Electronic Supplementary Information

A High-Field Solid-State $^{35/37}$Cl NMR and Quantum Chemical Investigation of the Chlorine Quadrupolar and Chemical Shift Tensors in Amino Acid Hydrochlorides

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Single-Crystal X-ray Diffraction

Suitable crystals were selected, mounted on a thin glass fibre using paraffin oil, and cooled to the data collection temperature of 203 K for **1**, 200 K for **3** and 217 K for **6**. Data were collected on a Bruker AXS SMART 1K CCD diffractometer. For **1** and **6** data collection was performed with three batch runs at Φ= 0.00º (650 frames), at Φ = 120.00º (650 frames), and at Φ = 240.00º (650 frames). For **3,** data collection was performed with four batch runs at Φ = 0.00º (650 frames), at Φ = 90.00º (650 frames), at Φ = 180.00º (650 frames), and at Φ = 270.00º (650 frames). Initial unit cell parameters were determined from 60 data frames collected at different sections of the Ewald sphere. Semi-empirical absorption corrections based on equivalent reflections were applied.[1] The systematic absences and unit cell parameters were consistent with $P1$ for **3**, $P2_1$ for **6** and $P2_12_12_1$ for **1.** The structures were solved by direct methods, completed with difference Fourier syntheses, and refined with full-matrix least-squares procedures based on $F2$. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms except those of the water molecule in **1** were treated as idealized contributions. The hydrogen atoms of the water molecule in **1** were refined isotropically. All scattering factors and anomalous dispersion factors are contained in the SHELXTL 6.12 program library[2].

[1] R. Blessing, *Acta Crystallogr.*, 1995, **A51**, 33-38.
[2] G. M. Sheldrick, *SHELXTL*; Bruker AXS: Madison, Wisconsin, USA, 2001.

