A solid-state ^{87}Sr NMR investigation of some inorganic and organometallic strontium complexes

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An important aspect of the research conducted in our lab has been to demonstrate the practicality and utility of conducting NMR investigations involving non-traditional nuclei, including a ^{99}Ru study of some diamagnetic ruthenium compounds [1], a ^{115}In NMR investigation of several indium coordination complexes [2] and the structural characterization of some silver dialkyl salts using ^{109}Ag solid-state NMR spectroscopy [3]. Strontium plays an important role in such diverse fields of research as materials chemistry [4], medicine [5] and paleoanthropology [6]. Yet only a few applications of solid-state ^{87}Sr have been reported [7-9].

This paucity of Sr NMR data may be attributed to the nuclear properties of ^{87}Sr: a low natural abundance, 7.00 %, a low frequency ratio, Ξ = 4.33% and a large quadrupole moment, Q = 33.5 fm^2.

We have undertaken a solid-state ^{87}Sr NMR investigation of numerous compounds. Despite the challenges imposed by the nuclear properties discussed above, we have acquired spectra of samples at natural abundance. Spectra for samples at natural abundance with moderate quadrupole

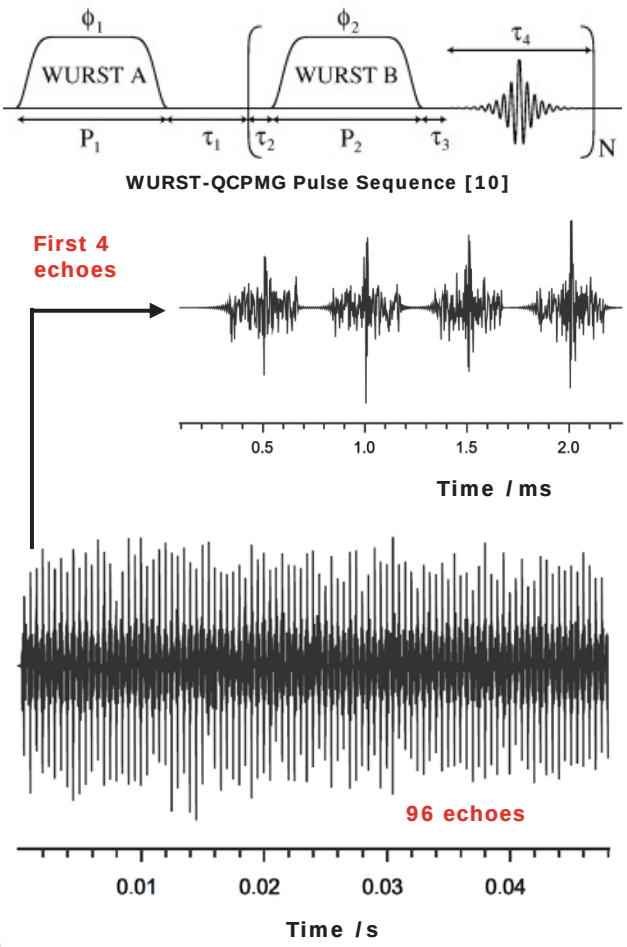
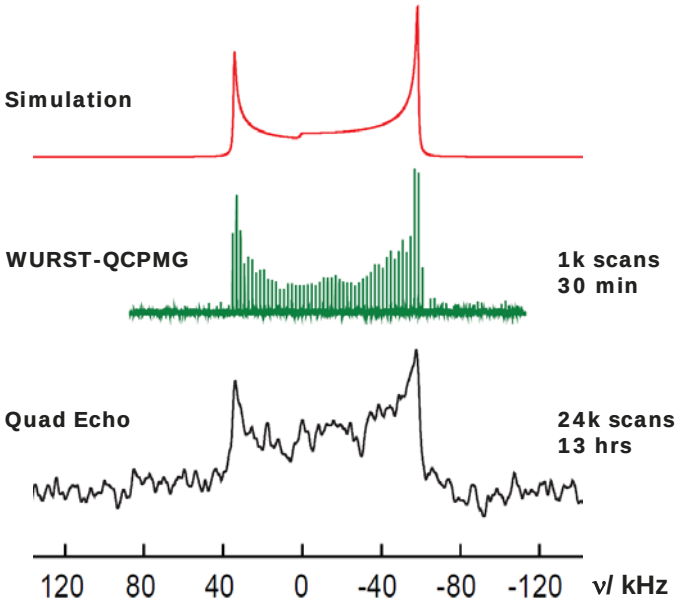
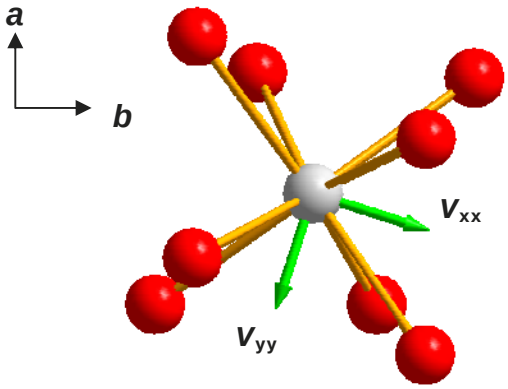


