

Ab Initio NMR Chemical-Shift Calculations Based on the Combined Fragmentation Method

Hwee-Jia Tan and Ryan P. A. Bettens

Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore 117543

Email: chmbrpa@nus.edu.sg

Phone: +65 6516 2846. Fax: +65 6779 1691

Supporting Information Available

Note that all coordinates are in Angstroms.

1 Chemical Shifts of the Fourteen Small Proteins

Table 1: Cartesian coordinates and isotropic shielding constants (in ppm) for 1OAI

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	-7.197000	43.748000	-10.846000	232.3405	232.3313	232.2697	232.3178	232.3068
2	C	-6.768000	42.330000	-10.685000	146.0922	146.1362	146.2507	146.1176	146.1039
3	C	-5.567000	42.024000	-11.578000	12.6889	12.6007	12.7383	12.7310	12.6825
4	O	-5.394000	40.881000	-12.033000	-40.1592	-39.6323	-37.1139	-40.2665	-40.2732
5	C	-7.918000	41.351000	-10.977000	164.3489	164.3734	164.3933	164.3541	164.3438
6	C	-9.224000	41.758000	-10.312000	5.5026	5.5284	5.5350	5.5153	5.5177

7	O	-9.220000	42.743000	-9.524000	27.3300	27.0250	26.8072	27.3227	27.3103
8	O	-10.315000	41.155000	-10.523000	8.5611	8.6961	8.3020	8.5186	8.4843
9	H	-7.974942	43.925963	-10.260137	24.8770	24.8859	24.8792	24.8719	24.8698
10	H	-6.451088	44.348888	-10.595702	29.2485	29.2489	29.2472	29.2423	29.2388
11	H	-7.449972	43.911186	-11.789120	29.7275	29.7335	29.7173	29.7246	29.7190
12	H	-6.479385	42.197085	-9.663269	28.9691	28.9789	28.9628	28.9665	28.9632
13	H	-8.070193	41.304125	-12.035083	30.8278	30.8467	30.8371	30.8307	30.8253
14	H	-7.640694	40.379176	-10.625489	30.1212	30.1544	30.1323	30.1267	30.1223
15	N	-4.754000	43.046000	-11.859000	156.6558	156.9895	156.9228	156.8820	156.8560
16	C	-3.490000	42.843000	-12.575000	142.3956	142.2998	142.2377	142.3210	142.3056
17	C	-2.373000	42.403000	-11.629000	10.3552	10.8869	10.8905	11.1036	10.8614
18	O	-2.284000	42.810000	-10.460000	-5.5372	-8.5094	-8.6165	-11.7234	-8.4700
19	C	-3.049000	44.144000	-13.324000	138.4829	138.3233	138.3137	138.4497	138.5097
20	O	-2.903000	45.188000	-12.411000	345.3258	345.0414	345.0477	344.9148	344.8748
21	H	-5.010086	43.960078	-11.577965	27.9656	27.9988	27.9777	27.9670	27.9588
22	H	-3.661880	42.066280	-13.290586	28.7822	28.8060	28.7857	28.7782	28.7769
23	H	-2.115911	43.970777	-13.818206	29.1206	29.1356	29.1249	29.1232	29.1197
24	H	-3.791623	44.406332	-14.048288	29.2111	29.2153	29.2138	29.2135	29.2133
25	H	-2.681273	44.759189	-11.592796	31.9834	32.0198	32.0124	32.0004	31.9969

26	N	-1.478000	41.607000	-12.188000	159.9620	159.5632	159.5286	159.3403	159.6300
27	C	-0.259000	41.228000	-11.546000	157.5243	157.5118	157.4996	157.5242	157.5543
28	C	-0.350000	39.831000	-10.952000	16.4979	16.4333	16.5019	16.5162	16.5211
29	O	-1.140000	38.999000	-11.384000	-4.1133	-4.0991	-4.2567	-3.8662	-3.9133
30	H	-1.661117	41.256373	-13.095540	27.6901	27.6544	27.6622	27.6524	27.6635
31	H	0.535030	41.251488	-12.262843	29.6446	29.6379	29.6519	29.6494	29.6464
32	H	-0.044356	41.926406	-10.764298	28.9529	28.9482	28.9531	28.9504	28.9543
33	N	0.505000	39.565000	-9.989000	150.5862	150.5483	150.7132	150.4878	150.4020
34	C	0.574000	38.240000	-9.365000	143.2378	143.7891	143.7894	143.7878	143.9679
35	C	-0.509000	38.063000	-8.342000	15.8631	16.1408	16.1200	16.0790	16.0563
36	O	-0.723000	38.940000	-7.548000	-8.0681	-6.3693	-7.2378	-9.2966	-9.9305
37	C	1.950000	38.035000	-8.740000	163.2590	163.4325	163.4748	163.4728	163.5789
38	C	2.190000	36.593000	-8.377000	53.2364	53.0385	53.5318	53.6318	53.7637
39	C	2.674000	35.702000	-9.324000	63.5646	62.8597	63.6071	63.5579	63.5110
40	C	1.894000	36.106000	-7.115000	64.8195	64.2542	64.6978	64.6582	64.6014
41	C	2.858000	34.378000	-9.030000	62.6550	62.3330	62.6496	62.6498	62.6438
42	C	2.102000	34.795000	-6.816000	68.2032	67.9093	68.0868	68.1389	68.1879
43	C	2.570000	33.927000	-7.746000	67.3479	66.6084	67.4711	67.3918	67.3565
44	H	1.117674	40.277489	-9.677406	28.0303	28.0001	28.0599	28.0394	28.0414

