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Title:	Operator-based analytic theory of decoherence in NMR
Authors:	Pandey, Manoj Kumar (/jspui/browse?type=author&value=Pandey%2C+Manoj+Kumar) Ramachandran, Ramesh (/jspui/browse?type=author&value=Ramachandran%2C+Ramesh)
Keywords:	Analytic models Analytic theory Analytical theory
Issue Date:	2011
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Citation:	Molecular Physics, 109 (12), pp. 1545-1565
Abstract:	The operator-based analytic description of polarization transfer in NMR spectroscopy is often fraught with difficulty due to (a) the dimension and (b) the non-commuting nature of the spin Hamiltonians. In this article, an analytic model is presented to elucidate the mechanism of polarization transfer between dilute spins I 1 and I 2 coupled to a reservoir of abundant S-spins (i.e. [I 1 - I 2]S N) in the solid state. Specifically, the factors responsible for the decoherence observed in double cross-polarization (DCP) experiments are outlined in terms of operators via effective Floquet Hamiltonians. The interplay between the various anisotropic interactions is thoroughly investigated by comparing the simulations from the analytic theory with exact numerical methods. The analytical theory presents a framework for incorporating multi-spin effects within a reduced subspace spanned by spinsI 1 and I 2. The simulation results from the analytic model comprising eight spins are in excellent agreement with the numerical methods and present an attractive tool for understanding the phenomenon of decoherence in NM
URI:	http://www.tandfonline.com/doi/abs/10.1080/00268976.2011.572088 (http://www.tandfonline.com/doi/abs/10.1080/00268976.2011.572088)
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