Title:	Unraveling multi-spin effects in rotational resonance nuclear magnetic resonance using effective reduced density matrix theory
Authors:	Sivaranjan, U. (/jspui/browse?type=author&value=Sivaranjan%2C+U.) Ramachandran, Ramesh (/jspui/browse?type=author&value=Ramachandran%2C+Ramesh)
Keywords:	Nuclear magnetic resonance Rotational resonance Matrix theory Unraveling multi-spin effects
Issue Date:	2014
Publisher:	American Institute of Physics Inc.
Citation:	Journal of Chemical Physics, 140(5)
Abstract:	A quantum-mechanical model integrating the concepts of reduced density matrix and effective Hamiltonians is proposed to explain the multi-spin effects observed in rotational resonance (R2) nuclear magnetic resonance (NMR) experiments. Employing this approach, the spin system of interest is described in a reduced subspace inclusive of its coupling to the surroundings. Through suitable model systems, the utility of our theory is demonstrated and verified with simulations emerging from both analytic and numerical methods. The analytic results presented in this article provide an accurate description/interpretation of R2 experimental results and could serve as a test-bed for distinguishing coherent/incoherent effects in solid-state NMR.
URI:	https://aip.scitation.org/doi/10.1063/1.4863212 (https://aip.scitation.org/doi/10.1063/1.4863212) http://hdl.handle.net/123456789/3058 (http://hdl.handle.net/123456789/3058)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
need to add pdf....odt (/jspui/bitstream/123456789/3058/1/need%20to%20add%20pdf....odt)		8.12 kB	OpenDocument Text	View/Open (/jspui/bitstream/1234

Show full item record (/jspui/handle/123456789/3058?mode=full)
(/jspui/handle/123456789/3058/statistics)