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Supporting Information

Accurate Determination of ^{1}H-^{15}N Dipolar Couplings Using Inaccurate Settings of the Magic Angle in Solid-State NMR Spectroscopy

Kai Xue, Max Mühlbauer, Salvatore Mamone, Riddhiman Sarkar, and Bernd Reif**

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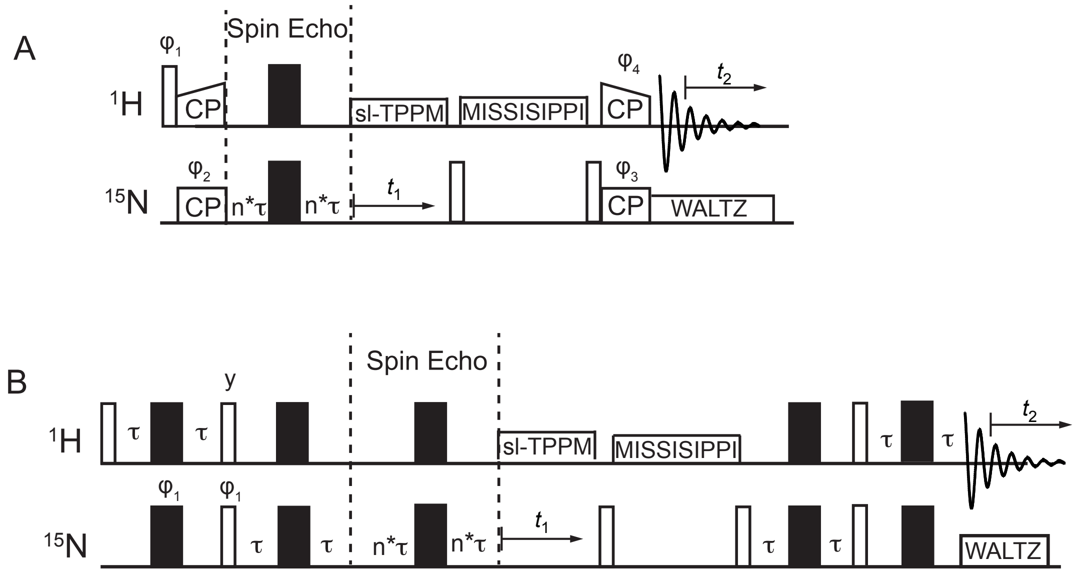

Figure S1. NMR pulse sequences employed in this study. (A) CP and (B) INEPT based methods to yield ^{15}N-^{1}H correlations as a function of spin echo delay.

