Electronic Supplementary Information

Application of Multinuclear Magnetic Resonance and Gauge-Including Projector-Augmented Wave Calculations to the Study of Solid Group 13 Chlorides

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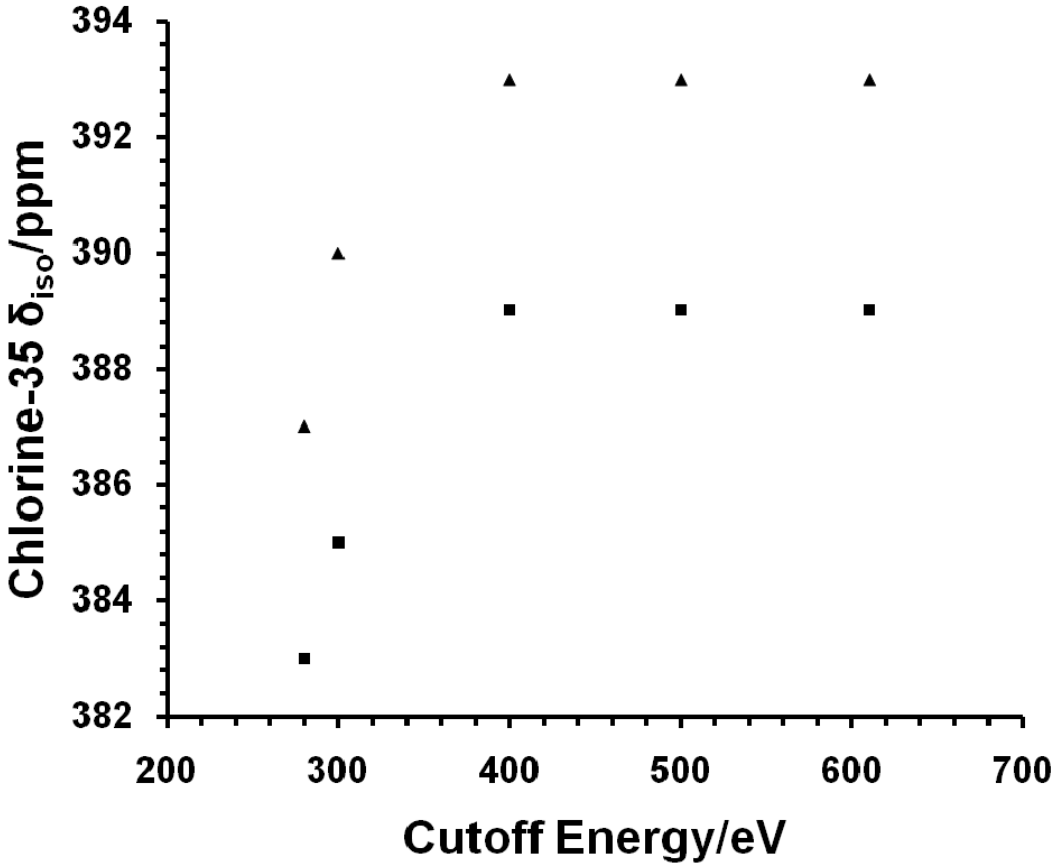

Figure 1S. Convergence of the chlorine chemical shift with increasing plane-wave cutoff energy, for $AlCl_3$. Site one: squares; site two: triangles. A cutoff energy of 610 eV was used for all calculations presented in the manuscript.

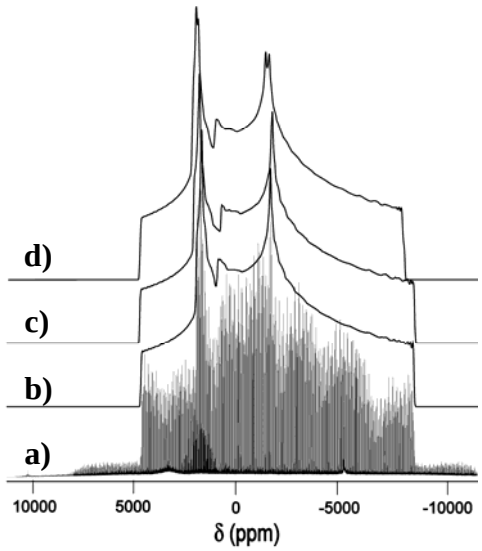

Figure 2S. Experimental and simulated solid-state chlorine-35 NMR spectra of aluminum trichloride at 21.1 T. Best-fit simulation is shown in (b), simulation assuming no CSA is shown in (c) and a simulation based on the GIPAW-DFT calculated parameters is shown in (d).

