SpinWorks Installation Guide for Windows

SpinWorks is a free program developed by Kirk Marat. It can process 1D and 2D NMR data, perform spectral simulations to determine chemical shifts and J-couplings on second-order spectra, as well as analyze dynamic behaviors using DNMR3 or Mexico. This installation guide is based on Windows 7 64 bit OS but should work on other Windows versions. There is a Java version available which works for MacOS and Linux (please read the READMEandFAQ file on the SpinWorks web site for details).

- Download SpinWorks 4.2.8 (SpinWorks_4.2.8.zip) or a newer version from the link at https://science.umanitoba.ca/chemistry/davinci/SpinWorks/

- Unzip and run setup. Use the default location and confirm that the program installed correctly if asked. You can then delete installation programs.

- Run SpinWorks and agree to create c:\Temp if asked.

To test DNMR3 and familiarize yourself with its operation set up and run an AB<>BA mutual exchange simulation:

- Set Simulation -> Simulation Mode to DNMR3/Mexico

- Open Spin System -> Edit Chemical Shifts...

  Set Group 1 fields to: 1 a H 1/2 500

  and Group 2 fields to: 1 b H 1/2 550

NOTE: You must use Hz for the shift option, ppm works for NUMMRIT but does not work for DNMR3. If you use ppm to enter shifts, you need to click on Hz to convert shifts to Hz before run DNMR3 simulation.

- Open Spin System -> Edit Scalar (J) Couplings...

  Set the one listed value to J(1,2)

- Open Spin System -> Edit Simulation Options and DNMR Parameters

  Set RC(1,2) to 5 (this is confusingly k(1,2) in other parts of the program)

  Set the first 2 fields of Permutation Vector 2 to: 2 1

  Mutual Exchange should be checked, no need to set Population of Sites for mutual exchange.

- To run DNMR3 simulations

Click Simulation -> Run DNMR3 Simulation (or, click on Simulate button at far lower right then click on DNMR3 in popup window).

- After confirming that you see a simulated AB pattern, change the rate constant from 5 to 20 and observe that the lines broaden. Then try 50, 100, 500 and 1000 to observe coalescence into a singlet.

This value is RC(1,2) in Spin System -> Edit Simulation Options and DNMR Parameters, OR k(1,2) in the Simulate popup window.