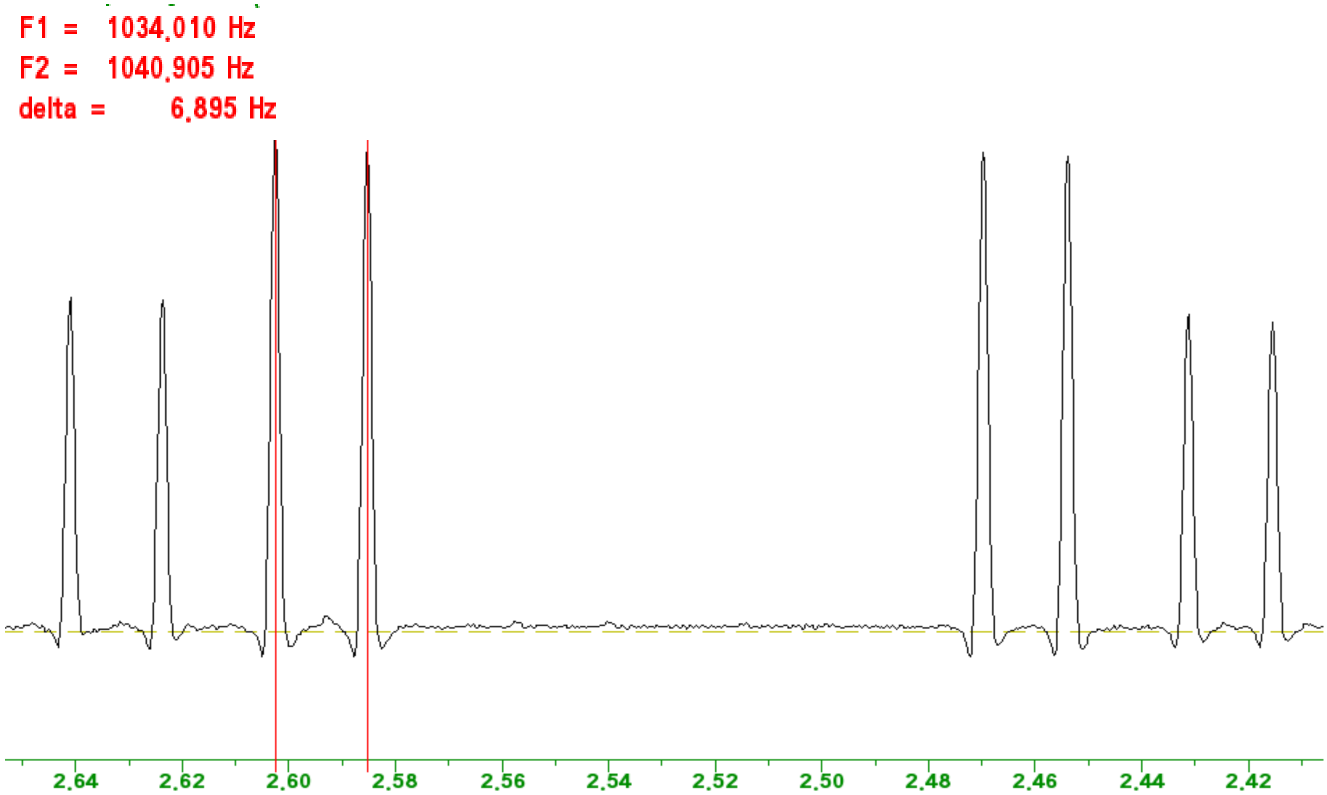
Group 1 1/2
Group 2 1/2
Group 3 1/2
Group 4 1/2
Group 5 1/2
Group 6 1/2
Group 7 1/2
Group 8 1/2
Group 9 1/2
Group 1/2

Figure 12: Edit Isotope Spin Values window



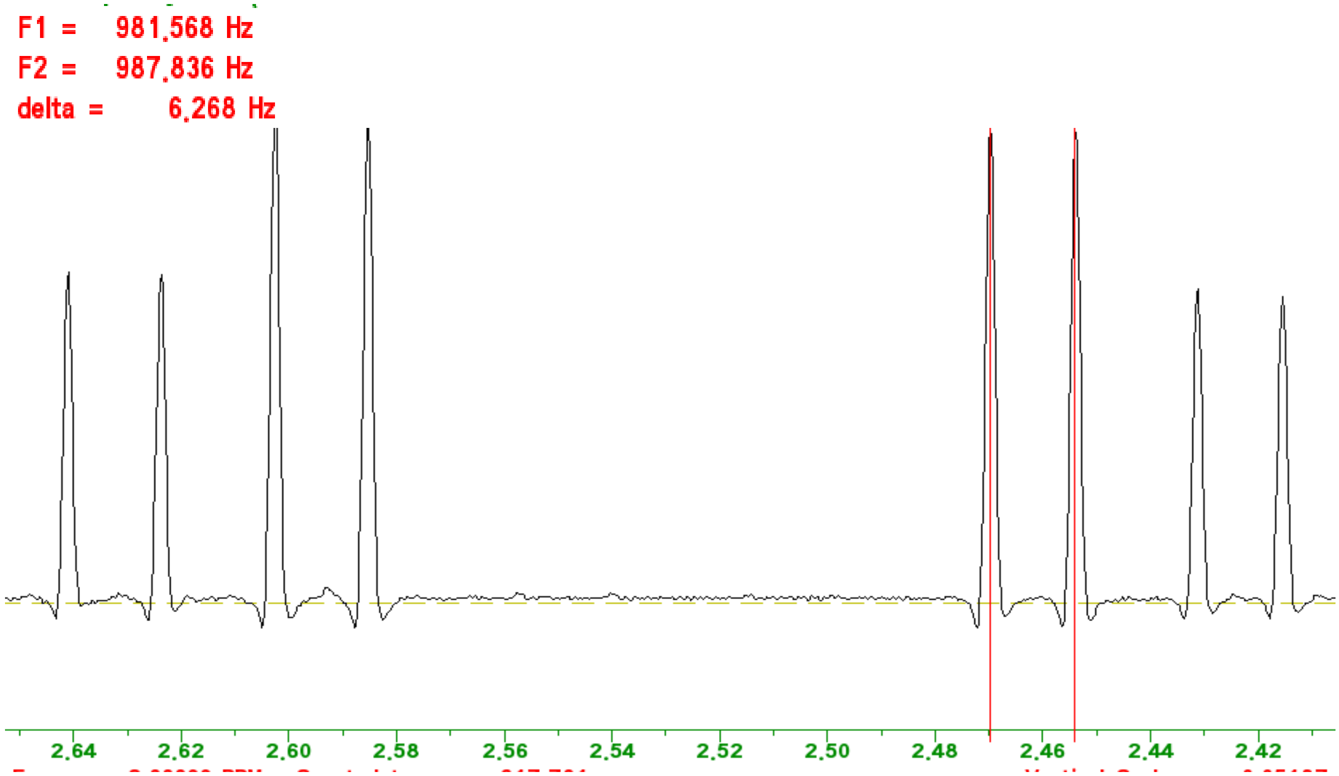
F1 = 972.480 Hz
F2 = 987.836 Hz
delta = 15.356 Hz