Figure 1: ^{87}Sr WURST-QCPMG NMR echo-train in a polycrystalline powder sample of strontium tungstate, $SrWO_4$.





Coordination environment of Sr in $SrWO_4$, oxygen - red, Sr - grey [11]. Sr-site has a 4-fold rotation-inversion symmetry. V_{zz} component of the EFG tensor is along the *c* axis, perpendicular to the plane of view.

Figure 2: Experimental and simulated ^{87}Sr NMR spectra for strontium tungstate, $SrWO_4$, at 21.1 T. Experimental and DFT calculated ^{87}Sr NMR parameters are as follows. Exp: δ_{iso}=27±5 ppm, C_Q=22.4 MHz, η_Q=0.0, DFT CASTEP: δ_{iso}=11 ppm, C_Q=-20.6 MHz, η_Q=0.0.

coupling constants can be acquired in several hours. For samples with large quadrupole coupling constants, we have found the QCPMG technique, combined with WURST, to be particularly effective; see Figure 2 for ^{87}Sr NMR spectra of strontium tungstate. A full manuscript describing our research is being prepared and will be submitted in the nearest future.

References

[1] K.J. Ooms and R.E. Wasylishen, *J. Am. Chem. Soc.* **126** (2004) 10972-10980.
[2] F. Chen, G. Ma, R.G. Cavell, V.V. Terskikh and R.E. Wasylishen, *Chem. Commun*. (2008) 5933-5935.
[3] F. Chen and R.E. Wasylishen, *Magn. Reson. Chem*. **48** (2010) 270-275.
[4] W. Ma and H. Dong, *Thermal Barrier Coatings* (2011) 25-52.
[5] P. J. Marie, D. Felsenberg and M. L. Brandi, *Osteoporosis International* **22** (2011) 1659-1667.
[6] M.J. Schoeninger, *Nature* **474** (2011) 43-45.
[7] C. Gervais, D. Veautier, M.E. Smith, F. Babonneau, P. Belleville and C. Sanchez, *Solid State Nucl. Magn. Reson.* **26** (2004) 147-152.
[8] G.M. Bowers, A.S. Lipton and K.T. Mueller, *Solid State Nucl. Magn. Reson.* **29** (2006) 95-103.
[9] G.M. Bowers, R. Ravella, S. Komarneni and K.T. Mueller, *J. Phys. Chem. B* **110** (2006) 7159-7164.
[10] L.A. O'Dell and R.W. Schurko, *Chem. Phys. Lett*. **464** (2008) 97-102.
[11] E. Guermen, E. Daniels, J.S. King, *J. Chem. Phys.* **55** (1971) 1093-1097.