45	H	0.422466	37.499484	-10.122346	29.5835	29.6540	29.6418	29.6319	29.6344
46	H	2.699267	38.348233	-9.436695	30.3590	30.3449	30.3475	30.3464	30.3486
47	H	2.023933	38.633685	-7.856252	30.3422	30.3432	30.3550	30.3561	30.3666
48	H	2.908521	36.057660	-10.305532	25.4199	25.2504	25.4260	25.4163	25.4124
49	H	1.499147	36.764904	-6.370126	26.3172	25.7288	26.2773	26.2774	26.2778
50	H	3.217697	33.700540	-9.776033	25.2771	25.0579	25.2721	25.2665	25.2624
51	H	1.892110	34.442471	-5.827785	28.0108	25.5283	27.9309	27.9502	27.9593
52	H	2.717483	32.897811	-7.493179	25.8605	25.3733	25.8521	25.8471	25.8435
53	N	-1.203000	36.913000	-8.377000	160.0628	160.7972	160.6476	160.5848	160.3352
54	C	-2.108000	36.586000	-7.307000	147.1210	146.9139	146.9054	147.0123	146.8809
55	C	-1.953000	35.139000	-6.895000	9.6422	9.9761	9.9117	10.2110	10.2540
56	O	-1.597000	34.275000	-7.727000	-17.0323	-18.8769	-20.8598	-21.9632	-22.4329
57	C	-3.476000	36.949000	-7.571000	145.8471	145.6004	145.5943	145.7777	145.7751
58	O	-3.911000	36.148000	-8.505000	335.5883	335.8440	335.7903	335.7291	335.7834
59	H	-1.091750	36.290669	-9.138858	28.2091	28.1959	28.2532	28.2363	28.2313
60	H	-1.829006	37.194692	-6.472401	29.0692	28.9963	29.0383	29.0550	29.0596
61	H	-4.063128	36.829032	-6.684553	29.6166	29.5871	29.6094	29.6014	29.5952
62	H	-3.526089	37.963456	-7.907556	29.7994	29.7338	29.8210	29.7980	29.7879
63	H	-3.315261	35.408407	-8.480541	32.0502	32.0837	32.0398	32.0468	32.0341

64	N	-2.223000	34.881000	-5.643000	145.8896	144.8785	144.9773	144.7517	144.2147
65	C	-2.199000	33.509000	-5.117000	144.3086	144.0879	144.0990	144.2950	144.4283
66	C	-3.574000	32.853000	-5.142000	26.0216	25.7421	25.8466	25.8331	25.8378
67	O	-4.553000	33.449000	-4.898000	8.4279	8.8670	9.1095	9.0485	9.1163
68	C	-1.728000	33.557000	-3.664000	161.8079	161.9043	161.8417	161.8154	161.8366
69	C	-0.297000	33.983000	-3.491000	49.7733	50.1471	49.5557	49.6369	49.6160
70	C	0.027000	35.337000	-3.357000	58.1957	59.0982	58.1836	58.1889	58.1818
71	C	0.719000	33.048000	-3.389000	60.0001	60.7661	60.0469	60.0144	60.0158
72	C	1.349000	35.708000	-3.155000	64.0566	64.7944	64.0127	64.0709	64.0839
73	C	2.049000	33.437000	-3.192000	59.7540	60.4909	59.8043	59.7889	59.7889
74	C	2.339000	34.779000	-3.062000	65.6557	66.9118	65.7016	65.7064	65.7035
75	H	-2.449251	35.627904	-5.033866	27.4695	27.3832	27.4511	27.4323	27.4283
76	H	-1.542671	32.934443	-5.736691	28.8047	28.8309	28.8318	28.8270	28.8357
77	H	-2.352504	34.240394	-3.127468	30.3349	30.3387	30.3617	30.3496	30.3518
78	H	-1.845881	32.583026	-3.236942	30.1384	30.1573	30.1436	30.1422	30.1420
79	H	-0.739315	36.081893	-3.409876	25.0647	25.2392	25.0476	25.0584	25.0643
80	H	0.482675	32.006998	-3.462252	24.9266	25.1132	24.9282	24.9274	24.9290
81	H	1.594874	36.745945	-3.070646	25.0909	25.3075	25.0770	25.0862	25.0903
82	H	2.828025	32.705136	-3.143060	24.8064	24.9876	24.8029	24.8047	24.8067

83	H	3.347376	35.091260	-2.887156	25.2221	25.3201	25.2259	25.2259	25.2262
84	N	-3.654000	31.562000	-5.253000	179.1563	179.2286	179.1525	179.2129	179.1973
85	C	-4.888000	30.739000	-5.293000	153.0723	153.1645	153.1272	153.1038	153.0984
86	C	-5.841000	30.951000	-6.462000	6.4631	6.5904	6.6188	6.5937	6.5586
87	O	-5.645000	31.816000	-7.350000	-53.7453	-51.3698	-50.2337	-53.2821	-53.8412
88	H	-2.796193	31.072088	-5.318217	29.1009	29.0576	29.1167	29.1015	29.0991
89	H	-4.594392	29.710071	-5.293518	29.4312	29.4298	29.4278	29.4295	29.4245
90	H	-5.432451	30.922755	-4.390389	28.9660	28.9602	28.9677	28.9615	28.9579
91	N	-6.929000	30.184000	-6.458000	160.2947	160.6680	160.4829	160.2669	160.2394
92	C	-7.792000	30.078000	-7.625000	143.7389	143.6753	143.6479	143.7608	143.7202
93	C	-8.798000	31.203000	-7.852000	13.9827	13.6661	13.7084	14.1347	14.0674
94	O	-9.448000	31.239000	-8.891000	5.8251	3.8916	3.9749	1.1056	2.4885
95	C	-8.585000	28.800000	-7.473000	137.7138	137.8157	137.8197	137.8291	137.8154
96	O	-9.444000	28.795000	-6.308000	341.8374	342.0773	342.1185	342.0906	342.0706
97	H	-7.156654	29.673159	-5.641106	27.8225	27.8362	27.8412	27.8184	27.8148
98	H	-7.132393	30.117559	-8.466578	29.0557	28.9985	29.0422	29.0505	29.0509
99	H	-9.189630	28.665711	-8.345519	29.0405	29.0278	29.0381	29.0325	29.0319
100	H	-7.902255	27.979441	-7.399232	29.4545	29.4351	29.4379	29.4376	29.4381
101	H	-9.875581	27.949101	-6.334321	31.9339	31.9419	31.9410	31.9333	31.9312

102	N	-8.891000	32.156000	-6.928000	141.5022	140.6975	140.7021	140.9145	141.1633
103	C	-9.887000	33.229000	-7.072000	143.9838	144.0186	144.0154	143.9427	143.9250
104	C	-9.670000	34.025000	-8.351000	12.7690	12.7582	12.8017	12.7924	12.7960
105	O	-8.535000	34.310000	-8.712000	68.6052	69.3417	69.1182	68.9603	68.9191
106	C	-9.827000	34.163000	-5.878000	170.7442	170.8523	170.8752	170.7694	170.7846
107	C	-11.048000	35.083000	-5.730000	176.1817	176.1378	176.1107	175.9967	175.9305
108	C	-10.945000	35.929000	-4.463000	172.3933	172.4082	172.4006	172.3528	172.3610
109	C	-10.910000	35.084000	-3.174000	152.7065	152.7135	152.7104	152.6646	152.6494
110	N	-10.223000	35.789000	-1.999000	234.8027	234.8216	234.7525	234.8077	234.8009
111	O	-10.614000	34.389000	-9.074000	45.9469	45.9674	45.9344	45.8791	45.9281
112	H	-8.288865	32.142904	-6.142276	27.7398	27.6927	27.7179	27.7164	27.7195
113	H	-10.851954	32.769374	-7.122074	29.9665	29.9678	29.9926	29.9821	29.9853
114	H	-9.738085	33.572542	-4.990107	31.8000	31.7926	31.7940	31.7984	31.7940
115	H	-8.952367	34.772707	-5.968413	31.8838	31.9124	31.9109	31.9108	31.9078
116	H	-11.105684	35.729719	-6.580486	31.3829	31.3926	31.3756	31.3909	31.3962
117	H	-11.934332	34.485470	-5.682313	31.9680	31.9581	31.9388	31.9403	31.9315
118	H	-10.052002	36.516293	-4.513423	31.8743	31.9173	31.8765	31.8749	31.8722
119	H	-11.787421	36.587298	-4.419754	30.9337	30.9463	30.9328	30.9294	30.9277
120	H	-11.914953	34.848939	-2.891659	29.5046	29.5124	29.5037	29.4965	29.4923