Figure 13: AB coupling constant



F1 = 1034.010 Hz
F2 = 1040.905 Hz
delta = 6.895 Hz

Figure 14: AX coupling constant



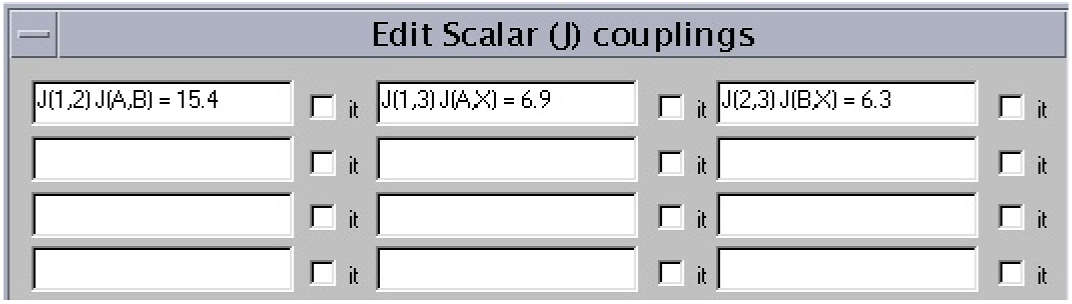
F1 = 981.568 Hz
F2 = 987.836 Hz
delta = 6.268 Hz

Figure 15: BX coupling constant

**11. Open the Edit Scalar (J) Couplings window** in the Simulation window shown on the right, by clicking on the **Js** button. Enter all known or estimated coupling values (negative or positive) by replacing 0.000000 with an approximate numerical value. Leave any irrelevant coupling constants at 0.000000.

Only edit the numeric portion of these fields,
**DO NOT edit the coupling labels such as J(1,2) J(A,B)=**.

When finished the Edit Scalar (J) Couplings window should look like shown in Figure 16.
Note that values beyond one decimal point (e.g. 15.4) are irrelevant. They are neither reproducible nor important for the simulation as these values are only *starting points* (and will change through the calculation).



J(1,2) J(A,B) = 15.4 ☐ it
J(1,3) J(A,X) = 6.9 ☐ it
J(2,3) J(B,X) = 6.3 ☐ it

Figure 16: Edit Scalar (J) Couplings window after entering the values obtained in Figures 13 to 15

**12. Save the initial chemical shifts and coupling constants** with *File: Save Spin System As...*.

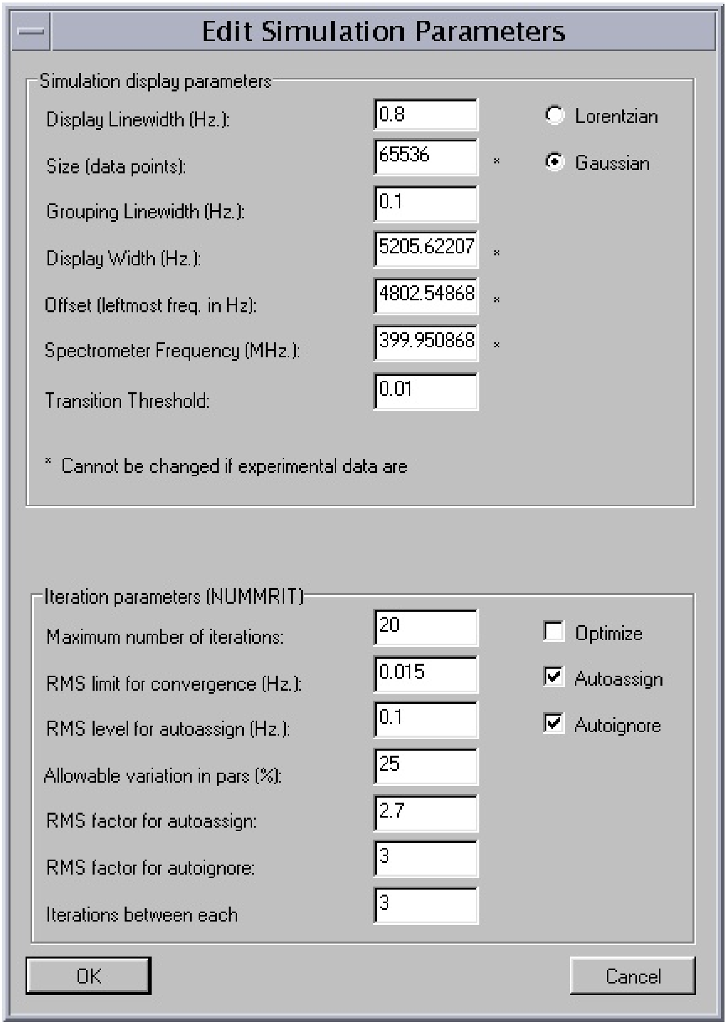
**13. Run the ABX simulation** by clicking on NUMMRIT in the Simulation window.

**14. The simulated spectrum is displayed** in blue (upper spectrum) and the experimental spectrum in black (lower spectrum Figure 17). To adjust the vertical scale and position of the simulated spectrum use the corresponding blue buttons + − and ↑ ↓ (the black ones are for the experimental spectrum).

The **linewidth of the simulated spectrum** can be adjusted to match the linewidth of the experimental spectrum by opening the Edit Simulation Parameters window (Figure 18), accessible via the Par button in the Simulation window. Select a suitable value for Display Linewidth (Hz) to closely match the experimental linewidth. Select Lorentzian or Gaussian lineshape and run the simulation again.

Strongly resolution-enhanced spectra like those shown in Figures 6 and 7 have a Gaussian lineshape. The natural lineshape of NMR lines without resolution enhancement is Lorentzian. Theory aside, most important is to select parameters that create a simulated spectrum as similar as possible to the experimental spectrum.

