For the Fe Crystal, I redid the fits with the previous boundary conditions (Z Z X) and switched datax and dataz, to keep with Michelle’s orientation.



From the fits, I got a 7Li shift tensor:

Diagonalizing this tensor, I got eigenvalues:

Leading to a pseudocontact tensor:

Which is traceless. I then did the 31P fits according to the same criteria as in 7Li



From the fits, I got a 31P shift tensor:

The lattice parameters (in angstroms) were averaged between materials project and Michelle’s data:

The Fe positions I used were:

Running the ChiTensor\_build code, I got a susceptibility tensor of:

The phosphorus site used was:

Using Chi to separate out the hyperfine term from 31P data:

The trace of pc is not 0, but pretty close, relatively speaking (92ppm, 92ppm/3390ppm = 2.7%). The eigenvectors and eigenvalues of the hyperfine term are

The vectors are plotted in VESTA.

For the Mn Crystal, I redid the fits with new boundary conditions (Y Y X) and switched datax and dataz, to keep with Michelle’s orientation.



From the fits, I got a 7Li shift tensor:

Diagonalizing this tensor, I got eigenvalues:

Leading to a pseudocontact tensor:

Which is traceless. I then did the 31P fits according to the same criteria as in 7Li



From the fits, I got a 31P shift tensor:

The lattice parameters (in angstroms) were averaged between materials project and Michelle’s data:

The Mn positions I used were:

Running the ChiTensor\_build code, I got a susceptibility tensor of:

The phosphorus site used was:

Using Chi to separate out the hyperfine term from 31P data:

The trace of pc is not 0, a little high (52ppm, 52ppm/8533ppm = .06%). The eigenvectors and eigenvalues of the hyperfine term are

The vectors are plotted in VESTA.