

# **Supplementary Material:**

## **$^{14}\text{N}$ Overtone NMR Spectra under Magic Angle Spinning Experiments and Numerically Exact Simulations**

Luke A. O'Dell<sup>†</sup> and Andreas Brinkmann\*

Measurement Science and Standards, National Research Council Canada, 1200 Montreal  
Road, M40, Ottawa, ON, K1A 0R6, Canada

\*Corresponding author e-mail: [Andreas.Brinkmann@nrc-cnrc.gc.ca](mailto:Andreas.Brinkmann@nrc-cnrc.gc.ca)

<sup>†</sup>Present address: Institute for Frontier Materials, Deakin University, Waurn Ponds  
Campus, Geelong, Victoria, 3220, Australia

### **S1. Dependence of the $^{14}\text{N}$ overtone NMR signal on sample spinning frequency**

The simulations in Figure S1 illustrate the dependence of the  $^{14}\text{N}$  overtone NMR signal on the magic-angle-spinning frequency  $\omega_r$ , calculated for a powdered sample of glycine. All simulations were done employing an rf pulse of 0.1  $\mu\text{s}$  duration with  $\omega_{rf}^{14\text{N}}/2\pi = 161.5$  kHz. Figure S1a shows the simulated static spectrum and overtone sideband patterns. The positions of the centerband, +1 and +2 overtone sidebands are indicated by visual guides. Figure S1b depicts the center-of-mass frequency  $\Omega_{\text{CM}}$  of the static powder pattern and +2 overtone sidebands as a function of the MAS frequency  $\omega_r$ . The fitted value for the slope of the straight line is given by 2.

### **S2. Width of $^{14}\text{N}$ overtone MAS +2 sideband powder lineshape**

Figure S2 depicts the width  $\Delta$  of the simulated  $^{14}\text{N}$  overtone MAS +2 sideband powder lineshape for  $\eta_Q = 0.0$  as a function of  $\omega_Q^2/(2\pi\omega_0)$ . All simulations were done employing an rf pulse of 0.2  $\mu\text{s}$  duration with  $\omega_{rf}^{14\text{N}}/2\pi = 161.5$  kHz. The results can be fitted to a straight line with slope 42.3.

Figure S1.

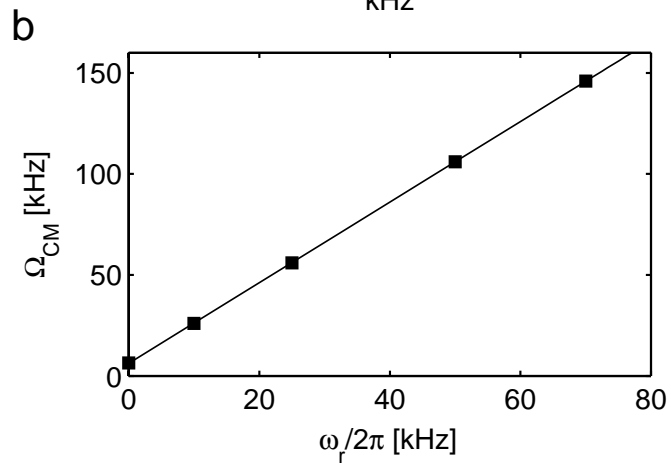
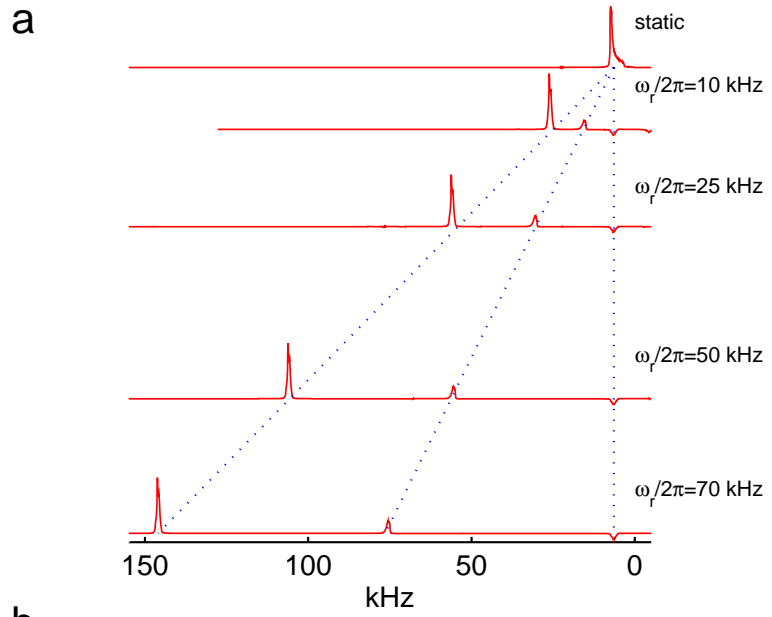


Figure S2.