Figure 17: Simulated spectrum at the top in blue, experimental spectrum at the bottom in black



Simulation display parameters

Display Linewidth (Hz.): 0.8
Size (data points): 65536 *
Grouping Linewidth (Hz.): 0.1
Display Width (Hz.): 5205.62207 *
Offset (leftmost freq. in Hz): 4802.54868 *
Spectrometer Frequency (MHz.): 399.950868 *
Transition Threshold: 0.01

○ Lorentzian
● Gaussian

* Cannot be changed if experimental data are

Iteration parameters (NUMMRIT)

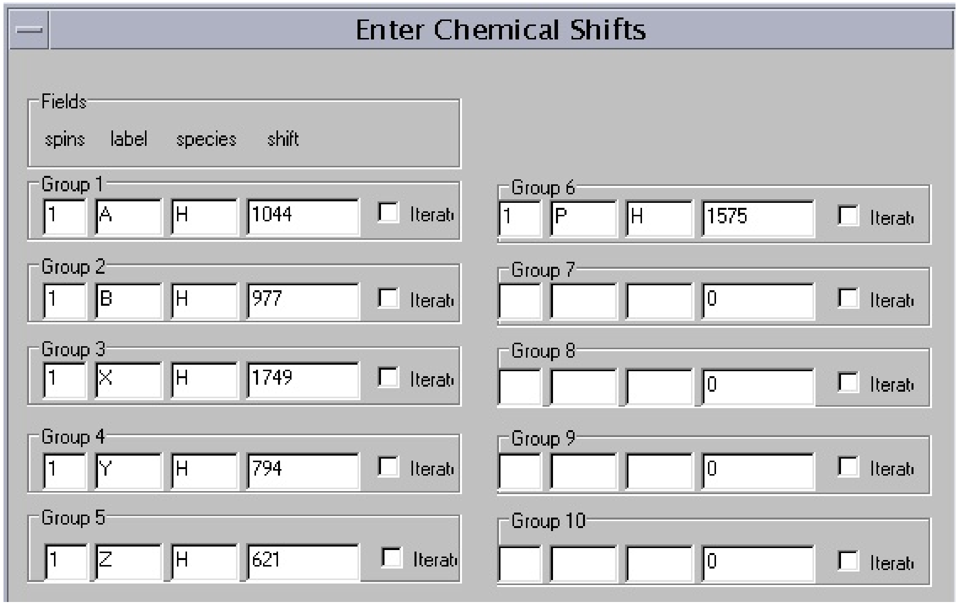
Maximum number of iterations: 20
RMS limit for convergence (Hz.): 0.015
RMS level for autoassign (Hz.): 0.1
Allowable variation in pars (%): 25
RMS factor for autoassign: 2.7
RMS factor for autoignore: 3
Iterations between each 3

☐ Optimize
☑ Autoassign
☑ Autoignore

Figure 18: Edit Simulation Parameters window

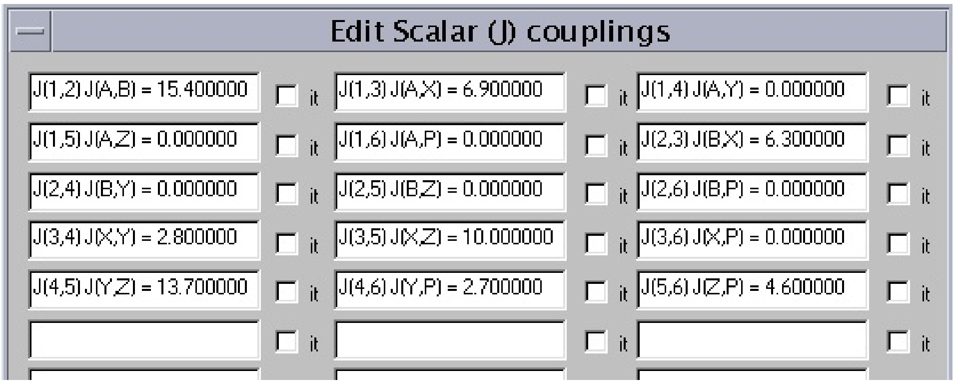
**14. The X portion** in the above simulation appears as a triplet which is obviously incorrect, whereas the AB part is quite close to the experimental. In order to correctly simulate the H(X) resonance, more interacting spins need to be added for the simple reason that H(X) is also coupled to H(Y) and H(Z) as can be expected by looking at the structure in Figure 1.

Figures 19 and 20 show chemical shift and scalar couplings information for the Y, Z and P spins.



| Group | spins | label | species | shift | |
|---|---|---|---|---|---|
| Group 1 | 1 | A | H | 1044 | ☐ Iterat |
| Group 2 | 1 | B | H | 977 | ☐ Iterat |
| Group 3 | 1 | X | H | 1749 | ☐ Iterat |
| Group 4 | 1 | Y | H | 794 | ☐ Iterat |
| Group 5 | 1 | Z | H | 621 | ☐ Iterat |
| Group 6 | 1 | P | H | 1575 | ☐ Iterat |
| Group 7 | | | | 0 | ☐ Iterat |
| Group 8 | | | | 0 | ☐ Iterat |
| Group 9 | | | | 0 | ☐ Iterat |
| Group 10 | | | | 0 | ☐ Iterat |

Figure 19: Enter Chemical Shifts window with information added for the Y, Z and P spins



J(1,2) J(A,B) = 15.400000 ☐ it
J(1,3) J(A,X) = 6.900000 ☐ it
J(1,4) J(A,Y) = 0.000000 ☐ it
J(1,5) J(A,Z) = 0.000000 ☐ it
J(1,6) J(A,P) = 0.000000 ☐ it
J(2,3) J(B,X) = 6.300000 ☐ it
J(2,4) J(B,Y) = 0.000000 ☐ it
J(2,5) J(B,Z) = 0.000000 ☐ it
J(2,6) J(B,P) = 0.000000 ☐ it
J(3,4) J(X,Y) = 2.800000 ☐ it
J(3,5) J(X,Z) = 10.000000 ☐ it
J(3,6) J(X,P) = 0.000000 ☐ it
J(4,5) J(Y,Z) = 13.700000 ☐ it
J(4,6) J(Y,P) = 2.700000 ☐ it
J(5,6) J(Z,P) = 4.600000 ☐ it

Figure 20: Enter Scalar (J) Couplings window with additional XY, XZ, YZ, YP and ZP coupling constants added

In **first order** systems the width in Hz of the entire multiplet (from most left to most right line) is equal to the **sum of all coupling constants** that create this multiplet. In cases where one J value cannot be measured in the experimental spectrum (typically because the multiplet is too complicated or overlapping) the missing coupling constant can be calculated. For example, as can be seen in Figure 21, the total width of the H(**X**) signal is 27.4 Hz. J(XZ) cannot be extracted from H(Z) but calculated by subtracting all the Js that are known for H(X) from its total width:

$$J_{XZ} = \text{total width} - (J_{AX}+J_{BX}+J_{XY}) = 27.4 - (6.9+6.3+2.8) = 11.4 \text{ Hz}$$

