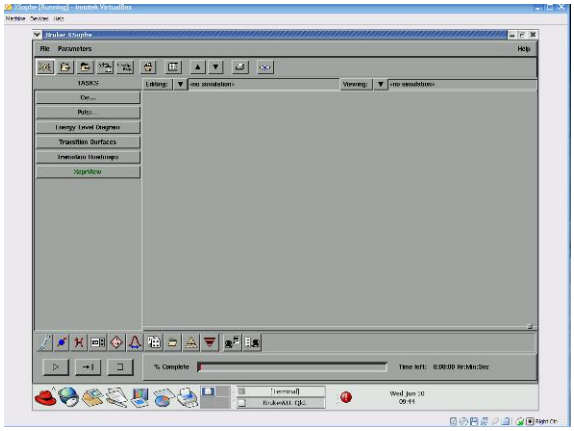
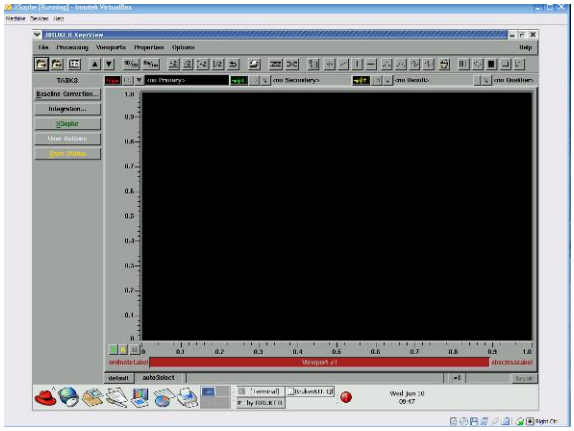
Tutorial on Simulation Program XSophe version 1.1.4

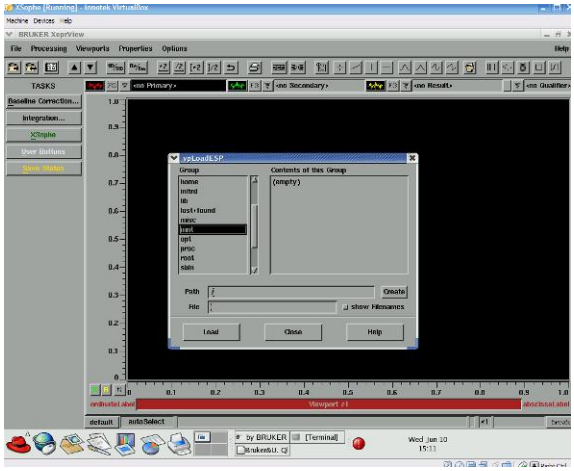
- Open **Bruker XSophe**

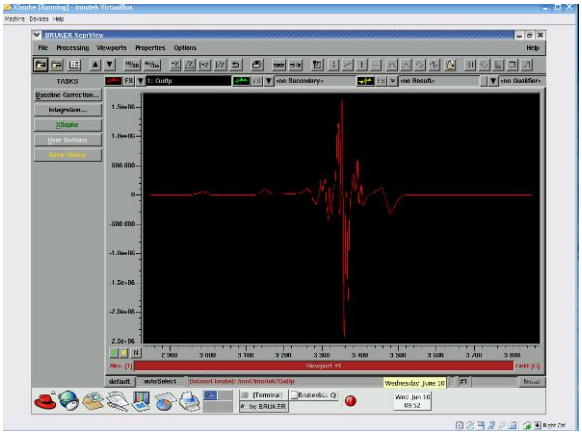


- Open **XeprView**



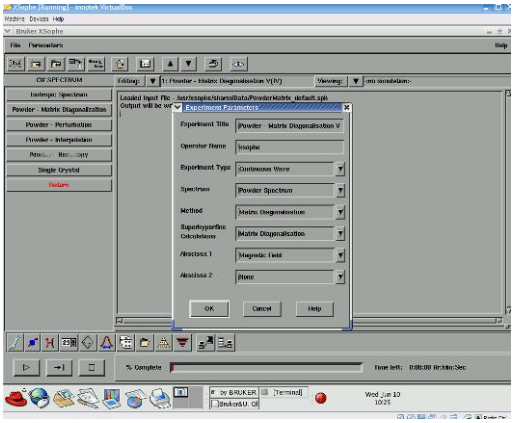
- Load experimental spectrum: File – load Navigate to e.g. /Server/workshop12/x/sol/ to simulate Cu(DTP)2



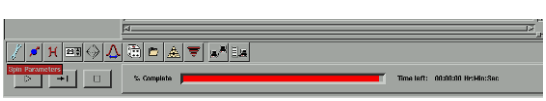


- Go back to the **Bruker XSophe** window
- Select **CW- Powder-Matrix Digitalization**