121	H	-10.389416	34.171521	-3.377161	29.4134	29.4176	29.4150	29.4202	29.4214
122	H	-10.234019	35.196053	-1.206288	28.8911	28.9051	28.8902	28.8934	28.8909
123	H	-9.286266	35.998140	-2.241673	29.2984	29.3382	29.3045	29.3029	29.3008
124	H	-10.705011	36.628136	-1.790157	29.0859	29.1074	29.1002	29.0866	29.0844

Table 2: Cartesian coordinates and isotropic shielding constants (in ppm) for 2ONW

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	6.410000	2.130000	2.642000	236.2566	236.2788	236.2685	236.2370	236.2327
2	C	7.582000	2.918000	3.128000	143.2670	143.2598	143.2376	143.2659	143.2628
3	C	8.876000	2.139000	2.922000	16.1565	16.1157	16.0483	16.1799	16.1853
4	O	8.852000	0.916000	2.802000	-30.7470	-30.2018	-30.9248	-30.9545	-31.0308
5	C	7.415000	3.275000	4.607000	139.4185	139.4075	139.4133	139.4149	139.3947
6	O	7.225000	2.112000	5.395000	345.1995	345.1799	345.1903	345.1937	345.1742
7	H	5.580280	2.651107	2.783819	28.9115	28.9029	28.8990	28.9124	28.9105
8	H	6.518482	1.938478	1.676779	28.6645	28.6587	28.6672	28.6552	28.6529
9	H	6.354382	1.278093	3.143259	27.9477	27.9287	27.9424	27.9421	27.9398
10	H	7.632500	3.823144	2.559613	29.0636	29.0500	29.0585	29.0626	29.0581
11	H	8.290781	3.788502	4.944970	29.0318	29.0240	29.0341	29.0395	29.0330
12	H	6.566556	3.917224	4.719210	29.0319	29.0248	29.0353	29.0328	29.0295
13	H	7.133168	2.438362	6.282443	31.5767	31.5659	31.5829	31.5756	31.5728
14	N	10.005000	2.843000	2.884000	162.8968	162.9720	163.0495	163.5765	163.3386
15	C	11.285000	2.190000	2.618000	143.4747	143.1668	143.1848	143.4715	143.3325

16	C	12.490000	2.926000	3.202000	12.5213	12.7722	12.8293	12.9547	12.9801
17	O	12.447000	4.133000	3.435000	-31.4201	-33.7125	-33.6379	-35.1037	-34.7881
18	C	11.475000	2.001000	1.109000	138.9944	138.6707	138.6954	138.7925	138.8730
19	O	11.511000	3.245000	0.432000	342.4625	342.6265	342.6397	342.6303	342.6749
20	H	9.977251	3.820592	3.037764	27.5843	27.5773	27.5852	27.6210	27.6136
21	H	11.241818	1.242255	3.112788	28.6105	28.5784	28.5933	28.6108	28.6065
22	H	12.393897	1.481266	0.934632	29.4835	29.4570	29.4825	29.4774	29.4697
23	H	10.664718	1.417187	0.724935	29.2830	29.2548	29.2724	29.2730	29.2603
24	H	11.790096	3.867574	1.093065	32.4779	32.4580	32.4720	32.4787	32.4757
25	N	13.556000	2.167000	3.447000	159.2380	159.4744	159.4470	159.1830	158.9652
26	C	14.858000	2.708000	3.830000	138.4186	138.4083	138.3974	138.3433	138.2764
27	C	15.909000	2.001000	2.975000	13.8993	14.3175	14.3128	14.4633	14.3949
28	O	15.943000	0.773000	2.940000	-3.7101	-7.3082	-7.6929	-8.5629	-8.0317
29	C	15.154000	2.471000	5.327000	132.5197	132.4422	132.4428	132.4252	132.4113
30	O	14.063000	2.960000	6.118000	316.0425	315.8021	315.8018	315.7415	315.6260
31	C	16.438000	3.180000	5.750000	179.5072	179.5949	179.5905	179.5754	179.5742
32	H	13.461527	1.184901	3.365415	27.8353	27.7834	27.7814	27.8030	27.8101
33	H	14.870614	3.766118	3.671487	28.8740	28.8629	28.8692	28.8731	28.8736
34	H	15.276380	1.419250	5.481094	29.5318	29.5483	29.5440	29.5341	29.5301

35	H	16.619215	2.999838	6.789039	31.5348	31.5400	31.5352	31.5316	31.5286
36	H	17.258563	2.805176	5.174602	32.2172	32.1936	32.1897	32.1989	32.2020
37	H	16.336229	4.231953	5.582857	31.9843	31.9747	31.9716	31.9718	31.9698
38	H	13.306514	2.479576	5.802688	31.4712	31.4618	31.4437	31.4499	31.4496
39	N	16.760000	2.760000	2.285000	156.8452	156.3795	156.3927	156.3183	156.3672
40	C	17.698000	2.159000	1.328000	145.1786	145.1105	145.1045	145.1376	145.1252
41	C	19.025000	2.904000	1.180000	14.4960	14.3901	14.4143	14.4619	14.4897
42	O	19.088000	4.119000	1.341000	-7.7147	-7.4448	-7.4777	-7.6319	-7.6400
43	C	17.032000	2.032000	-0.044000	139.4191	139.4107	139.3944	139.4480	139.4675
44	O	16.484000	3.271000	-0.459000	340.2549	340.2342	340.1705	340.2469	340.2306
45	H	16.759813	3.740860	2.419217	27.5587	27.5104	27.5165	27.5192	27.5278
46	H	17.941262	1.198319	1.731505	28.7040	28.6635	28.6715	28.6830	28.6847
47	H	17.760398	1.712720	-0.759819	29.6367	29.6091	29.6166	29.6237	29.6251
48	H	16.250583	1.303123	0.010994	29.4004	29.3733	29.3777	29.3812	29.3835
49	H	17.056503	3.924785	-0.075196	32.4034	32.3853	32.3988	32.3939	32.3976
50	N	20.075000	2.150000	0.857000	151.5855	151.5682	151.5356	151.5160	151.4512
51	C	21.412000	2.702000	0.636000	148.7604	148.8710	148.7631	148.7578	148.7550
52	C	22.098000	1.960000	-0.511000	13.8687	13.9631	13.8571	13.8939	13.8705
53	O	22.063000	0.733000	-0.560000	25.3172	26.8991	25.9126	25.7405	25.3608

