

2D Off-Resonance Nutation NQR Spectroscopy of Spin 3/2 Nuclei*

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The effects of off-resonance irradiation in nutation NQR experiments are demonstrated both experimentally and theoretically. The theoretical description of the off-resonance effects in 2D nutation NQR spectroscopy is given, and general exact formulas for the asymmetry parameter are obtained. It is shown that the outcome of the off-resonance nutation experiments depends on the data acquisition procedure, leading to one- or three-line nutation spectra. To explain this fact and to describe the off-resonance nutation experiment properly, the transient response theory of a quadrupolar spin system to an RF pulse was modified using the wave-function approach. The 2D separation of interactions technique has been applied to separate a static and a randomly time-fluctuating dynamic part of the quadrupole interaction in the antiferroelectric phase of polycrystalline ammonium dihydrogen arsenate.

Two-dimensional off-resonance nutation NQR spectroscopy has been used to determine the full quadrupolar tensor of spin-3/2 nuclei in several molecular crystals containing the ^{35}Cl and ^{75}As nuclei. The off-resonance phenomena in 2D NQR are very important from the practical point of view (determination of η in multiple or broad-line spectrum) and also provide interesting information on the dynamic properties of a quadrupolar spin system.

Key words: Nuclear Quadrupole Resonance; 2D Nutation Spectroscopy; Off-resonance Irradiation; Electric Field Gradient Tensor.

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