

About SIMPOW6

Program SIMPOW6 generates a powder spectrum for a spin 1/2 system with two nuclei (calculated to second order) and four super-hyperfine spins for which there can be more than one equivalent nucleus. All hyperfine matrices can be rotated in any direction. The three Euler angles are read in the order alpha, beta, and gamma. The Euler angles conform to the convention of M.E. Rose, Elementary Theory of Angular Momentum (New York: Dover, 1995). Spectra are integrated using a two dimensional 4-point Gauss-point integration.

The program includes strain in the g tensor and the two primary hyperfine tensors calculated to first order.

See the file "simpow6.txt" for further instructions.

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For bug reports, inquiries, additional examples and suggestions, contact the developer at e-mail: mjnilges@uiuc.edu.

The most recent version of the software can be found at the web site: <http://ierc.scs.uiuc.edu/~nilges/software.html>.