54	C	22.241000	2.596000	1.907000	177.5788	177.5665	177.5540	177.5728	177.5776
55	H	19.944832	1.173169	0.762352	27.8904	27.8869	27.8674	27.8766	27.8777
56	H	21.323277	3.735647	0.374079	28.9458	28.9682	28.9431	28.9366	28.9393
57	H	23.215221	3.002558	1.732344	32.0669	32.0894	32.0630	32.0642	32.0656
58	H	21.761806	3.142824	2.692020	31.6782	31.7065	31.6757	31.6724	31.6756
59	H	22.329102	1.568056	2.190672	31.7838	31.8072	31.7866	31.7795	31.7817
60	N	22.714000	2.699000	-1.433000	140.7091	140.9809	140.8312	140.8158	140.7934
61	C	23.397000	2.092000	-2.581000	150.7555	150.8189	150.7739	150.7643	150.7612
62	C	24.750000	2.741000	-2.846000	16.4311	16.3972	16.3951	16.4262	16.4273
63	O	25.580000	2.190000	-3.570000	67.6240	67.7934	67.8158	67.6368	67.6407
64	C	22.524000	2.177000	-3.820000	177.6978	177.6950	177.6550	177.6932	177.6959
65	O	25.048000	3.827000	-2.351000	56.6111	56.6915	56.6308	56.6075	56.6159
66	H	22.710723	3.684699	-1.340871	27.8655	27.8903	27.8643	27.8617	27.8618
67	H	23.572293	1.063739	-2.342566	29.0002	29.0180	28.9976	28.9973	28.9983
68	H	23.034896	1.730904	-4.647577	31.8597	31.8733	31.8597	31.8569	31.8580
69	H	21.605439	1.656725	-3.645470	31.9482	31.9615	31.9502	31.9424	31.9444
70	H	22.316329	3.203283	-4.040264	32.1643	32.1792	32.1641	32.1604	32.1619

Table 3: Cartesian coordinates and isotropic shielding constants (in ppm) for 3DRF

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	19.307000	45.799000	20.873000	231.2037	231.2043	231.2130	231.2091	231.2106
2	C	18.108000	45.529000	21.642000	148.6771	148.6693	148.7607	148.6669	148.6557
3	C	18.160000	46.354000	22.960000	23.3594	23.3808	23.4450	23.3543	23.3286
4	O	19.142000	46.351000	23.651000	-3.7629	-3.4996	-3.6472	-3.7281	-3.8133
5	C	17.997000	43.962000	21.838000	176.5242	176.5301	176.5166	176.5200	176.5136
6	H	19.283539	45.278161	20.031408	28.8521	28.8433	28.8741	28.8561	28.8521
7	H	19.353118	46.765150	20.661983	28.6535	28.6522	28.6776	28.6636	28.6599
8	H	20.103096	45.538062	21.400487	28.4521	28.4480	28.4369	28.4584	28.4544
9	H	17.213317	45.838398	21.143287	29.3336	29.3169	29.3540	29.3437	29.3394
10	H	17.117956	43.734751	22.404162	31.3157	31.3068	31.3113	31.3199	31.3167
11	H	17.938054	43.486195	20.881426	31.4103	31.4054	31.4363	31.4159	31.4119
12	H	18.859967	43.605941	22.360886	31.4504	31.4467	31.4395	31.4514	31.4479
13	N	17.064000	47.025000	23.271000	160.1549	160.1408	160.0564	160.1957	160.2179
14	C	17.063000	47.951000	24.393000	144.2287	144.2225	144.2405	144.2143	144.2130
15	C	15.656000	48.024000	25.017000	32.1375	32.1475	32.1834	32.1437	32.1312

16	O	14.715000	47.605000	24.472000	-1.5850	-1.1578	-1.1870	-1.5139	-1.6597
17	C	17.556000	49.320000	23.946000	139.2285	139.2236	139.2361	139.2284	139.2285
18	O	16.637000	49.824000	23.016000	336.1183	336.1313	336.0788	336.1636	336.1458
19	H	16.239898	46.896612	22.737641	27.5254	27.5190	27.5282	27.5278	27.5280
20	H	17.735008	47.596785	25.146549	28.7265	28.7198	28.7228	28.7326	28.7285
21	H	17.615890	49.976589	24.788736	29.4126	29.4150	29.4235	29.4234	29.4178
22	H	18.519381	49.227087	23.489749	29.5229	29.5203	29.5276	29.5281	29.5253
23	H	15.841166	49.330725	23.176710	32.7842	32.7775	32.7984	32.7949	32.7938
24	N	15.601000	48.568000	26.202000	162.9300	162.9424	162.8291	162.9737	162.9997
25	C	14.326000	48.835000	26.891000	146.4918	146.4367	146.4118	146.4519	146.5125
26	C	13.673000	50.063000	26.276000	25.3426	25.3804	25.3930	25.3303	25.2858
27	O	14.326000	51.018000	26.056000	15.1873	15.7328	15.9468	15.3261	15.0822
28	C	14.515000	49.083000	28.410000	160.2866	160.2090	160.1941	160.2696	160.3488
29	C	15.099000	47.889000	29.154000	24.8795	24.8781	24.8554	24.7791	24.7554
30	O	16.193670	47.925394	29.628539	-16.9264	-15.7659	-15.6875	-16.2044	-16.2796
31	N	14.315411	46.840482	29.267620	175.5582	175.6948	175.6563	175.6412	175.6260
32	H	16.447321	48.810316	26.654905	28.4781	28.5026	28.5096	28.5058	28.4954
33	H	13.710787	47.967637	26.772282	29.1082	29.0904	29.0969	29.1044	29.1094
34	H	15.168176	49.920309	28.541053	30.9897	31.0058	31.0061	30.9938	30.9952

