This programs simulates powder or single-crystal EPR spectra for spin states with 0<**S**<16 using full diagonalisation of the spin Hamiltonian matrix.

Note: Spin.exe requires a processor supporting Advanced Vector Extensions 2. SpinSSE2.exe uses the older SSE2 processor instruction set, suitable for older processors.

Installation:

Save the exe file in a directory of your choice. No installation is required.

If the program refuses to start or to work, download a Microsoft file from

https://aka.ms/vs/17/release/vc\_redist.x64.exe

and install it on your computer

Usage:

Start the program and click File. Select 'Load Bruker spectrum' or other format, navigate to the directory where spectra are stored and load one you wish. It will be displayed automatically. The program looks for the \*.spc files and for the new-style Bruker \*.dta files.

To open a file created at the Magnetlab use 'Load Van Tol's file'. In such case two spectra from two channels of the phase-sensitive detector are loaded with the red one being considered by the program as ‘simulated’ and the blue one as ‘experimental’. If the red plot is better, use ‘File/transfer red to blue’ before simulation.

Note: the two traces are normalized independently and shown with the same amplitude. To see the real intensity ratio use ‘set common scale’ in File menu.

To convert a spectrum to text file select 'Save red spectrum as text' or 'Save blue spectrum as text' in File menu. Data will be saved under the name you give with the extension .txt appended automatically

You may edit your text file to add at the beginning all or some of the lines

freq=whatever

temp=whatever

hister=whatever

then, if you load such a file with this program, frequency, temperature and hysteresis (for the Magnetlab spectra) will be read.

Dragging the mouse with the left or right button pressed shows the cursors. Cursors positions may be also controlled by keys F1 through F4. Spectrum may be expanded between cursors by using Expand. To reset an expanded and/or magnified spectrum click Reset. Numbers at the bottom of the window show field values under the cursors and the difference between them.

The intensity and the point number in the ‘active’ spectrum that is currently under the left cursor is shown in the right upper corner. The ‘active’ spectrum (simulated – red, experimental – blue) is toggled by pressing SPACE. In the left bottom corner the g value under the left cursor is shown.

Arrows (beneath Delete, End, Page down) change the vertical position and the intensity of a spectrum.

The window in that the program works may be resized.

It is possible to print spectra directly from the program - select File/Plot on printer. The picture currently on screen (i.e. expanded or magnified) will be printed on a printer of your choice. The printout size depends on the current size of the program window.

Instrument settings and comment will be also printed out (only for Bruker spectra).

Bruker instruments save each spectrum as a pair of files: a spectrum let say 'tempo' will be saved as a text file tempo.par that contains experimental parameters and a binary file tempo.spc that contais the intensity. New Bruker instruments use files \*.dsc and \*.dta in a very different format.

The experimental parameters may be accessed by File/Show experimental parameters

Parameters like frequency and field range are loaded from the Bruker parameter file and from the Van Tol's files. For the spectra loaded as text files the magnetic field range is determined automatically and the frequency will be read if the line freq=whatever is present.

Simulation:

Go to Parameters and set values. The zero-field splitting parameters D, E and B4i are entered in Gauss. To convert between Gauss and cm-1 use

(D, E or B in cm-1) = (D, E or B in Gauss) **·** 4.6686**·**10-5 **·** 2.0023

Spin values like 5/2 may be entered as 5/2 or 2.5

The default parameters are gxyz=2, D=38200 Gauss, E=0. These are parameters for frozen oxygen, which is very often seen below 30 K.

Set the theta and fi steps for simulation – the steps should not be divisors of 90 to avoid calculating equivalent orientations like 90+alpha and 90-alpha.

Go to Linewidth and set values.

Click Simulation

After the spectrum has been simulated you may change Linewidth without resimulating the spectrum, provided that isotropic linewidth was used