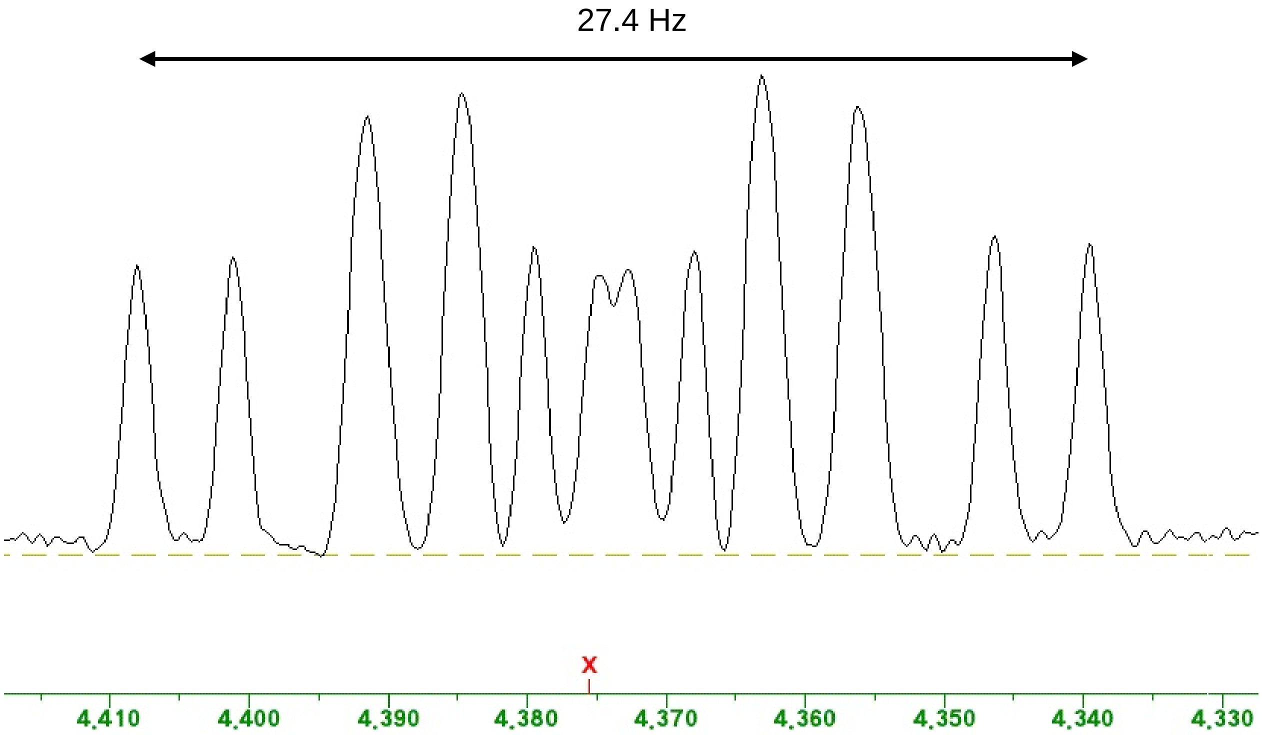


Figure 21: The 27.4 Hz wide H(**X**) multiplet contains 12 lines due to 4 coupling constants

According to first order rules, **4 coupling constants** should result in 2 x 2 x 2 x 2 = **16 lines**. In Figure 5 it can be seen that four lines are more intense than the rest and in Figure 21, although intensities are severely distorted by the very strong resolution enhancement, the same four lines that were higher are now broader than the rest. This indicates clearly that each of those four lines is the result of two lines with an extremely small difference in chemical shift, so small that even with strong resolution enhancement they cannot be separated. This is quite a common situation and no reason to give up!

Like in step 12 for the ABX, the initial chemical shifts and coupling constants for the ABXYZP spectrum can be saved with *File: Save Spin System As...*.

**15. To simulate the new ABXYZP system** with parameters added under 14, click on Sim to get to the simulation window, then on NUMMRIT to run the simulation.

As can be seen in Figure 22, H(X) is now much closer to the experimental spectrum than in Figure 17 and the new spins that were added appear as well. H(A), H(B), H(X) and H(Y) are nearly as they should be but P in particular is way too simple, the result of missing couplings to adjacent protons (analogous to the initial problem with the H(X) spin). This is normal: almost always some more spins can be added, but often this is not needed as only a portion of the molecule needs to be analyzed in great detail.

If the simulation result is satisfactory, the process can be stopped here. However, it is possible and **recommended to refine the result** further by using an **iterative process** after assigning the lines between the experimental and calculated spectrum.

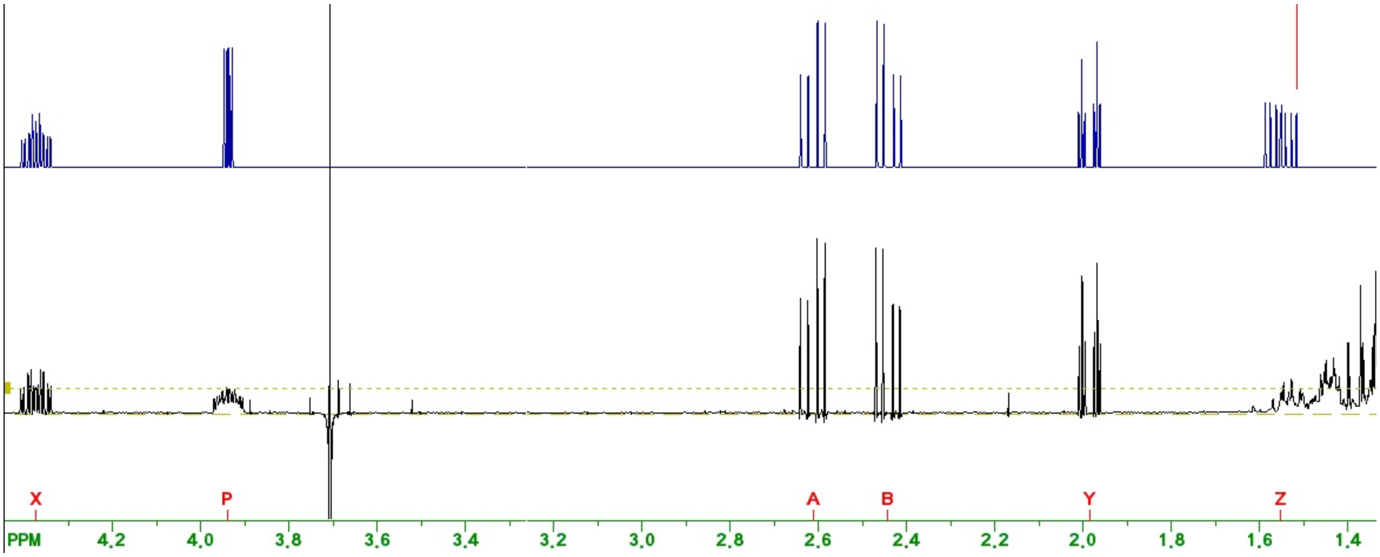


Figure 22: The ABXYZP spectral simulation on top and the experimental spectrum at the bottom

**16. To assign the simulated peaks to experimental peaks** use the Simulation Window. Activate the red transition cursor corresponding to the simulated spectrum with Find Cursor. Then right click on the corresponding experimental peak. Use the left arrow key to move to the next simulated peak and repeat the assignment. Often multiple hits on the left arrow key on the keyboard are needed because what appears as one single line is often an overlap of many in-distinguishable yet different lines. **Do not make line assignments that are ambiguous**, like here spin Z, due to spectral overlap.

