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Second-order quadrupolar line shapes under molecular dynamics: an additional transition in the extremely fast regime

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ABSTRACT

NMR spectroscopy is a powerful tool for probing molecular dynamics. For the classic case of two-site exchange, NMR spectra go through the transition from exchange broadening through coalescence and then motional narrowing as the exchange rate increases passing through the difference between the resonance frequencies of the two sites. For central-transition spectra of half-integer quadrupolar nuclei in solids, line shape change due to molecular dynamics occurs in two stages. The first stage occurs when the exchange rate is comparable to the second-order quadrupolar interaction. The second spectral transition comes at a faster exchange rate which approaches the Larmor frequency and generally reduces the isotropic quadrupolar shift. Such a two-stage transition phenomenon is unique to half-integer quadrupolar nuclei. A quantum mechanical formalism in full Liouville space is presented to explain the physical origin of the two-stage phenomenon and for use in spectral simulations. Variable-temperature \textsuperscript{17}O NMR of solid NaNO\textsubscript{3} in which the NO\textsubscript{3}\textsuperscript{−} ion undergoes 3-fold jumps confirms the two-stage transition process. The spectra of NaNO\textsubscript{3} acquired in the temperature range of 173 – 413 K agree well with simulations using the quantum mechanical formalism. The rate constants for the 3-fold NO\textsubscript{3}\textsuperscript{−} ion jumps span eight orders of magnitude (10\textsuperscript{2} – 10\textsuperscript{10} s\textsuperscript{−1}) covering both transitions of the dynamic \textsuperscript{17}O line shape.

1. Introduction

NMR spectroscopy is a powerful tool not only for structure elucidation but also for probing molecular dynamics. Molecular motion can be probed by monitoring spectral line shapes and a variety of relaxation measurements which cover a wide range of motional time constants from seconds down to nanoseconds. The classic case that revealed the effects of molecular dynamics on NMR spectral line shapes in the early days of NMR [1, 2] is the exchange between
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