R2SR for Windows

K.Worvill
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Abstract

This program calculates the NMR spectrum of a two proton system using density matrix methods. Relaxation is formulated using the Redfield theory and covers the following types:

Random Field (Field at nucleus A , correlation and asymmetry)
Spin Rotation (as above with different parameter interpretation)
Dipolar coupling modulation
Scalar coupling to a rapidly relaxing quadrupolar nucleus

Also AB to BA chemical exchange

The author hopes that it will be useful as a teaching aid for basic NMR. It allows rapid "what if" calculations so that students can appreciate the effects of changing chemical shift, coupling constant, relaxation and exchange rates and RF power in the simplest A2,AX,AB cases.

It should run happily on most Students Windows PCs/Laptops and can be distributed freely.

The Density Matrix selection tab allows for more advanced “experiments” such as tracking of the level populations in the spin system and observation of the off diagonal elements contributing to the normal absorption or dispersion modes.

Originally developed in FORTRAN on cards to run on an ICL 1905E mainframe in 1972 the reference to the original work is:

Journal of Magnetic Resonance 9,394-410 (1973) R.K.Harris & K.M.Worvill

Some other details are available from the menu items Help/About and Help/Help .

Installation

To install just copy the image file to the directory of your choice. The program has been tested on Windows 95/98/NT/2000 and XP(Pro & Home) .

Usage

Data is preset for a simple AB spectrum so the first test is just to click on calculate
- wait for the pop up box saying "calculation finished" then plot for a screen display of the spectrum. The print function has been tested with several different inkjet and laser printers at UEA and should format the results for your default PC printer.

This version includes a standard print dialogue which will allow output in landscape format as well as allowing scaling depending on the available printer drivers installed.

In this version two diagnostic files (NMR.csv & NMR.txt) are output to C:\TEMP on request (see the printing tab option) so if you switch this option on you'll need

to create this directory if it does not exist. The .csv file created is the calculated spectrum and can be used as input to e.g. Excel . The other file lists the input parameters and the matrix which is the set of simultaneous equations of the density matrix to be solved at the first frequency increment only. These files are overwritten at each calculation.

The plotting vertical scale is calculated to be approx. 125% of the maximum peak height but a fixed value (e.g. to compare sequences of spectra) can be set by:

1. selecting the density matrix tick box on tab H1 AND
2. setting the required value in the normalisation box on tab H0 to > 1.0

H0 Tab

The parameters on the H0 tab are for general spectrum frequency range and scaling as well as the proper high resolution Hamiltonian H0 parameters of chemical shift and coupling constant. The preset values just give you a typical AB spectrum as a starting point for trial calculations.

H1 Tab

The parameters on the H1 tab are:

RF Field:
the strength in nano Tesla of the radio frequency magnetic field
a typical range would be 0.1 to 100.0 from unsaturated to saturated spectra.

Dispersion mode %:
for allowing a small amount of the dispersion mode as a phase error
or for switching to 100% dispersion mode as an alternative observation.

Tick box:
If the tick box to select mode by density matrix is set then the “observed” magnetisation is controlled by the elements selected on that tab and the % value here is ignored.

Spectrometer window:
This is just a factor to allow for instrumental broadening of the observed lines in the spectrum.

HR Tab

The parameters on the HR tab represent the relaxation as described by Redfield theory.

Random Field: colour coded green

Field at nucleus A + Asymmetry + Correlation:

> a measure of the random field strength at nucleus A with the field at B being determined by any asymmetry and correlation. Further details on these parameters can be found in the reference given above.

Dipolar Field: colour coded red

> A measure of the fluctuating dipolar coupling field causing relaxation .

Exchange Mean Life: colour coded yellow

> The mean lifetime in seconds of a nucleus at any one site in AB to BA chemical exchange.

Scalar 2 relaxation: colour coded blue

> Scalar coupling to a rapidly relaxing quadrupolar nucleus as a mechanism of relaxation is defined by two parameters. A field strength and a scalar coupling ratio .

The field strength parameters in all the above cases have units rad/sec when squared.

Density Matrix Tab

The tick boxes on the density matrix tab form control which elements contribute to the calculated spectrum (i.e. the linear combination of unknowns to solve for in the set of simultaneous equations)

Elements in red (p11,p22,p33,p44) represent the energy level populations of the spin system. Other elements (off diagonal) represent the transitions of the spin system of each particular quantum nature. So we have the single quantum transitions represented by p12,p13,p24,p34 and the zero quantum p23 and double quantum p14 elements. The diagonal elements (populations) are real and the off diagonal (transitions) are complex. In the calculation the absorption mode spectrum is given by the sum of imaginary parts of the single quantum transition elements and the dispersion mode by the sum of real parts of those elements.

The equations can be solved for any particular combination (.e.g. to “observe” one of the level populations changes) by ticking just that box and deselecting all others.

Printing Options Tab

These should be self explanatory. Output of the spectrum to a CSV file is an option if you want to use external plotting or analysis programs such as Excel.

Kevin Worvill (k.worvill@uea.ac.uk) (k.worvill@gmail since 2009 retirement !)
IT & Computing Service
University of East Anglia
Norwich
UK