**Automatic assignments**. To auto-assign, make sure the dashed yellow threshold line is below the black experimental peaks but not in the spectral noise. **Auto assign works only in the displayed region** of the spectrum. It clearly works best when only applied to expanded regions not the entire spectrum. Click Assign to start the process.

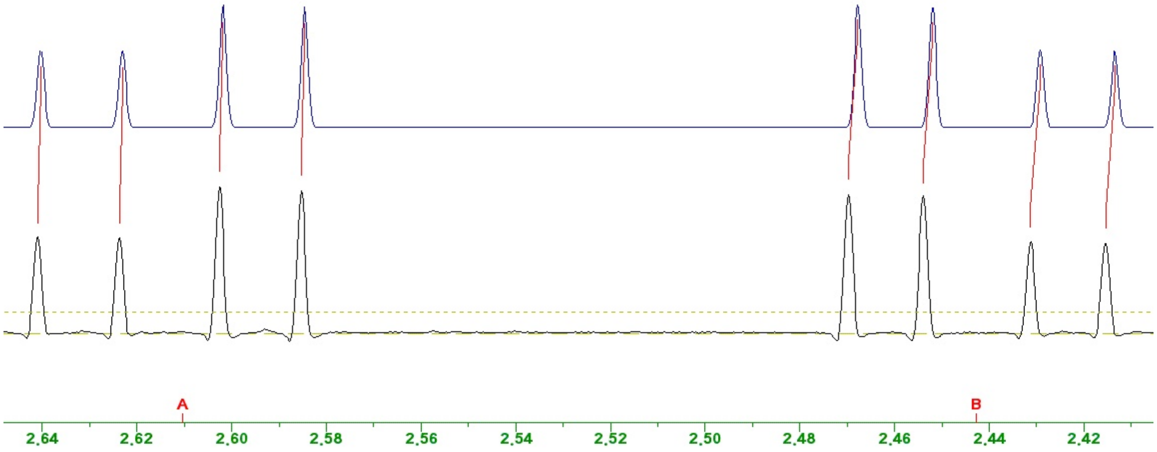


Figure 23: Expansion of the AB portion after line assignments

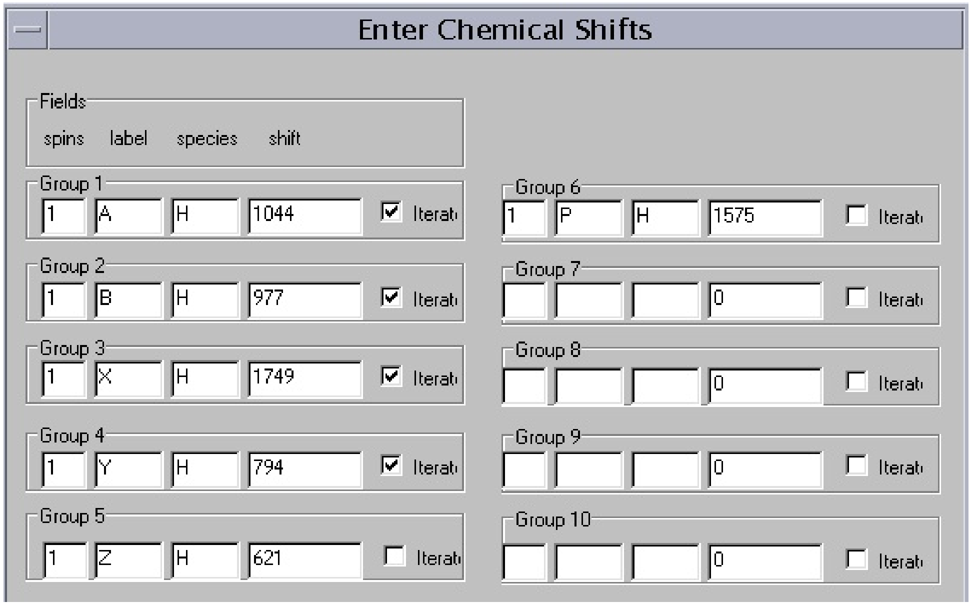
The result is rarely perfect so some adjustments may have to be made manually. If needed, use Delete to remove all the automatically assigned transitions **in the displayed region** or use again Find Cursor and move the cursor with the left or right arrow keys on the keyboard to find the undesired assignment then type **d** to remove it. Like for manual line assignments, when deleting manually, d may have to be typed multiple times to remove all assignments associated with a single line.

In general, the more lines that are assigned correctly, the closer simulated and experimental spectrum will match after the iteration (i.e. lower rms error). However, if unsure about which simulated and experimental lines belong together, rather leave them unassigned. Mis-assignments can lead to pretty weird results. See step 19 for information on how to undo an iteration that did not improve but rather made the calculated spectrum worse.

**17. Save the assigned transitions** with *File: Save Assigned Transitions as…*.

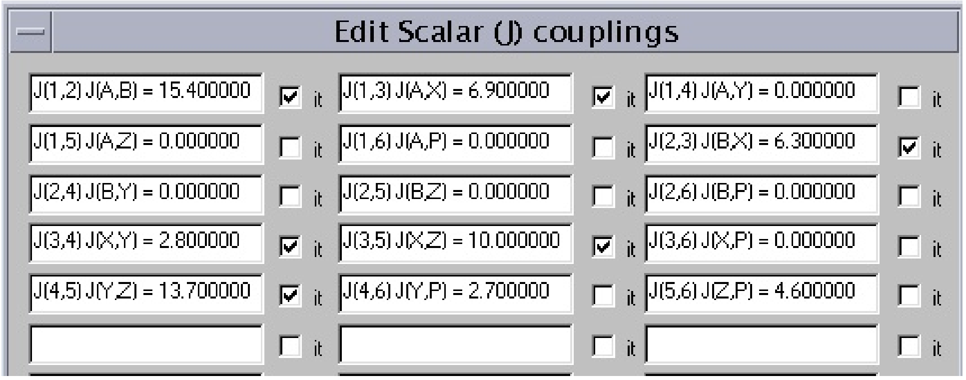
**18. Iteration.** Once all the desired peak assignments have been made, use Shifts and Js in the Simulation Window and put a tick mark in each of the fields that should be optimized by the iteration process (Figures 24 and 25).

