# **Supporting Information**

On the performance of Spin Diffusion NMR Techniques in Oriented Solids: Prospects for Resonance Assignments and Distance Measurements from Separated Local Field Experiments

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## SUPPORTING INFORMATION TABLE I

| Atom | H1     | H2      | Н3      | H4      | H5      | H6     | H7      | H8     | Н9      | H10     | N2     |
|------|--------|---------|---------|---------|---------|--------|---------|--------|---------|---------|--------|
| N1   | -913.8 | 127.2   | 298.1   | -149    | -5544.2 | -38.7  | -31.0   | -107.0 | -90.7   | -29.6   | 3.2    |
| H1   |        | -2290.5 | -1002.9 | -2182.1 | 4034.6  | 1087.7 | 508.6   | 1426.8 | 3580.8  | 380.4   | -60.7  |
| H2   |        |         | -2108.1 | 395.9   | -309.8  | 474.2  | 137.4   | 172.4  | 513.7   | 214.5   | -38.1  |
| H3   |        |         |         | 7126.0  | -39.1   | 374.6  | 212.0   | 999.8  | 340.0   | 670.8   | -64.9  |
| H4   |        |         |         |         | 1579.2  | 1523.2 | 463.4   | 1823.6 | 344.4   | 1891.6  | -270.6 |
| H5   |        |         |         |         |         | 275.2  | 209.4   | 703.8  | 521.4   | 262.8   | -27.4  |
| H6   |        |         |         |         |         |        | -3159.1 | 1250.4 | 6265.5  | -2268.0 | 652.5  |
| H7   |        |         |         |         |         |        |         | 2986.4 | 1524.9  | -996.0  | 125.3  |
| H8   |        |         |         |         |         |        |         |        | -3950.5 | 885.8   | -113.0 |
| Н9   |        |         |         |         |         |        |         |        |         | -725.4  | 78.6   |
| H10  |        |         |         |         |         |        |         |        |         |         | 4525.7 |

Homo and heteronuclear dipolar couplings (in Hz) used in the simulation shown in Figure 13.

PDSD experiments on the NAL single crystal. All 12 cross-peaks are shown from the spectra as expressed as the cross-peak intensity ( $Int_c$ ) divided by diagonal peak intensities ( $Int_d$ ). Note that the maximum value along the y-axis is 0.2, corresponding to a 20% transfer efficiency.



PDSD experiments on the NAVL single crystal. All 12 cross-peaks are shown from the spectra as expressed as the cross-peak intensity (Int<sub>c</sub>) divided by diagonal peak intensities (Int<sub>d</sub>).



PMPT experiments on the NAL single crystal. The <sup>1</sup>H RF amplitude was varied between 0-70 kHz for three different <sup>15</sup>N spinlocks (21, 37.5, and 52.5 kHz). The mixing time was fixed at 10 msec for all points. Cross-peak intensities are plotted in arbitrary units. The dip in the curves is due to the Hartmann-Hahn match.



Same as **Supporting Information Figure 3**, except that the <sup>1</sup>H RF amplitude is plotted in units of percentage mismatch from that of the <sup>15</sup>N RF amplitude.



PMPT experiments on the NAVL single crystal. The <sup>1</sup>H RF amplitude was varied for a <sup>15</sup>N spinlock of 57.5 kHz. The mixing time was fixed at 10 msec for all points. Cross-peak intensities are plotted in arbitrary units. The dip in the curves is due to the Hartmann-Hahn match.



Same as **Supporting Information Figure 5**, except that the <sup>1</sup>H field is plotted in units of percentage mismatch from that of the <sup>15</sup>N RF amplitude (57.5 kHz).

