

Lineshape Analysis of 2D NMR and NQR Nutation Spectra of Integer and Half-Integer Quadrupolar Nuclei

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A lineshape analysis of the NMR and NQR powder nutation spectra of integer and half-integer quadrupolar nuclei is presented. Simulated NMR nutation spectra of spin $I = 1$ and 3 nuclei are reported. For $I = 1$ the formulas for the singularities of the NMR nutation powder patterns as a functions of η , e^2Qq and γB_1 are given. The NQR nutation powder patterns for spin $I = 3/2$, $5/2$, $7/2$, and $9/2$ for different induced transitions are calculated, and some experimental aspects of the method are discussed. A universal empirical formula to facilitate the determination of the asymmetry parameter from the NQR nutation frequency singularities for any arbitrary spin or transition is found. The NQR nutation spectra for half-integer and integer spins are compared. For integer spins the two-frequency excitation of the nutation spectrum is analysed. Application of the 2D-nutation lineshape analysis for the determination of the quadrupole interaction parameters is emphasised.

Key words: 2D Nutation Spectroscopy; NQR; NMR; Electric Field Gradient Tensor.