k(1,2)= 0



| Group | spins | label | species | shift | Iterate |
|---|---|---|---|---|---|
| Group 1 | 1 | A | H | 1044 | ☑ |
| Group 2 | 1 | B | H | 977 | ☑ |
| Group 3 | 1 | X | H | 1749 | ☑ |
| Group 4 | 1 | Y | H | 794 | ☑ |
| Group 5 | 1 | Z | H | 621 | ☐ |
| Group 6 | 1 | P | H | 1575 | ☐ |
| Group 7 | | | | 0 | ☐ |
| Group 8 | | | | 0 | ☐ |
| Group 9 | | | | 0 | ☐ |
| Group 10 | | | | 0 | ☐ |

Figure 24: H(A), H(B), H(X) and H(Y) have been selected for chemical shift iteration

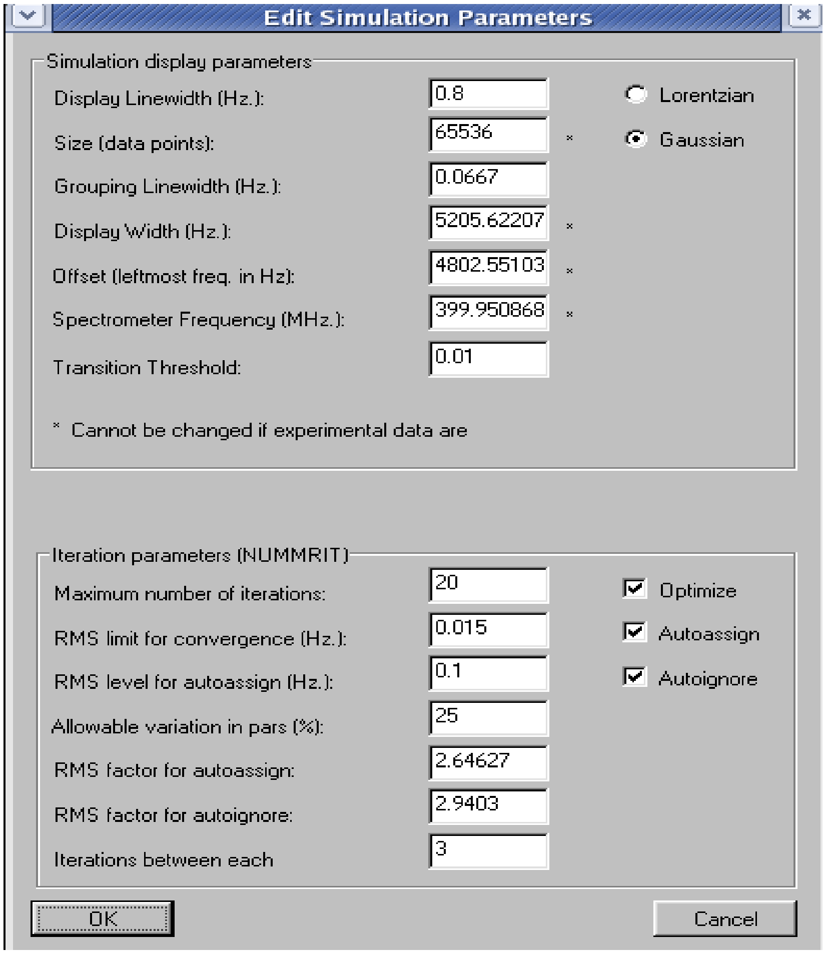


| | | | | | |
|---|---|---|---|---|---|
| J(1,2) J(A,B) = 15.400000 | ☑ it | J(1,3) J(A,X) = 6.900000 | ☑ it | J(1,4) J(A,Y) = 0.000000 | ☐ it |
| J(1,5) J(A,Z) = 0.000000 | ☐ it | J(1,6) J(A,P) = 0.000000 | ☐ it | J(2,3) J(B,X) = 6.300000 | ☑ it |
| J(2,4) J(B,Y) = 0.000000 | ☐ it | J(2,5) J(B,Z) = 0.000000 | ☐ it | J(2,6) J(B,P) = 0.000000 | ☐ it |
| J(3,4) J(X,Y) = 2.800000 | ☑ it | J(3,5) J(X,Z) = 10.000000 | ☑ it | J(3,6) J(X,P) = 0.000000 | ☐ it |
| J(4,5) J(Y,Z) = 13.700000 | ☑ it | J(4,6) J(Y,P) = 2.700000 | ☐ it | J(5,6) J(Z,P) = 4.600000 | ☐ it |
| | ☐ it | | ☐ it | | ☐ it |

Figure 25: Coupling constants selected for iteration

**18. Open the Edit Simulation Parameters window** (Figure 26) by clicking on Par and make sure **Optimize, Autoassign and Autoignore are all selected**. You can adjust the Display Linewidth (Hz), if desired, then click on OK and NUMMRIT to run the iteration.

If experienced enough with simulations and iterations, you can also change other parameters such as the number of iterations etc. **For a start it is best to leave the default values unchanged.**



Edit Simulation Parameters

Simulation display parameters

Display Linewidth (Hz.): 0.8

Size (data points): 65536 *

Grouping Linewidth (Hz.): 0.0667

Display Width (Hz.): 5205.62207 *

Offset (leftmost freq. in Hz): 4802.55103 *

Spectrometer Frequency (MHz.): 399.950868 *

Transition Threshold: 0.01

○ Lorentzian

● Gaussian

* Cannot be changed if experimental data are

Iteration parameters (NUMMRIT)

Maximum number of iterations: 20

RMS limit for convergence (Hz.): 0.015

RMS level for autoassign (Hz.): 0.1

Allowable variation in pars (%): 25

RMS factor for autoassign: 2.64627

RMS factor for autoignore: 2.9403

Iterations between each 3

☑ Optimize

☑ Autoassign

☑ Autoignore

Figure 26: Edit Simulation Parameters window prior to iteration

**19. The new simulated and iterated spectrum** displayed in Figure 27 should be a very close match to the experimental spectrum. Zoom in on spins of interest, check for mis-assignments and correct them, if necessary, by deleting incorrect line assignments and reassigning them correctly. Load the new parameters with *Spin System: Load Optimized Parameters*, then re-run the simulation with NUMMRIT. The rms deviation (displayed in green in the top left corner of the spectrum) should be less than 0.1 Hz. If not, repeat steps 16 to 18 with different coupling constants and/or different chemical shifts selected for iteration.

