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Artefact-free broadband 2D NMR for separation of quadrupolar and paramagnetic shift interactions

Deuterium (^{2}H) NMR is well-suited for probing the structure and dynamics of materials. The study of ^{2}H via NMR has gained popularity owing to the abundance of hydrogen in materials and the ease to substitute with ^{2}H and most importantly due to favorable NMR properties of ^{2}H. ^{2}H has spin $I = 1$, and has a quadrupole moment, the interaction of which with the electric-field gradient (EFG) affords invaluable information about the local hydrogen environment and any motional processes.

However, in paramagnetic materials, the combination of paramagnetic shift anisotropy (SA), quadrupolar broadening and inhomogeneous broadening due to bulk magnetic susceptibility (BMS) leads to featureless spectra, hence impeding extraction of individual NMR parameters. This issue has been addressed by introducing static 2D experiments which separate and correlate the shift (including isotropic shift, SA and BMS effects) and first-order quadrupole interactions. To date, two elegant experiments have been proposed for separation of the interactions which also provide information about the relative orientation between the two tensors, however, both methods, among other drawbacks, suffer from major artefacts in the quadrupolar dimension [1,2].

Here we present two new pulse sequences for separating the shift and quadrupolar interactions, which incorporate short high-power adiabatic pulses (SHAPs) [3]. The new experiments yield artefact free spectra and achieve greater excitation bandwidth. Application of the pulse sequences has provided unprecedented structural information on local hydride environments of deuterated forms of the oxyhydride ion conductor $BaTiO_{3-x}H_y$. These experimental data were of sufficient quality to provide insight into the local hydride structure of these materials, with the aid of quantum chemical/density-functional theory (DFT) calculations.

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