Boltzmann-statistics analysis of solid state NMR experiments

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A data analysis approach employing Boltzmann-statistics variation of Maximum Entropy is introduced to determine distances using solid-state NMR data from rotational-echo double-resonance (REDOR) experiments [Gehman *et al.*, 2007]. Using structural studies of amyloid-beta peptide from Alzheimer's disease, we demonstrate that this approach can provide the means to determine an unconstrained population distribution of fractional contributions for some data sets governed by amenable complex analytic forms. These examples illustrate the general utility of the Boltzmann statistics approach, as the fitting of nonlinear physical data is often a hazardous affair. As in our examples, frequently an analytical model governing a measured process is firmly grounded in theory, and the measured signal is a sum of contributions from one or more fractional components. One needs to fix the number of components used in a fit, thereby constraining the conceivable population distribution to relatively few discrete contributions. Often there is not enough information to be unequivocal about the number of components to use; too few and the fit will be poor, too many improves the fit but with large error estimates that can render the characteristic parameters for each component meaningless. Imperfect data blurs the boundary between too few and too many. The Boltzmann-statistics approach thereby extracts a relatively model-free distribution of internuclear distances present in a sample measured by REDOR, and allows NMR time to be spent obtaining better signal-to-noise on fewer data points.

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