**To undo the last iteration, uncheck Optimize** in the Edit Simulation Parameters window displayed with Par (Figure 26), then re-run the simulation with NUMMRIT.

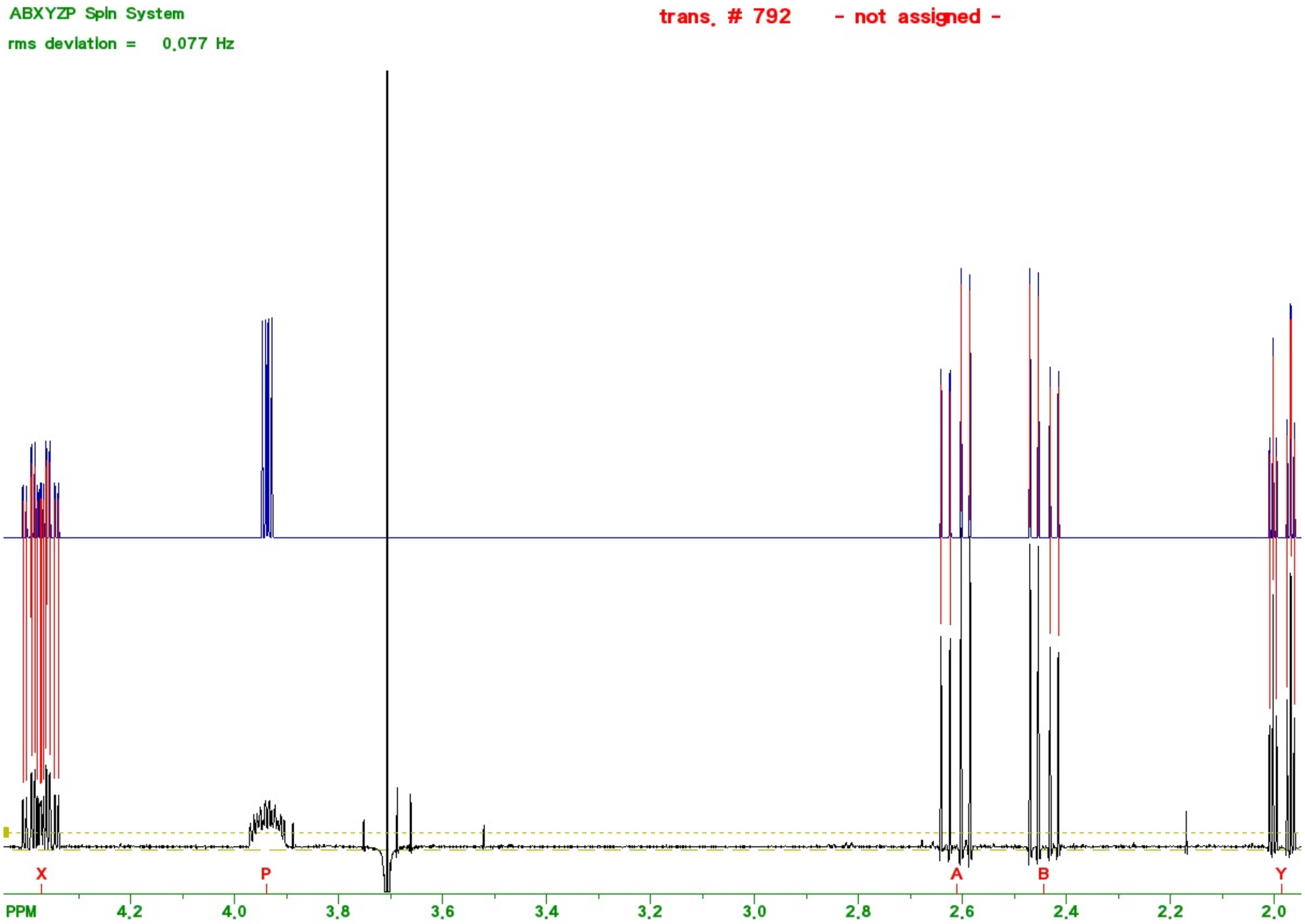


Figure 27: The simulated (top) and experimental (bottom) spectra after optimized parameters are loaded and NUMMRIT is re-run. The rms deviation is less than 0.1 Hz.

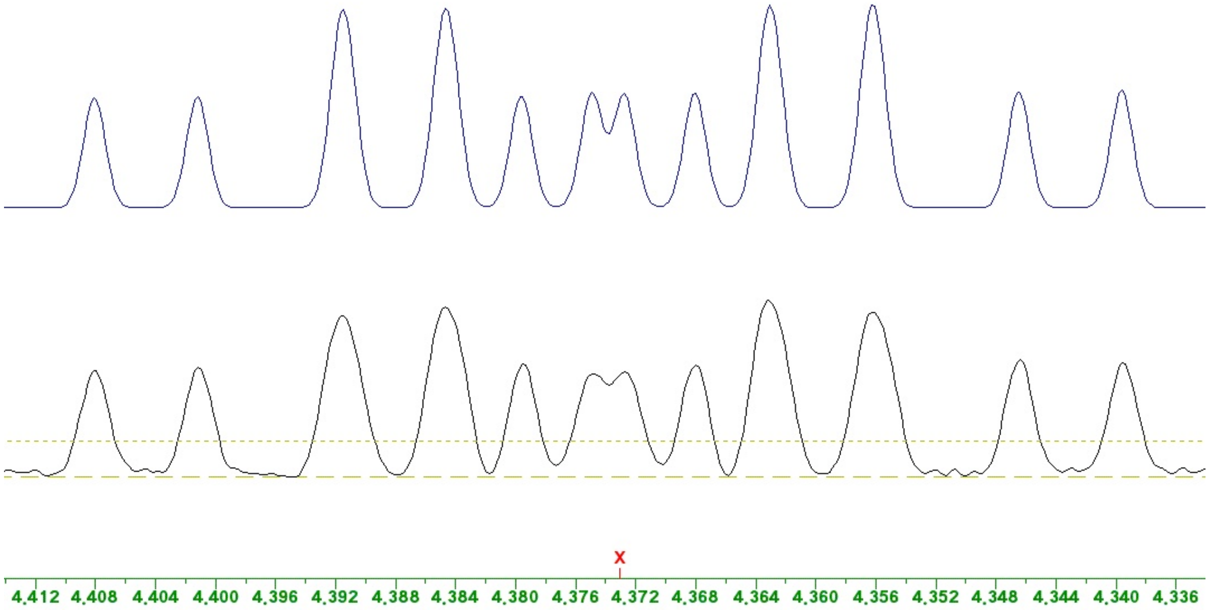


Figure 28: Expansion of the H(X) part, taken from in Figure 27. Simulated (top) with 0.8 Hz linewidth, experimental LB = -1, GB = 0.33 (bottom)

**20. The simulation and iteration output** can be viewed with *Simulation: List Simulation Output* which starts a Text Editor window. **The Chemical Shifts and Js in their respective panels** (Figures 19 and 20) **are not updated automatically in the iteration process.** Only a much abbreviated version of the very long document is shown here. The file is called sim_out.txt and can be opened independently from running SpinWorks. Search for term 'final iteration' to find what is really important. Shown here is the output with 3 decimal places as produced by the program. That does not mean they are all relevant!

