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Supplementary Information

Quantitative analysis of 14N Quadrupolar Couplings Using Proton Detected 14N Solid-State NMR

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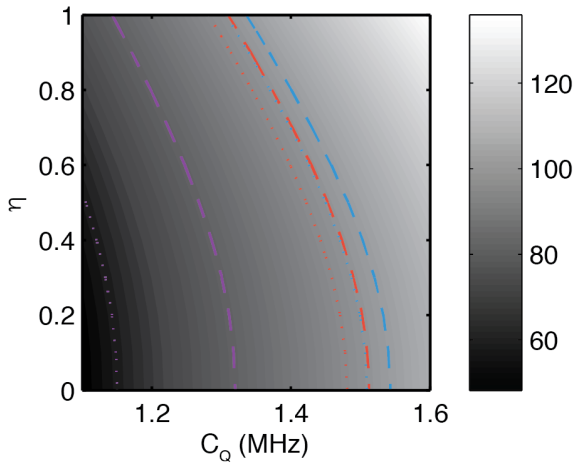
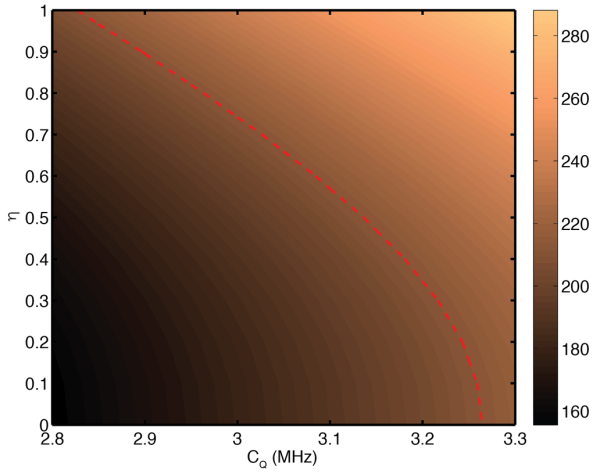
Supplementary Figure S1



Supplementary Figure S1. Plot of δ_{CS}^{iso} as a function of C_Q and η at 14.1T. The δ_{CS}^{iso} is plotted in ppm as a function of C_Q and η, calculated from Equation 1. Plot is for a magnetic field of 14.1T. Dotted and dashed lines indicate the experimentally determined and calculated values for the δ_{CS}^{iso}, respectively, of $-NH_3^+$, (purple), Nε (blue) and Nδ (red) sites in His.HCl.H_2O.

Supplementary Figure S2



Supplementary Figure S2. Plot of δ_{CS}^{iso} as a function of C_Q and η at 20.T. The δ_{CS}^{iso} is plotted in ppm as a function of C_Q and η, calculated from Equation 1. Dashed lines indicate the experimentally determined values for the δ_{CS}^{iso} of the amide nitrogen in NAV.

Supplementary Figure S3

Supplementary Figure S3. Simulations of 2D $^{1}H/^{14}N$ correlation spectrum of NAV showing influence of relative orientations (α_Q^{PM}, β_Q^{PM}, 0) of the quadrupolar interaction and the ^{14}N-^{1}H dipolar coupling tensors (C_Q=3.2 MHz, η=0.32, CSA omitted) on lineshape (A, ^{1}H x-axis 8 to 10 ppm, ^{14}N y-axis 250 to 400ppm) and the corresponding skyline projections of the ^{14}N dimenion. (B, normalized to maximum intensity, and plotted between 250 and 400 ppm). Spectra were simulated for a field of 19.96T with a spinning speed of 78 kHz. Simulations were performed with a rotor grid rank of 55 and summed over 1202 powder points and processed with 200 Hz linebroadening in both dimensions.

Supplementary Figure S4

Supplementary Figure S4. Simulations of 2D $^{1}H/^{14}N$ correlation spectrum of NAV showing influence of relative orientations (α_Q^{PM}, β_Q^{PM}, 0) of the quadrupolar interaction and the ^{14}N-^{1}H dipolar coupling tensors (C_Q=3.2 MHz, η=0.32, with CSA included as described in Table 1) on lineshape (A, ^{1}H x-axis 8 to 10 ppm, ^{14}N y-axis 250 to 400ppm) and the corresponding skyline projections of the ^{14}N dimenion. (B, normalized to maximum intensity, and plotted between 250 and 400 ppm). Spectra were simulated for a field of 19.96T with a spinning speed of 78 kHz. Simulations were performed with a rotor grid rank of 55 and summed over 1202 powder points and processed with 200 Hz linebroadening in both dimensions.