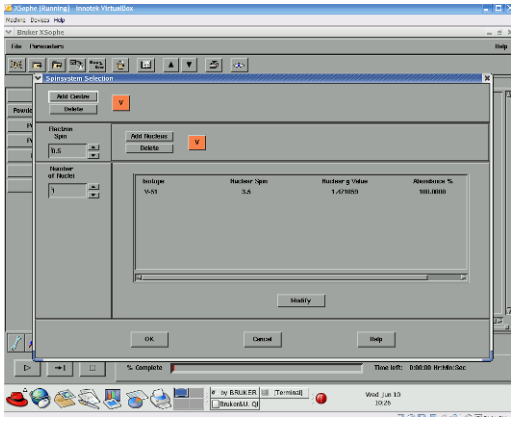
- **Experimental parameters** window comes up
- Press **cancel**



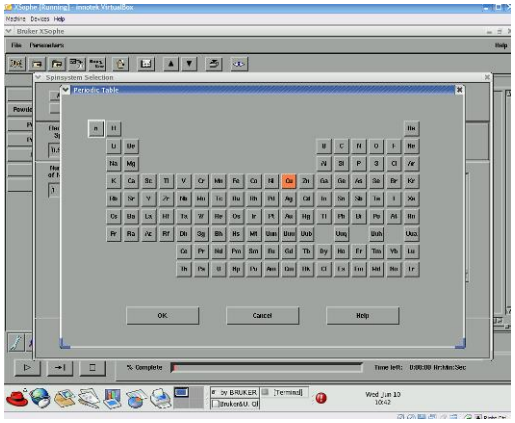
- Open the **Spinsystem selection** window



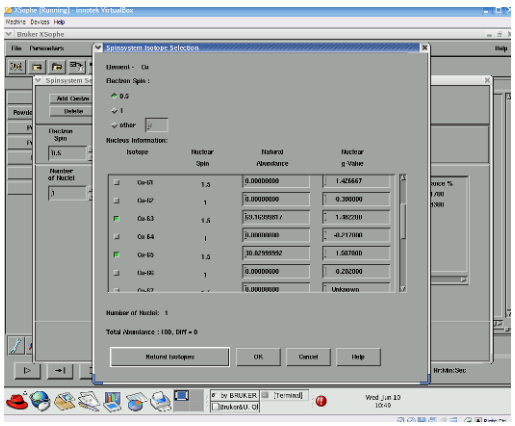
- Spinsystem selection



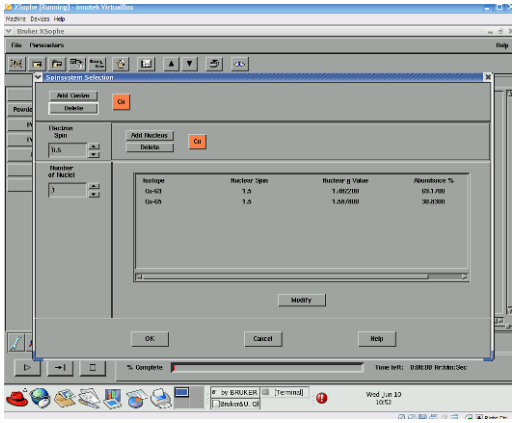
- Delete **V**
- **Add centre**
- Select atom from periodic table (Cu for Cu(dtp))



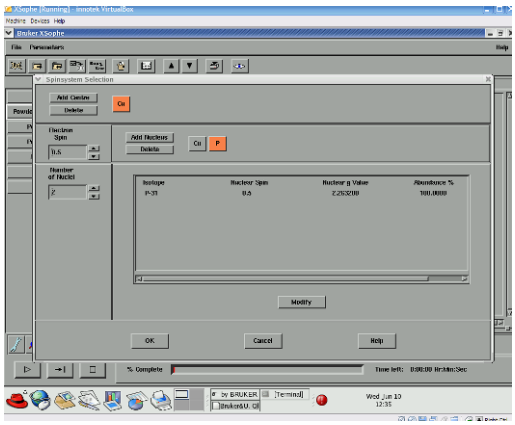
- Select **natural isotopes**



- Press **OK**

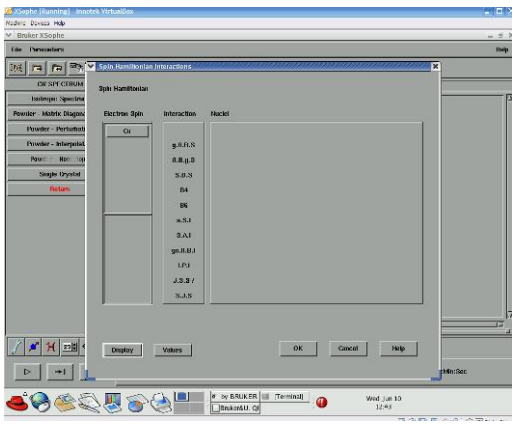


- **Add nucleus**
- Select from periodic table (P for $Cu(dtp)_2$)
- Select **natural isotopes** and nr of nuclei (2 for Cu(dtp)2)