**DO NOT PRINT THE ENTIRE DOCUMENT**

copy and paste only the essential information into a Text Editor then print

```
***  after final iteration:
***    current iteration count                    =              10
***    transitions now assigned                   =             128
***    current RMS                                =        0.077198

***    Final parameters after 10 iterations are:

v[1]          =         v[A]     1044.256 Hz        +/- 0.0138 Hz
v[2]          =         v[B]      977.795 Hz        +/- 0.0138 Hz
v[3]          =         v[X]     1749.254 Hz        +/- 0.0136 Hz
v[4]          =         v[Y]      793.656 Hz        +/- 0.0137 Hz
v[5]          =         v[Z]      621.000 Hz
v[6]          =         v[P]     1575.000 Hz

j[1][2]       =        j[A][B]     15.377 Hz        +/- 0.0193 Hz
j[1][3]       =        j[A][X]      6.768 Hz        +/- 0.0196 Hz
j[1][4]       =        j[A][Y]      0.000 Hz
j[1][5]       =        j[A][Z]      0.000 Hz
j[1][6]       =        j[A][P]      0.000 Hz
j[2][3]       =        j[B][X]      6.487 Hz        +/- 0.0196 Hz
j[2][4]       =        j[B][Y]      0.000 Hz
j[2][5]       =        j[B][Z]      0.000 Hz
j[2][6]       =        j[B][P]      0.000 Hz
j[3][4]       =        j[X][Y]      2.727 Hz        +/- 0.0193 Hz
j[3][5]       =        j[X][Z]     11.392 Hz        +/- 0.0273 Hz
j[3][6]       =        j[X][P]      0.000 Hz
j[4][5]       =        j[Y][Z]     13.638 Hz        +/- 0.0273 Hz
j[4][6]       =        j[Y][P]      2.700 Hz
j[5][6]       =        j[Z][P]      4.600 Hz
```

Note that values without a +/- error were not optimized by the iteration (see Figures 24 and 25).

**21. The title of the spectrum** can be edited using *Edit: Plot Title...* Use *File: Print Preview* and *File: Print* to print your experimental and simulated spectra on the same page.

**22. Data in filename.fid folder** (Figure 29) The results from an simulation/iteration can be retrieved most effectively later on if one is aware of what files are essential.

| | |
|---|---|
| **processed spectrum:** | 1D_image, 1D_par and 1D_real |
| **chemical shifts, scalar couplings:** | spin_system |
| **assigned transitions:** | asn_trans |

These files can be opened using

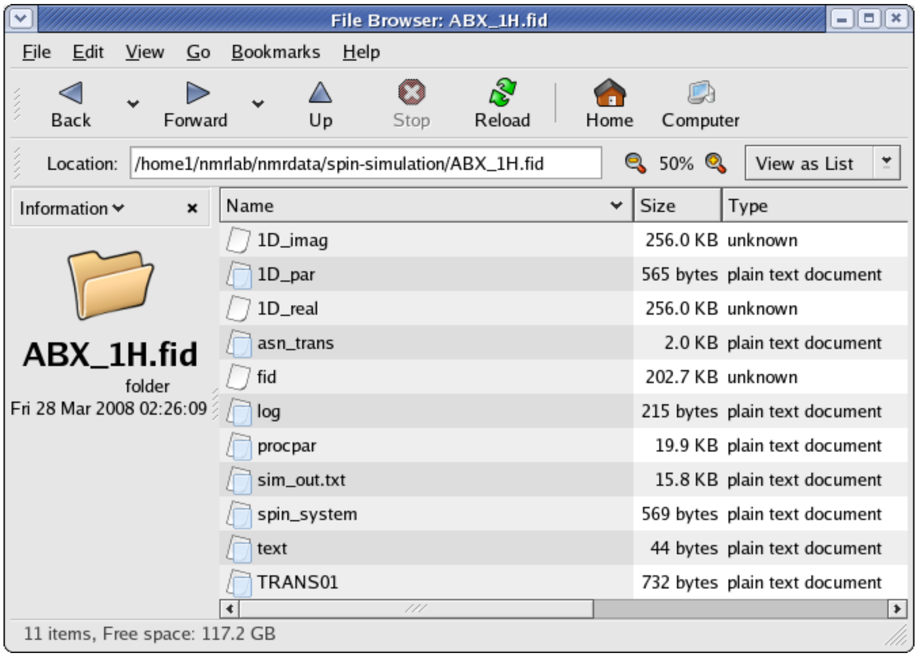
| | |
|---|---|
| 1) *File: Open...* | open *fid* |
| 2) *File: Load Processed Data* | retrieve data as processed in this program (phasing, window functions) |
| 3) *File: Read Spin System File...* | load the chemical shifts and coupling constants |

After NUMMRIT is run, proceed to iteration:

| | |
|---|---|
| 4) *File: Read Assigned Transitions....* | load assigned transitions and continue at step 18 |

**23. The entire collection of files** can be viewed in the File Browser.

**The files: *fid*, *log*, *procpar* and *text*** belong to the original VNMRJ *filename.fid* folder and **should <u>not</u> be deleted!**



Location: /home1/nmrlab/nmrdata/spin-simulation/ABX_1H.fid

| Name | Size | Type |
|---|---|---|
| 1D_imag | 256.0 KB | unknown |
| 1D_par | 565 bytes | plain text document |
| 1D_real | 256.0 KB | unknown |
| asn_trans | 2.0 KB | plain text document |
| fid | 202.7 KB | unknown |
| log | 215 bytes | plain text document |
| procpar | 19.9 KB | plain text document |
| sim_out.txt | 15.8 KB | plain text document |
| spin_system | 569 bytes | plain text document |
| text | 44 bytes | plain text document |
| TRANS01 | 732 bytes | plain text document |

<u>Figure 29</u>: Contents of the *filename.fid* folder

For more information refer to the electronic manual *Help: View Manual(pdf)*. Spin simulations are discussed on pages 38 - 41 and 67 - 70.