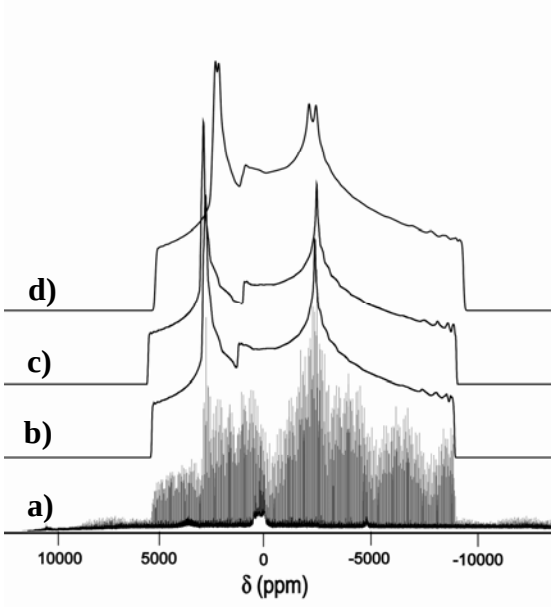

Figure 3S. Experimental and simulated solid-state chlorine-35 NMR spectra of indium trichloride at 21.1 T. Best-fit simulation is shown in (b), simulation assuming no CSA is shown in (c) and a simulation based on the GIPAW-DFT calculated parameters is shown in (d).

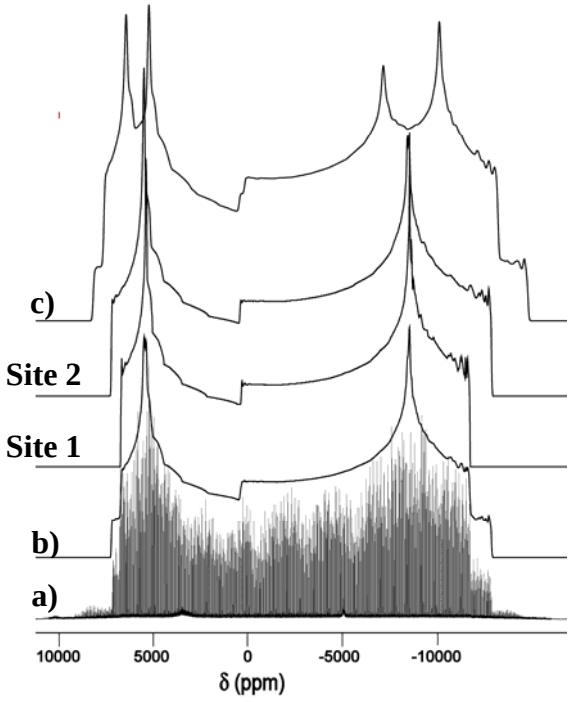

Figure 4S. Experimental and simulated solid-state chlorine-35 NMR spectra of gallium dichloride at 21.1 T. Best-fit simulation is shown in (b), with individual simulations of the two sites shown above. Simulation based on the GIPAW-DFT calculated parameters is shown in (c).

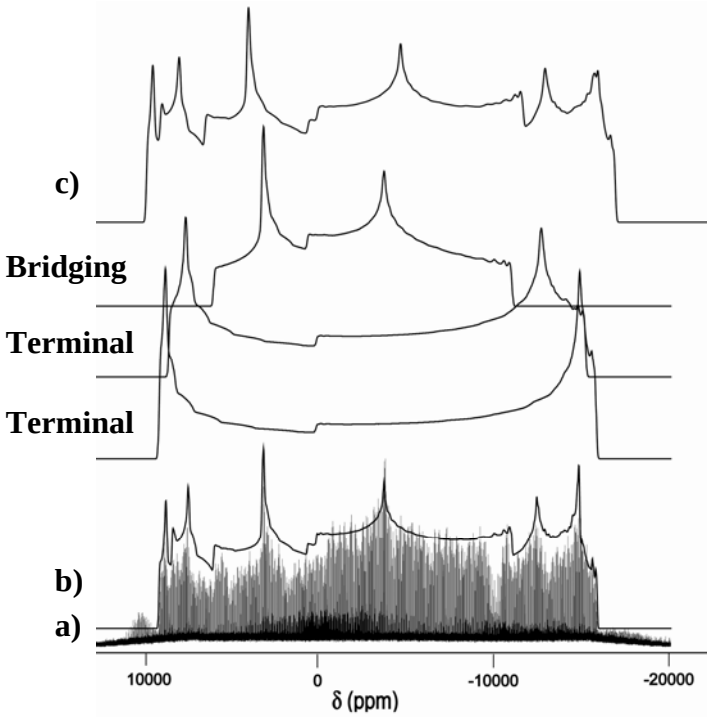

Figure 5S. Experimental and simulated solid-state chlorine-37 NMR spectra of gallium trichloride at 21.1 T. Best-fit simulations are shown in (b), with individual simulations of the three sites shown above. Simulation based on GIPAW-DFT calculated parameters is shown in (c).