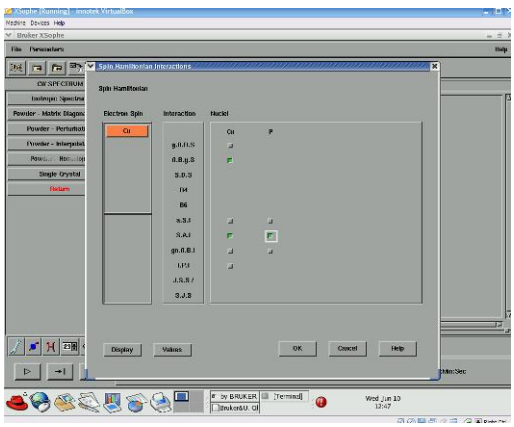
- Open the **Spin Hamiltonian Parameters** window

- Spin Hamiltonian interaction

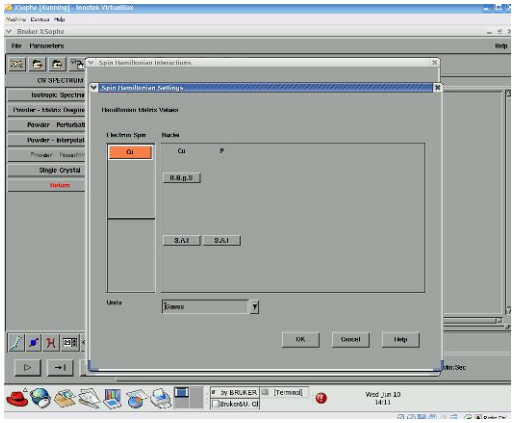


- Select **Cu**
- Select βBgS for g values for anisotropic spectra

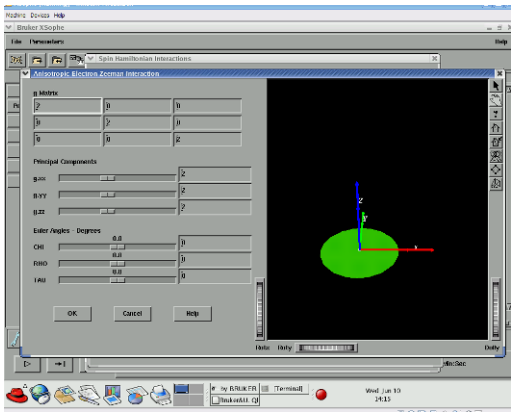
- Select SAI for A values for anisotropic spectra



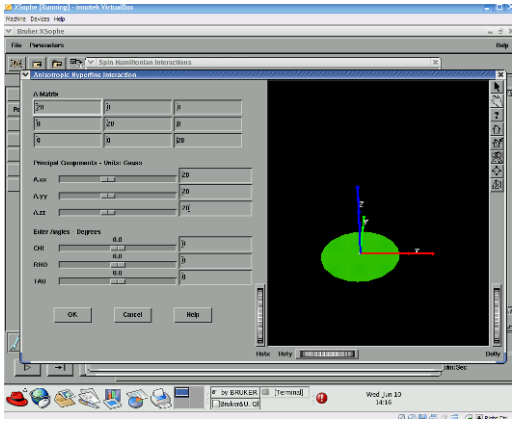
- Select **values** from the **Spin Hamiltonian Settings** windows
- Change units in Gauss
- Select **Cu**



- Select **βBgS** to assign g values

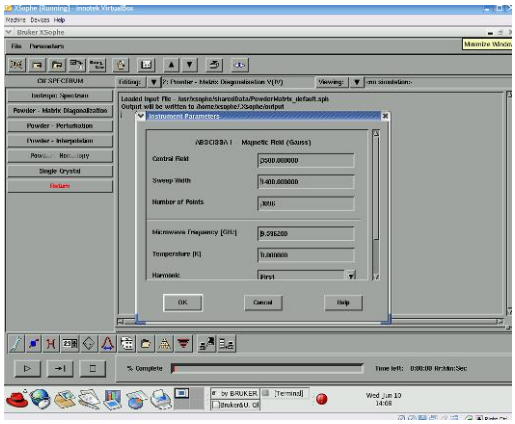


- Select **SAI** for hyperfine values (Cu and P for Cu(dtp))