35	H	13.563875	49.320980	28.838516	30.7211	30.7201	30.7212	30.7394	30.7422
36	H	13.413618	46.849883	28.859232	28.4330	28.4323	28.4102	28.4227	28.4167
37	H	14.626780	46.041035	29.761618	28.3862	28.3935	28.3930	28.3889	28.3839
38	N	12.368000	49.965000	26.010000	162.2674	162.5043	162.3680	162.3282	162.3410
39	C	11.575000	51.065000	25.431000	144.8160	144.9377	144.8938	144.8412	144.8417
40	C	10.278000	51.240000	26.223000	31.0599	31.2493	31.2682	31.1456	31.0992
41	O	9.674000	50.317000	26.607000	16.0162	18.4807	17.7597	16.8338	16.2082
42	C	11.301000	50.828000	23.928000	132.6004	132.6136	132.6127	132.6016	132.6106
43	O	12.538000	50.960000	23.154000	334.3192	334.1877	334.3094	334.2786	334.2636
44	H	11.909964	49.110823	26.211705	28.1026	28.1124	28.1216	28.1121	28.1124
45	H	12.138085	51.972053	25.502348	28.9037	28.9232	28.9055	28.9108	28.9107
46	H	10.903092	49.844017	23.792547	29.5547	29.5750	29.5673	29.5658	29.5649
47	H	10.589053	51.547545	23.581177	29.5394	29.5624	29.5474	29.5488	29.5469
48	H	12.274553	50.799939	22.255403	32.1091	32.1161	32.1102	32.1196	32.1177
49	N	9.913000	52.485000	26.427000	156.7972	157.2854	157.0628	156.9872	156.7565
50	C	8.679000	52.842000	27.113000	141.4790	141.2976	141.2598	141.4265	141.4581
51	C	7.470000	52.593000	26.222000	18.7671	18.6236	18.6603	18.6967	18.6814
52	O	7.391000	53.089000	25.122000	38.3767	38.3062	38.7948	38.1967	38.0928
53	C	8.682000	54.344000	27.401000	165.0781	165.1166	165.1062	165.1369	165.1372

54	C	9.894000	54.770000	28.256000	171.1867	170.9304	170.9299	171.1188	171.1034
55	C	7.427000	54.752000	28.067000	183.8725	184.0593	184.0605	184.0260	184.0193
56	C	9.994000	56.334000	28.415000	184.4038	184.3546	184.3566	184.3448	184.3208
57	H	10.501414	53.211243	26.100749	28.5874	28.5918	28.6075	28.6008	28.5909
58	H	8.622354	52.253062	28.004540	29.9519	29.9422	29.9387	29.9431	29.9428
59	H	8.757873	54.841474	26.456721	31.8823	31.8701	31.8737	31.8694	31.8637
60	H	9.805855	54.328037	29.226463	32.3669	32.3213	32.3278	32.3445	32.3405
61	H	10.788750	54.411043	27.791810	31.7103	31.7150	31.7372	31.7070	31.6890
62	H	7.450757	55.804426	28.258661	31.8471	31.8445	31.8571	31.8495	31.8470
63	H	6.596069	54.523646	27.432722	32.4704	32.4146	32.4378	32.4435	32.4551
64	H	7.325731	54.223262	28.991706	32.7939	32.7837	32.7947	32.7945	32.7917
65	H	10.846845	56.577865	29.013402	32.0423	32.0322	32.0400	32.0373	32.0341
66	H	10.094757	56.784903	27.449891	32.4940	32.4797	32.4845	32.4870	32.4842
67	H	9.108324	56.701598	28.889710	31.9461	31.9489	31.9430	31.9411	31.9393
68	N	6.550000	51.803000	26.713000	145.3612	145.4183	145.2913	145.3042	145.3214
69	C	5.365000	51.416000	25.959000	148.1375	148.2185	148.1337	148.1242	148.1172
70	C	4.159000	52.253000	26.419000	5.2885	5.3773	5.3842	5.3086	5.2396
71	O	4.080000	52.635000	27.607000	-11.2040	-9.6952	-9.9786	-10.4173	-11.2362
72	C	5.080000	49.886000	26.140000	177.2627	177.2714	177.2263	177.2470	177.2559

73	H	6.663477	51.454614	27.632701	27.8773	27.8431	27.8452	27.8534	27.8575
74	H	5.535094	51.602082	24.919124	28.7479	28.7478	28.7497	28.7431	28.7457
75	H	4.208043	49.617069	25.581192	31.7510	31.7596	31.7471	31.7529	31.7544
76	H	5.918141	49.322771	25.786175	31.6687	31.6776	31.6734	31.6687	31.6697
77	H	4.919185	49.673297	27.176241	31.7543	31.7701	31.7485	31.7528	31.7549
78	N	3.261000	52.534000	25.490000	154.9130	155.0947	155.0082	155.0005	154.9289
79	C	2.082000	53.359000	25.796000	142.8436	142.8889	142.8654	142.8659	142.8591
80	C	0.981000	52.643000	26.556000	22.8830	22.8533	22.8628	22.8746	22.8809
81	O	0.277000	53.290000	27.275000	14.2297	14.3135	14.4190	13.8754	13.8387
82	C	1.558000	53.988000	24.540000	140.8700	140.8541	140.8580	140.8613	140.8624
83	O	1.164000	53.010000	23.604000	343.1374	343.1268	343.1469	343.1195	343.1218
84	H	3.384204	52.183087	24.572514	27.3824	27.3715	27.3892	27.3776	27.3802
85	H	2.420668	54.117670	26.470259	29.0820	29.0952	29.0698	29.0748	29.0745
86	H	0.715359	54.601867	24.780880	29.2271	29.2300	29.2243	29.2222	29.2227
87	H	2.323624	54.597972	24.107966	29.3725	29.3692	29.3670	29.3664	29.3688
88	H	0.852638	53.507486	22.856965	31.8774	31.8722	31.8760	31.8735	31.8741
89	N	0.895000	51.336000	26.452000	164.6018	164.6664	164.5608	164.6855	164.6953
90	C	-0.177000	50.638000	27.132000	154.6253	154.6337	154.6279	154.6252	154.6216
91	C	0.321000	50.177000	28.457000	25.4932	25.4885	25.4889	25.4823	25.4778

92	O	1.057000	49.218000	28.441000	67.4732	67.4223	67.6116	67.6090	67.6234
93	O	0.032000	50.700000	29.508000	66.6401	66.7719	66.4732	66.6140	66.6310
94	H	1.556536	50.832960	25.914022	27.6789	27.6622	27.6703	27.6710	27.6711
95	H	-1.006400	51.299792	27.269942	29.5551	29.5623	29.5582	29.5475	29.5466
96	H	-0.483150	49.794293	26.549479	30.2842	30.2820	30.2729	30.2803	30.2794