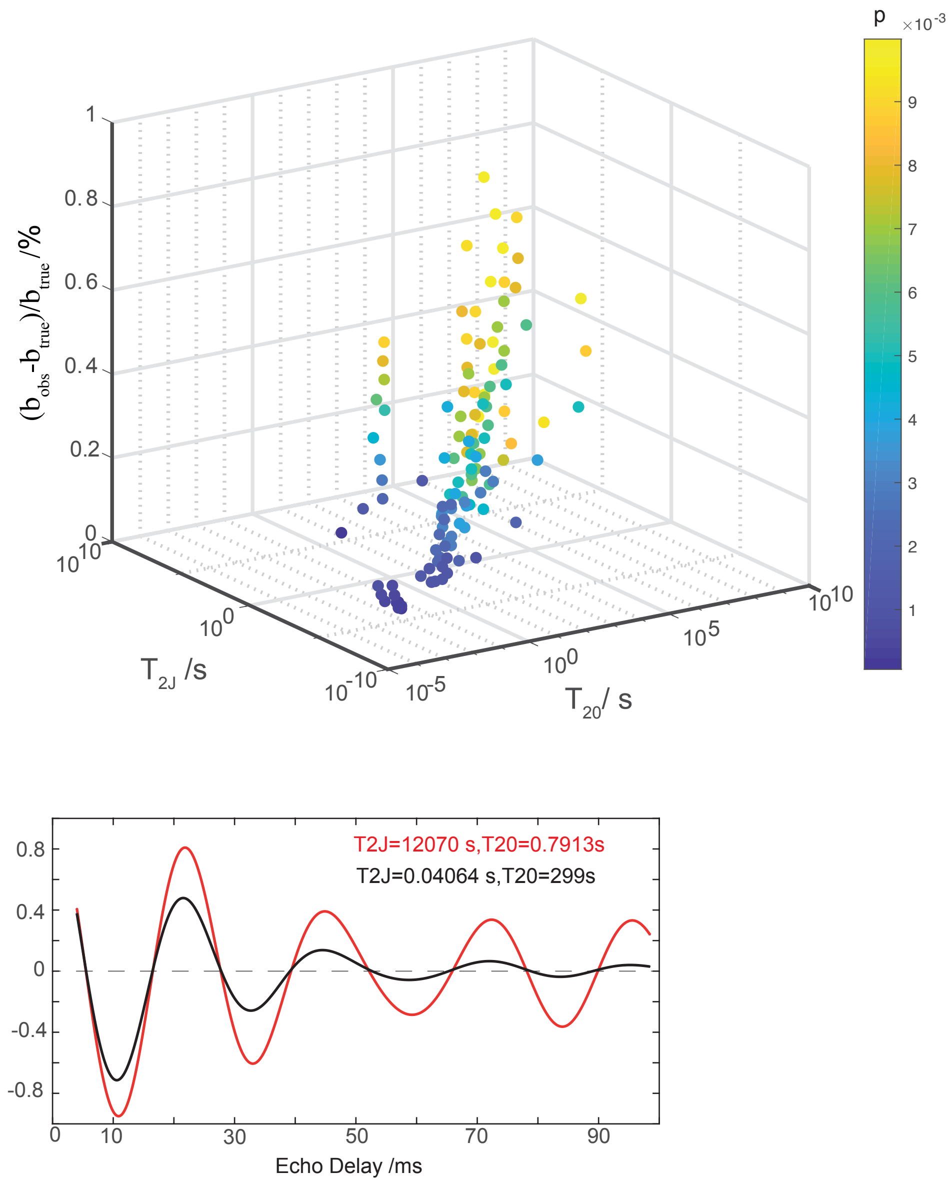

Figure S2: The influence of {p, T_2 and T_{2J}} parameters on the uncertainty of measurement of ^{15}N-^{1}H dipolar coupling for a small range of p, which is observed experimentally. The spin-echo curves at very different T_2 and T_{2J} values (bottom panel) still produce a small error on the determination of the dipolar coupling values.

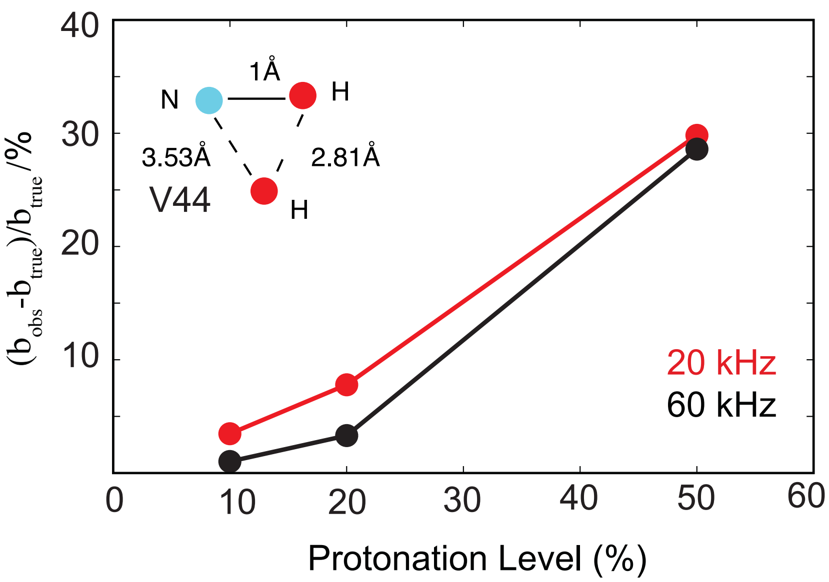

Figure S3: The influence of remote protons on the measured value of ^{15}N-^{1}H dipolar coupling is evaluated under 20 kHz and 60 kHz MAS, respectively. The local proton network around residue V44 in SH3 domain was taken from PDB (2NUZ). A two-spin simulation assuming only the directly bonded ^{15}N and ^{1}H and a three-spin simulation assuming the geometry above were performed. Subsequently, a weighted sum of the two simulations were performed, where the weight reflects the degree of protonation in the sample.

