Tutorial on Simulation Program XSophe version 1.1.4

- Open Bruker XSophe

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- Open XeprView



- Load experimental spectrum: File – load Navigate to e.g. /Server/workshop12/x/sol/ to simulate Cu(DTP)2





- Go back to the **Bruker XSophe** window
- Select CW- Powder-Matrix Digitalization



- **Experimental parameters** window comes up
- Press cancel



- Open the Spinsystem selection window



- Spinsystem selection



- Delete V
- Add centre

- Select atom from periodic table (Cu for Cu(dtp))



- Select natural isotopes



- Press OK

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- Add nucleus
- Select from periodic table (P for Cu(dtp)₂)
- Select **natural isotopes** and nr of nuclei (2 for Cu(dtp)2)

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- Open the **Spin Hamiltonian Parameters** window

- Spin Hamiltonian interaction

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- Select Cu

- Select βBgS for g values for anisotropic spectra

- Select SAI for A values for anisotropic spectra



- Select values from the Spin Hamiltonian Settings windows
- Change units in Gauss
- Select Cu



- Select β BgS to assign g values



- Select ${\bf SAI}$ for hyperfine values (Cu and P for Cu(dtp))



- Open the Instrument parameters window

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- Instrument parameters



- Open the Lineshape parameter window



- Lineshape parameters

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- Change lineshape units
- Open line parameter vectors

- Angular dependence of g



- Open the Sophe Grid Parameters window



- Sophe grid

- Increase the number of partitions if the simulated spectrum has too many spikes.



- Run simulation



- Switch to the **Xepr View** window when the simulation is completed



- Select your experimental spectrum as secondary spectrum



- Adjust the scale of the primary and secondary spectrum

- Go to Proprieties Relative ordinate scale
- Select Primary set
- Select Secondary set