Table 4: Cartesian coordinates and isotropic shielding constants (in ppm) for 3DRJ

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	-1.904000	21.612000	-1.857000	228.6487	228.6279	228.6279	228.6433	228.6491
2	C	-1.080000	20.392000	-1.603000	145.4420	145.4175	145.4126	145.4163	145.4149
3	C	-1.111000	19.963000	-0.138000	19.4874	19.4703	19.4925	19.4728	19.4707
4	O	-0.920000	18.794000	0.174000	-8.7626	-8.2606	-8.4081	-8.5699	-8.5759
5	C	0.354000	20.645000	-2.017000	180.8964	180.8844	180.8989	180.8916	180.8958
6	H	-1.853118	21.850716	-2.816440	28.8598	28.8537	28.8636	28.8532	28.8525
7	H	-2.845848	21.431091	-1.611449	28.6908	28.6681	28.6765	28.6853	28.6867
8	H	-1.559076	22.362653	-1.311429	29.7063	29.6917	29.7063	29.7027	29.7034
9	H	-1.503141	19.599827	-2.184648	29.1287	29.1253	29.1349	29.1259	29.1248
10	H	0.938502	19.767924	-1.832621	31.4792	31.4732	31.4791	31.4766	31.4765
11	H	0.387491	20.883264	-3.059597	31.7090	31.7077	31.7122	31.7071	31.7066
12	H	0.749565	21.462633	-1.451399	32.6500	32.6367	32.6434	32.6420	32.6412
13	N	-1.340000	20.912000	0.759000	149.1490	149.2044	149.2402	149.2575	149.1500
14	C	-1.311000	20.608000	2.189000	147.8454	148.0313	148.0411	148.0610	148.3032
15	C	-2.718000	20.541000	2.717000	11.3858	11.4872	11.4795	11.4528	11.4951

16	O	-3.628000	21.222000	2.219000	14.7614	15.8094	16.2237	16.1509	16.3240
17	C	-0.530000	21.651000	2.926000	171.5554	171.5398	171.5554	171.5223	171.5107
18	C	0.717000	22.041000	2.226000	51.1885	51.1742	51.1990	51.2597	51.2920
19	N	0.992796	23.345875	1.871430	-33.4343	-33.5286	-33.4424	-33.4545	-33.5207
20	C	1.771255	21.303078	1.817449	78.6891	78.8016	78.8010	78.7572	78.7372
21	C	2.167701	23.390386	1.270974	53.3820	53.3477	53.3555	53.3480	53.3346
22	N	2.662284	22.164678	1.230552	106.7572	106.8119	106.7571	106.7618	106.7718
23	H	-1.532461	21.835222	0.457802	28.8988	28.8825	28.8958	28.8958	28.8935
24	H	-0.834107	19.661676	2.337133	28.1284	28.1399	28.1254	28.1250	28.1363
25	H	-1.143368	22.519482	3.046079	30.4688	30.4694	30.4687	30.4643	30.4668
26	H	-0.277124	21.271670	3.894020	29.8648	29.8768	29.8651	29.8640	29.8623
27	H	1.889280	20.245611	1.930286	25.8158	25.8113	25.8262	25.8211	25.8201
28	H	2.639515	24.268886	0.882993	24.7157	24.7071	24.7137	24.7119	24.7105
29	H	3.535384	21.909971	0.839499	24.7879	24.7848	24.7879	24.7882	24.7873
30	N	-2.890000	19.719000	3.738000	148.5630	148.4877	148.3591	148.4590	148.3876
31	C	-4.214000	19.419000	4.239000	151.2798	151.3480	151.3129	151.3538	151.3716
32	C	-4.226000	19.426000	5.755000	9.4893	9.3503	9.3712	9.3913	9.4005
33	O	-3.203000	19.140000	6.386000	-9.4050	-9.0910	-9.1512	-9.2686	-9.3326
34	C	-4.632000	18.076000	3.721000	176.9894	176.9037	176.9428	176.9703	176.9915

35	H	-2.100797	19.302240	4.166450	27.4199	27.4262	27.4371	27.4319	27.4359
36	H	-4.900903	20.167012	3.902039	28.5861	28.5729	28.5851	28.5879	28.5857
37	H	-5.610710	17.842217	4.084831	31.9886	31.9702	31.9795	31.9815	31.9831
38	H	-4.644125	18.094320	2.651226	31.7503	31.7329	31.7373	31.7388	31.7369
39	H	-3.939558	17.332752	4.057165	31.8470	31.8350	31.8446	31.8420	31.8438
40	N	-5.398000	19.712000	6.318000	154.2661	154.5337	154.4498	154.3867	154.2144
41	C	-5.540000	19.838000	7.789000	147.7429	147.8033	147.7284	147.7930	147.9872
42	C	-5.129000	18.525000	8.400000	8.5616	8.4840	8.4781	8.5246	8.5066
43	O	-5.596000	17.461000	7.965000	5.9749	11.8863	11.2882	9.2821	7.9417
44	C	-6.976000	20.132000	8.251000	172.9460	172.9265	172.9137	172.9416	172.9927
45	C	-7.801000	21.091000	7.437000	180.1076	179.8991	179.8233	179.8903	180.0258
46	C	-7.593000	22.549000	7.796000	178.5887	178.6164	178.5735	178.6053	178.6010
47	C	-8.438000	23.427000	6.937000	160.5080	160.5508	160.5013	160.5355	160.5494
48	N	-9.549000	22.666000	6.299000	237.1067	237.1390	237.1064	237.1388	237.1496
49	H	-6.192394	19.843497	5.742025	28.0484	28.0389	28.0573	28.0482	28.0546
50	H	-4.931083	20.662492	8.096135	29.3067	29.3459	29.3136	29.3146	29.3278
51	H	-7.502248	19.201066	8.287396	31.2529	31.2829	31.2501	31.2627	31.2648
52	H	-6.923974	20.514650	9.248884	31.5655	31.5964	31.5858	31.5811	31.5794
53	H	-7.556280	20.957374	6.403967	32.2711	32.2915	32.2559	32.2564	32.2575