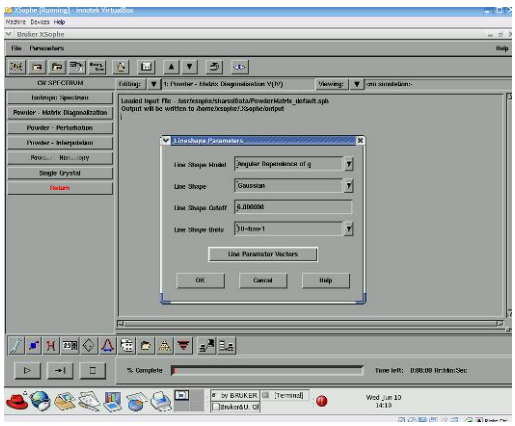
- Open the **Instrument parameters** window

- Instrument parameters



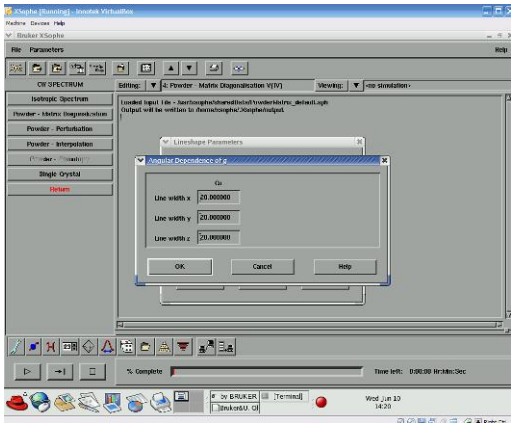
- Open the **Lineshape parameter** window

- Lineshape parameters



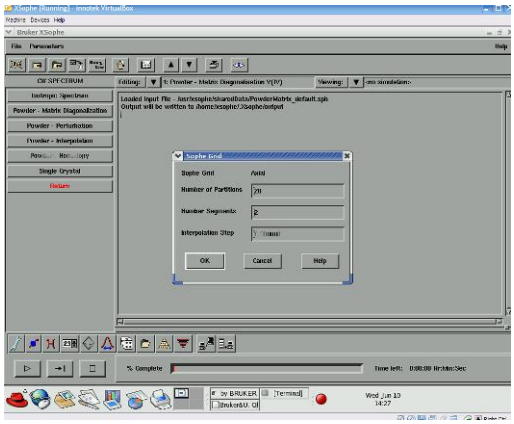
- Change lineshape units
- Open **line parameter vectors**

- Angular dependence of g

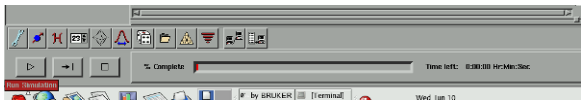


- Open the **Sophe Grid Parameters** window

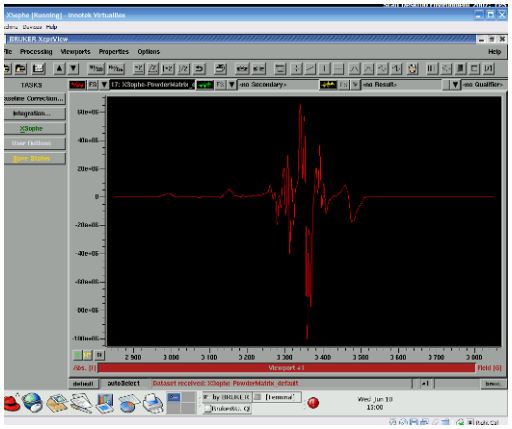
- Sophe grid
- Increase the number of partitions if the simulated spectrum has too many spikes.



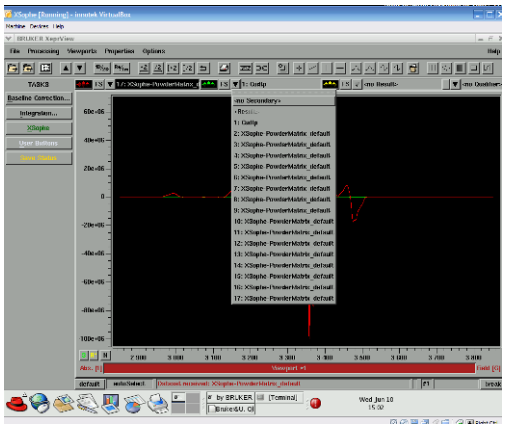
- Run simulation



- 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