Residue	T20(s)	error	T2J(s)	error	Dipolar_cou	error	J_coupling(H	error	P	error
8	25.13428	296490.134	0.03570006	0.00520563	9540.337	942.076	93.42285	1.21334	0.00092241	0.02093795
9	0.06717358	0.81775578	0.02871086	0.00934919	10274.8	2557.405	95.16529	3.11687	0.00958266	0.05836123
14	15.9661	15452.7361	0.1010473	0.02928465	10179.06	732.921	93.35833	1.13465	0.01028506	0.0295268
15	0.1125392	1.0849897	0.08467864	0.03343575	9362.38	1167.434	96.03527	1.69079	0.01599543	0.0519959
16	7.40331	5509.60631	0.08204134	0.03342495	9898.567	1283.616	96.106	1.8972	0.00982006	0.04687233
19	0.1301078	1.7331268	0.09566349	0.05376329	8694.816	1448.245	96.65581	2.0753	0.01765225	0.07068252
21	3.277557	94691.4776	0.04363398	0.01288808	6196.13	1481.152	92.20005	1.67893	0.00011037	0.04606708
24	31.40606	174977.806	0.06878922	0.02599721	9955.447	1315.283	91.0905	1.96322	0.00541219	0.0458015
25	0.1752358	2.3912848	0.1021192	0.04629972	9416.508	1151.883	96.7982	1.6731	0.0160525	0.05159505
26	13.91209	24228.1921	0.07125329	0.03165893	9716.488	1570.126	95.61766	2.29045	0.00916692	0.05465062
27	7.814704	9183.5817	0.06106736	0.0272082	9709.054	1808.384	97.60854	2.58787	0.00797642	0.0574376
28	0.0448445	0.2551226	0.06634763	0.02767551	10149.99	1509.885	96.00248	2.23907	0.02129396	0.07007217
29	0.06631153	0.41862473	0.08202696	0.03313317	10688.45	1250.914	96.38292	1.92266	0.01847763	0.05615795
30	13.66451	14688.9745	0.0770701	0.03182585	11066.55	1400.946	95.05184	2.19075	0.01266512	0.04762553
31	8.468865	9819.01287	0.04075319	0.00983015	10775.9	1409.015	95.22501	1.98794	0.00501418	0.03315721
32	12.81579	21395.0158	0.04664963	0.01338466	10346.18	1475.848	94.92173	2.1114	0.00623807	0.03910539
33	2.04E-05	0.01201576	0.07730999	0.06319259	9459.363	1941.661	99.36637	2.79741	0.2049264	0.19717264
35	12.13945	11882.6595	0.09263275	0.03446387	9965.981	1053.606	95.90414	1.57235	0.01052652	0.04025279
36	0.00023973	0.69894083	0.06038249	0.03204315	10680.53	1549.955	98.28657	2.29061	0.2831969	0.1341499
37	0.09394382	1.04234922	0.02708696	0.00730258	11144.94	2236.342	91.03071	2.77028	0.00988831	0.04433648
39	0.5457945	39.7895345	0.09864936	0.07230749	8843.358	1889.975	97.66589	2.71635	0.01361359	0.08295181
40	0.1663288	1.1472711	0.04809445	0.01164693	9758.737	1180.548	94.49042	1.65951	0.02105243	0.03636738
41	0.0828684	0.5850727	0.1194772	0.07050168	9554.041	1274.363	95.59153	1.87969	0.0225203	0.06590566
42	0.02773484	0.06060775	0.0456653	0.01225494	10492.12	1312.227	96.52358	1.87561	0.04006018	0.05771609
43	0.05994834	0.45209334	0.03727172	0.00997382	10093.36	1627.914	96.40643	2.17259	0.01230301	0.04868297
44	0.2054356	3.9585166	0.08574802	0.04411745	9714.52	1541.739	96.80952	2.25735	0.01571565	0.0624259
45	8.07254	7826.25454	0.03563829	0.01037504	10076.04	1908.659	95.39102	2.51259	0.00705564	0.0409883
49	12.49789	12514.6979	0.03356488	0.00525448	8287.183	1077.303	95.21008	1.26236	0.00602601	0.02333151
50	1.967345	670.338345	0.04746016	0.01136745	8766.909	1164.021	93.9225	1.57048	0.0042183	0.03464534
51	0.1170729	1.2402639	0.04720982	0.01262935	9825.984	1337.387	97.05542	1.86159	0.01187966	0.041998
52	2.775874	754.497974	0.08910141	0.03070187	10261.15	995.748	94.36545	1.52816	0.00822662	0.03798008
53	0.00223529	0.00190445	0.06266508	0.01590891	10154.13	707.916	94.96424	1.07191	0.2187681	0.0697079
55	1.03E-05	0.00343041	0.1466136	0.17138434	9517.005	1618.42	97.72966	2.35562	0.19502	0.17976347
56	0.03256413	0.12854429	0.07866387	0.04452562	8200.43	1617.335	98.95592	2.3309	0.04174295	0.10135494
57	0.00016338	0.18576298	0.08737418	0.02473227	10243.93	605.08	95.15642	0.92058	0.2534129	0.0593233
58	2.11E-05	0.0116615	0.1497075	0.15018799	9179.244	1350.98	98.54685	1.94312	0.2047222	0.15122194
59	6.409668	2222.52867	0.07221248	0.0223359	10717.6	1059.091	92.11649	1.65028	0.01397502	0.0360741
60	60.27905	821951.979	0.2473908	0.26683661	8292.518	1141.996	97.91121	1.66397	0.00624093	0.06655897
61	11.28416	65177.8842	0.05044886	0.0148511	10188.36	1388.651	93.26496	2.01456	0.00161829	0.03975002
62	3.504224	1566.77522	0.02487571	0.00285658	4603.179	1525.586	92.70464	0.80774	0.00288676	0.01776453

Table S1: List of {p, J, $\Delta\theta_{RL}$, b, T_2 and T_{2J}} best fit parameters for resolved residues are shown.