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Title: Multi-spin Analyses of Rotational Resonance (R2) NMR Using Rabi Oscillations and Reduced Density Matrix Theory

Authors: Uppala, Siva Ranjan (/jspui/browse?type=author&value=Uppala%2C+Siva+Ranjan)

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Abstract: An analytic framework integrating the concept of effective Hamiltonians and Reduced density matrix theory is proposed for describing polarization transfer in solid-state NMR. Specifically, the magnetization exchange between ^{13}C nuclei in Rotational Resonance (R2) experiments is described in the presence of coupling to protons reservoir. The factors responsible for depolarization in R2 experiments and the role of heteronuclear decoupling schemes during the dipolar mixing are thoroughly investigated. Additionally, implementation of fractional R2 experiments are discussed. The simulations emerging from the proposed analytic model are well substantiated through simulations emerging from exact numerical methods. The framework presented in the thesis is well-suited for describing both homonuclear and heteronuclear experiments in solid-state NMR.


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