Title:	A theoretical perspective on the accuracy of rotational resonance (R 2)-based distance measurements in solid-state NMR
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Abstract:	The application of solid-state NMR methodology for bio-molecular structure determination requires the measurement of constraints in the form of 13C- 13C and 13C- 15N distances, torsion angles and, in some cases, correlation of the anisotropic interactions. Since the availability of structurally important constraints in the solid state is limited due to lack of sufficient spectral resolution, the accuracy of the measured constraints become vital in studies relating the three-dimensional structure of proteins to its biological functions. Consequently, the theoretical methods employed to quantify the experimental data become important. To accentuate this aspect, we re-examine analytical two-spin models currently employed in the estimation of 13C- 13C distances based on the rotational resonance (R 2) phenomenon. Although the error bars for the estimated distances tend to be in the range 0.5-1.0 Å, R 2 experiments are routinely employed in a variety of systems ranging from simple peptides to more complex amyloidogenic proteins. In this article we address this aspect by highlighting the systematic errors introduced by analytical models employing phenomenological damping terms to describe multi-spin effects. Specifically, the spin dynamics in R 2 experiments is described using Floquet theory employing two different operator formalisms. The systematic errors introduced by the phenomenological damping terms and their limitations are elucidated in two analytical models and analysed by comparing the results with rigorous numerical simulations.
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