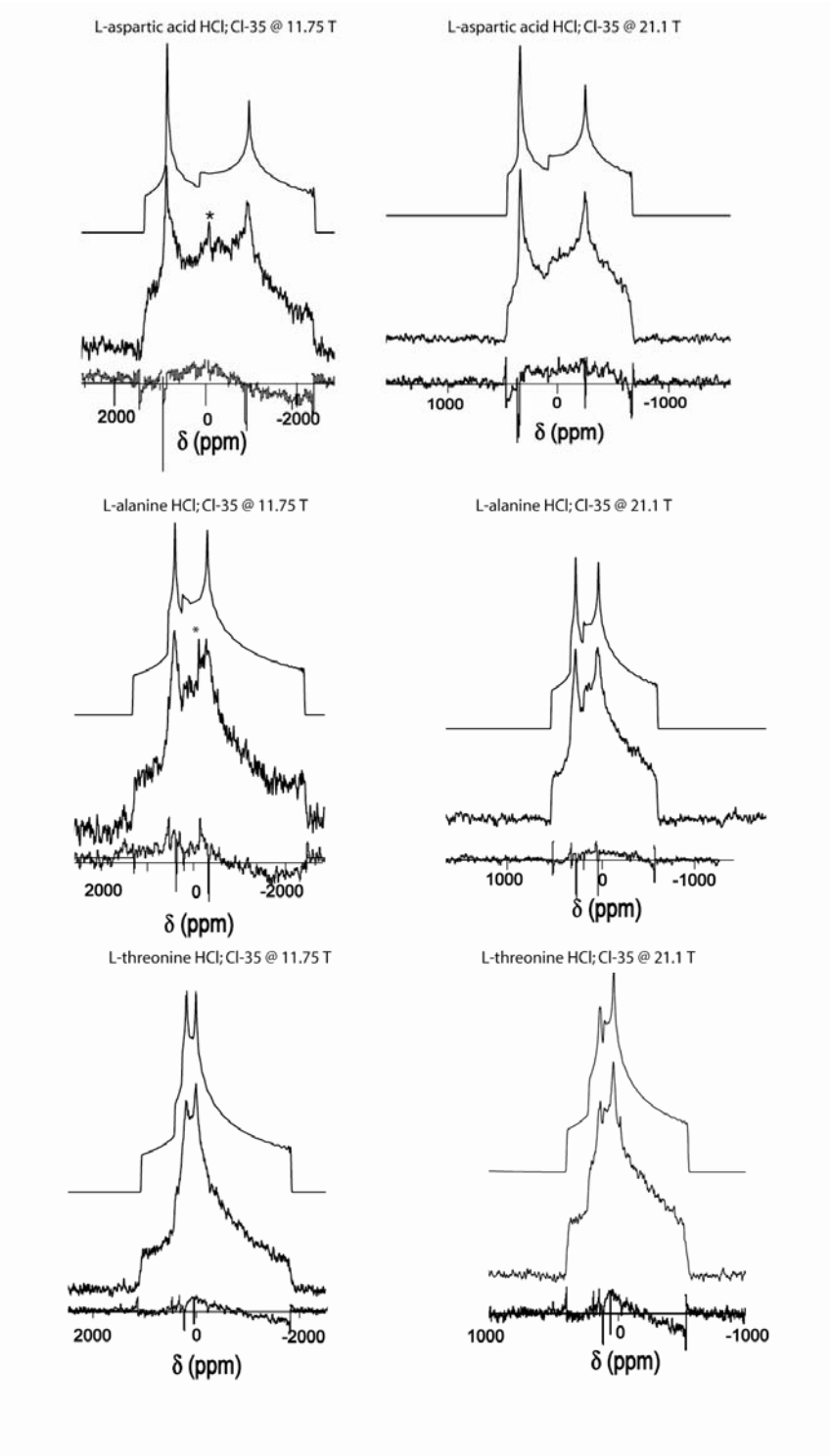
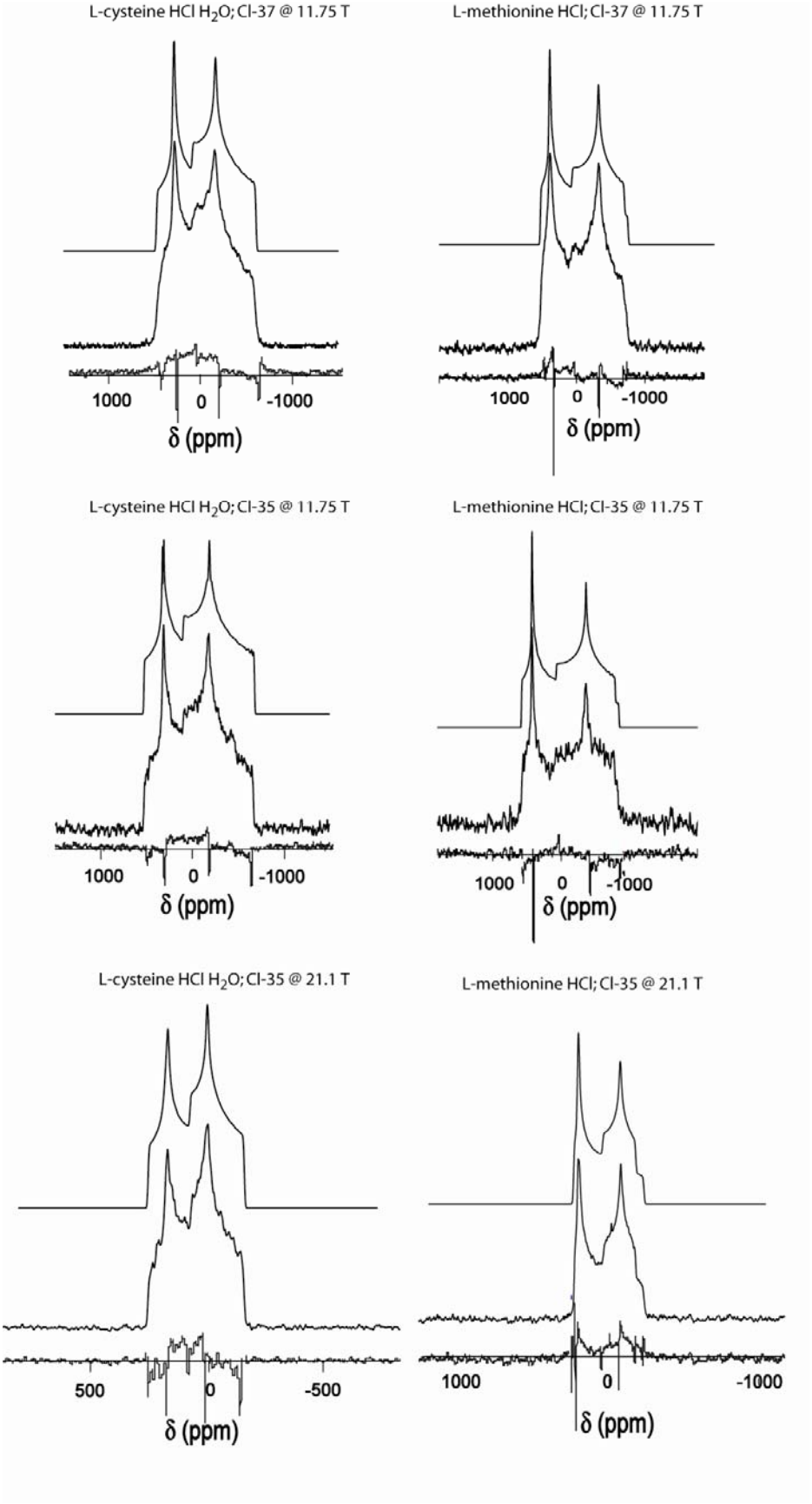


Figure 1S (continued next page): Difference spectra (experimental minus simulated) are shown in the lower trace for all spectra obtained for stationary samples. Discrepancies may be attributed to imperfect excitation of the experimental spectra which causes broad features in the difference spectra and/or sharper features in the simulated spectra which result in spikes in the difference spectra.


L-cysteine HCl H_2O; Cl-37 @ 11.75 T
1000
0
-1000
δ (ppm)
L-methionine HCl; Cl-37 @ 11.75 T
1000
0
-1000
δ (ppm)
L-cysteine HCl H_2O; Cl-35 @ 11.75 T
1000
0
-1000
δ (ppm)
L-methionine HCl; Cl-35 @ 11.75 T
1000
0
-1000
δ (ppm)
L-cysteine HCl H_2O; Cl-35 @ 21.1 T
500
0
-500
δ (ppm)
L-methionine HCl; Cl-35 @ 21.1 T
1000
0
-1000
δ (ppm)