

EWVoigt and EWVoigtN: Inhomogeneous line shape simulation and fitting programs

This package contains two programs, EWVOIGT and EWVOIGTN. EWVOIGTN is an extended version of EWVOIGT and is suitable for least squares simulations of two overlapping spin label nitroxide spectra. Some of EWVOIGTN extended features include:

- Second order perturbation approximation for calculating nitroxide spectra;
- Simulation of two nitroxides with different inhomogeneous line width parameters, for example, different width of the Gaussian envelope;
- Explicit accounting for ^{13}C satellite lines in the simulation;
- Extended equality constraints for fitting parameters.

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