54	H	-8.834688	20.851448	7.574856	31.8258	31.8325	31.7924	31.8010	31.8012
55	H	-7.856382	22.700544	8.821946	31.3264	31.3371	31.3216	31.3157	31.3113
56	H	-6.563283	22.803392	7.655045	31.2151	31.2229	31.2226	31.2144	31.2140
57	H	-8.851286	24.209867	7.538011	29.4062	29.4219	29.3994	29.3979	29.3946
58	H	-7.827086	23.859508	6.172395	29.5569	29.5831	29.5572	29.5478	29.5447
59	H	-10.088244	23.277706	5.737634	29.0714	29.0869	29.0573	29.0584	29.0537
60	H	-9.173345	21.944834	5.734285	28.8255	28.8454	28.8089	28.8083	28.8071
61	H	-10.123528	22.269873	7.001211	29.0699	29.0884	29.0569	29.0598	29.0565
62	N	-4.255000	18.572000	9.398000	145.7523	146.1090	146.0635	145.8177	145.7691
63	C	-3.810000	17.360000	10.062000	149.4118	149.4790	149.4537	149.4506	149.4667
64	C	-2.526000	17.551000	10.838000	13.8081	13.7462	13.7371	13.7878	13.7777
65	O	-1.947000	16.565000	11.320000	69.1699	69.4850	69.3030	69.1650	69.1799
66	C	-3.630000	16.234000	9.039000	179.1023	179.1084	179.0703	179.0949	179.0955
67	O	-2.051000	18.687000	10.994000	55.3777	55.5567	55.5364	55.4354	55.4439
68	H	-3.900867	19.447712	9.694341	27.3244	27.3717	27.3599	27.3507	27.3456
69	H	-4.570932	17.099354	10.767653	29.8199	29.8436	29.8256	29.8216	29.8199
70	H	-3.302219	15.346717	9.539189	32.0201	32.0515	32.0181	32.0221	32.0195
71	H	-4.562555	16.043945	8.550001	27.8894	27.9020	27.8717	27.8758	27.8754
72	H	-2.899502	16.524865	8.313279	32.6329	32.6679	32.6403	32.6282	32.6268

Table 5: Cartesian coordinates and isotropic shielding constants (in ppm) for 3DS1

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	5.374000	22.958000	43.943000	240.0413	239.7542	240.0421	240.1729	240.1569
2	C	3.910000	22.649000	43.902000	138.4691	138.4058	138.5321	138.4644	138.4673
3	C	3.691000	21.192000	44.261000	11.8693	12.5348	11.9715	12.0534	11.9382
4	O	4.638000	20.393000	44.255000	0.4338	-9.4767	-1.9610	-3.0832	-3.4332
5	C	3.222000	22.964000	42.538000	163.1082	162.1241	163.0329	162.5130	162.2832
6	C	3.737000	22.062000	41.422000	176.7511	176.6230	176.6311	176.4077	176.2967
7	C	3.359000	24.448000	42.186000	182.3635	181.9415	182.4331	182.3201	182.2982
8	C	2.707000	21.780000	40.314000	183.9575	184.5202	183.9871	183.7380	183.6795
9	H	5.517206	23.909145	43.708661	29.0661	28.9839	29.0411	29.0866	29.0833
10	H	5.722087	22.786506	44.853783	28.8154	28.7331	28.8233	28.8257	28.8221
11	H	5.851003	22.382723	43.293674	28.8328	28.7664	28.8585	28.8412	28.8406
12	H	3.449406	23.297088	44.618055	28.7601	28.9915	28.7910	28.7896	28.7724
13	H	2.178279	22.753042	42.643084	30.2492	31.2614	30.2565	30.2563	30.2740
14	H	4.594026	22.525000	40.979238	32.3693	32.2669	32.3856	32.3737	32.3635
15	H	4.038430	21.129244	41.850959	32.0289	32.0378	32.0881	32.0477	32.0393

16	H	2.879991	24.637823	41.248227	31.7039	31.5000	31.7472	31.6983	31.6878
17	H	2.897116	25.039572	42.948630	31.9670	31.8814	32.0060	31.9887	31.9788
18	H	4.395621	24.703543	42.115184	32.6590	32.5256	32.6480	32.6757	32.6668
19	H	3.144757	21.143404	39.573720	32.0602	32.0131	32.0642	32.0450	32.0403
20	H	1.850565	21.298188	40.737411	32.1502	32.1528	32.1593	32.1775	32.1867
21	H	2.409498	22.702328	39.860454	32.2108	32.0218	32.2441	32.2004	32.1947
22	N	2.437000	20.868000	44.564000	154.6153	156.3155	151.2340	152.0275	152.1481
23	C	2.067000	19.531000	45.005000	142.3289	141.9128	141.8759	142.0748	142.0454
24	C	1.136000	18.875000	43.977000	7.0008	8.0109	7.6656	7.4591	7.2484
25	O	0.666000	19.523000	43.032000	-34.8346	-44.9174	-26.9332	-25.9110	-23.0308
26	C	1.310000	19.595000	46.337000	131.0990	131.4629	131.3131	131.2647	131.1817
27	O	0.162000	20.455000	46.196000	295.9523	305.4576	294.8078	295.2350	294.8779
28	C	2.206000	20.129000	47.457000	175.6803	175.5300	175.4753	175.4711	175.4630
29	H	1.732120	21.558887	44.487058	24.8140	27.5127	24.7586	24.7374	24.7298
30	H	2.967682	18.964131	45.116052	28.3617	28.2289	28.3612	28.3488	28.3369
31	H	1.000060	18.603740	46.594374	29.1820	29.1314	29.1584	29.1723	29.1701
32	H	1.651945	20.162247	48.371778	31.9561	31.9106	31.9729	31.9545	31.9428
33	H	3.051579	19.484114	47.575394	32.1454	32.0858	32.1428	32.1323	32.1195
34	H	2.540893	21.113973	47.206850	31.7057	31.6953	31.6816	31.6848	31.6746

