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WURST-QCPMG sequence and "spin-lock" in ¹⁴N Nuclear Quadrupole Resonance

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Abstract

¹⁴N nuclear quadrupole resonance (NQR) is a promising method for the analysis of pharmaceuticals or for the detection of nitrogen based illicit compounds, but so far, the technique is still not widely used, mostly due to the very low sensitivity. This problem is already acute in the preliminary NQR stage, when a compound is being examined for the first time and the NQR frequencies are being searched for, by scanning a wide frequency range step-by-step. In the present work, we experimentally show how to increase the efficiency of this initial stage by using a combination of a wideband excitation achieved with frequency swept pulses (WURST) and a "spin-lock" state obtained with a quadrupolar-CPMG (QCPMG) sequence. In the first part we show that WURST pulses provide a much larger excitation bandwidth compared to common rectangular pulses. This increased bandwidth allows to increase the frequency step and reduces the total number of steps in a scanning stage. In the second part we show that the "spin-lock" decay time T_{2eff} obtained with the WURST-QCPMG combination is practically identical with the T_{2eff} obtained with the most common "spin-lock" sequence, the SLSE, despite a very different nature and length of excitation pulses. This allows for a substantial S/N increase through echo averaging in every individual step and really allows to exploit all the advantages of the wider excitation in the NQR frequency scanning stage. Our experimental results were obtained on a sample of trinitrotoluene, but identical behavior is expected for all compounds where a "spin-lock" state can be created.

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