



Total line shape analysis of high-resolution NMR spectra

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Abstract

Analysis of high-resolution NMR spectra consist in determining the parameters of the spin system that provide the best correspondence between the theoretical and experimental spectra. This review is devoted to modern approaches to the total line shape analysis of high-resolution NMR spectra; discussion of difficulties and pitfalls associated with both the fundamental features of high-resolution NMR spectra and the optimization of parameters values. The question of the accuracy of determining values of spin systems parameters is discussed. Practical examples of the spectra analysis are considered, as well as recommendations for obtaining experimental NMR spectra of high quality.

Keywords: Total line shape analysis, Spin-spin coupling constants, Multiplet structure elucidation, Broadening approach, Simulated annealing

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