Two-dimensional Exchange and Nutation Exchange Nuclear Quadrupole Resonance Spectroscopy

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A theoretical treatment of the 2D exchange NQR pulse sequence is presented and applied to a quantitative study of exchange processes in molecular crystals. It takes into account the off-resonance irradiation, which critically influences the spin dynamics. The response to the three-pulse sequence of a system of spins $I = 3/2$ in zero applied field, experiencing electric quadrupole couplings, is analysed. The mixing dynamics by exchange and the expected cross-peak intensities as a function of the frequency offset have been derived. The theory is illustrated by a study of the optimization procedure, which is of crucial importance for the detection of the cross- and diagonal-peaks in a 2D-exchange spectrum. The systems investigated are hexachloroethane and tetrachloroethylene. They show threefold and twofold reorientational jumps about the carbon-carbon axis, respectively.

A new method of direct determination of rotational angles based on two-dimensional nutation exchange NQR spectroscopy is proposed. The method involves the detection of exchange processes through NQR nutation spectra recorded after the mixing interval. The response of a system of spins $I = 3/2$ to the three-pulse sequence with increasing pulse widths is analyzed. It is shown that the 2D-nutation exchange NQR spectrum exhibits characteristic ridges, which manifest the motional mechanism in a model-independent fashion. The angles through which the molecule rotates can be read directly from elliptical ridges in the 2D spectrum, which are also sensitive to the asymmetry parameter of the electric field gradient tensor.

Key words: Nuclear Quadrupole Resonance; 2D Spectroscopy; Electron Field Gradient Tensor; Exchange; Nutation.