35	H	-0.250183	20.443745	47.051850	32.2576	32.1275	32.3277	32.3000	32.2539
36	N	0.871000	17.584000	44.163000	149.5624	150.2434	148.8094	148.0541	147.8388
37	C	-0.030000	16.861000	43.271000	142.0667	142.0382	142.2604	142.2541	142.2323
38	C	-1.433000	17.475000	43.382000	10.9036	12.2656	12.1159	11.8806	11.6134
39	O	-2.155000	17.571000	42.404000	-17.1146	-34.9643	-20.1272	-15.6487	-6.6478
40	C	-0.056000	15.378000	43.636000	164.7740	164.5553	164.6518	164.6030	164.6819
41	C	-0.942000	14.555000	42.761000	53.8256	53.0285	53.6560	53.7221	53.8342
42	C	-0.800000	14.583000	41.380000	60.2220	60.5599	60.1668	60.1438	60.1993
43	C	-1.924000	13.746000	43.315000	59.8605	60.9022	59.9712	59.9872	59.9608
44	C	-1.632000	13.817000	40.561000	61.1831	61.0262	61.2623	61.2820	61.2556
45	C	-2.746000	12.971000	42.490000	59.5148	61.9030	59.4847	59.4764	59.4163
46	C	-2.604000	13.014000	41.127000	64.1810	65.4901	64.1996	64.2316	64.1881
47	H	1.292700	17.105462	44.920146	27.6231	27.6867	27.5914	27.5734	27.5528
48	H	0.313198	16.943829	42.260924	28.4714	28.4732	28.3818	28.4227	28.4400
49	H	0.940315	14.993433	43.569926	29.7426	29.7961	29.6990	29.6986	29.6886
50	H	-0.391802	15.281977	44.647393	30.3624	30.4370	30.3262	30.3548	30.3545
51	H	-0.044399	15.198582	40.938383	24.8465	24.9039	24.7613	24.7907	24.7997
52	H	-2.052876	13.714895	44.376755	25.2331	25.2870	25.2362	25.2432	25.2386
53	H	-1.517274	13.851647	39.497733	25.0096	24.9836	24.9901	24.9990	24.9941

54	H	-3.491582	12.339552	42.926213	25.1035	25.1883	25.1051	25.1021	25.0944
55	H	-3.244591	12.426897	40.502617	25.1812	25.2310	25.1803	25.1839	25.1763
56	N	-1.793000	17.887000	44.590000	152.0688	157.7122	152.0059	152.0603	151.9392
57	C	-3.065000	18.569000	44.824000	142.2280	142.1194	141.7720	141.9100	142.0448
58	C	-3.250000	19.814000	43.956000	11.9670	12.6204	11.8656	11.9344	11.9181
59	O	-4.352000	20.092000	43.516000	1.3487	-9.6243	1.7700	2.3161	1.6118
60	C	-3.190000	18.917000	46.308000	170.8696	170.7031	171.0075	170.7688	170.7132
61	C	-3.299000	17.658000	47.156000	161.5969	160.8423	160.9903	161.0840	161.0592
62	C	-3.323000	17.960000	48.652000	9.4856	9.3743	9.3233	9.3533	9.4007
63	O	-4.263000	18.660000	49.103000	50.7836	52.1174	51.5651	51.4457	51.2177
64	O	-2.406000	17.501000	49.368000	23.9692	23.5284	24.8675	24.6385	24.4172
65	H	-1.183910	17.728482	45.354187	27.7414	28.0354	27.6426	27.6776	27.7037
66	H	-3.846239	17.895285	44.539967	29.7653	29.9685	29.8337	29.8361	29.8409
67	H	-2.327360	19.472003	46.612504	32.0757	32.1571	32.0454	32.0698	32.0821
68	H	-4.063708	19.516752	46.455755	31.2614	31.3825	31.3214	31.2853	31.2779
69	H	-4.198295	17.141135	46.893286	31.4111	31.4083	31.3903	31.4053	31.3852
70	H	-2.462387	17.025347	46.944509	31.6651	31.6644	31.6557	31.6346	31.6237
71	N	-2.173000	20.560000	43.725000	149.1990	150.6283	149.5566	149.2780	149.8143
72	C	-2.190000	21.734000	42.826000	142.7908	142.7462	143.4199	143.3352	143.3891

73	C	-2.482000	21.275000	41.398000	5.8745	6.9072	7.5738	7.2618	7.0566
74	O	-3.217000	21.939000	40.664000	-7.1405	-28.6602	-3.1183	-5.9720	-13.1363
75	C	-0.861000	22.482000	42.853000	162.8529	161.3505	163.1344	162.9518	163.2056
76	C	-0.541000	23.067000	44.224000	15.8791	17.5922	15.8678	15.9609	16.0245
77	O	-1.474000	23.453000	44.936000	38.2075	54.2458	39.4474	39.2600	38.5650
78	O	0.649000	23.142000	44.564000	56.1286	33.2590	53.1207	53.0084	52.7457
79	H	-1.324211	20.318984	44.173963	27.8658	28.5621	27.7440	27.8028	27.8508
80	H	-2.954001	22.400965	43.167117	28.7328	28.7800	28.7300	28.7666	28.7668
81	H	-0.079236	21.806204	42.575430	30.4942	31.5021	30.4967	30.5053	30.5026
82	H	-0.898633	23.277820	42.138750	31.0900	30.9382	31.1430	31.1237	31.1164
83	N	-1.904000	20.141000	41.004000	146.1745	157.3095	149.0950	148.8339	149.0333
84	C	-2.169000	19.603000	39.660000	145.1200	145.0183	144.6715	144.9604	144.9815
85	C	-3.629000	19.208000	39.551000	4.2233	4.8402	3.3105	3.5061	3.4960
86	O	-4.297000	19.556000	38.564000	-4.8009	-26.4199	-3.8943	-2.1079	-1.3902
87	C	-1.261000	18.418000	39.334000	163.7353	162.1450	163.8843	163.7129	163.7334
88	C	0.237000	18.763000	39.221000	174.1293	173.0494	173.7544	173.7954	173.6847
89	C	1.059000	17.506000	39.051000	175.0807	175.6824	175.1424	174.9682	174.9438
90	C	0.496000	19.700000	38.036000	177.0401	177.8493	176.8054	176.8033	176.8303
91	H	-1.294408	19.658836	41.617201	27.0636	27.9960	26.9648	27.0295	27.1393

92	H	-1.953891	20.367973	38.943449	29.0428	29.1125	29.1165	29.1035	29.1003
93	H	-1.380460	17.680739	40.100209	30.8313	31.9129	30.7871	30.8112	30.8473
94	H	-1.580444	17.993850	38.405048	31.9274	32.0655	31.9954	31.9658	31.9425
95	H	0.525340	19.257327	40.125102	31.5317	31.9723	31.5026	31.5277	31.5320
96	H	2.094450	17.764601	38.974395	31.8222	32.0187	31.8354	31.8280	31.8131
97	H	0.912584	16.867004	39.896663	31.6919	32.1457	31.6037	31.6531	31.6667
98	H	0.751864	16.996558	38.161598	32.0954	32.4478	32.1249	32.1119	32.0981
99	H	1.540871	19.923586	37.979837	32.0999	32.1304	32.0844	32.0968	32.0881
100	H	0.183936	19.223893	37.129999	32.3932	32.6545	32.3810	32.3903	32.3859
101	H	-0.055999	20.606639	38.170918	31.9847	31.9135	31.9562	31.9624	31.9714
102	N	-4.135000	18.518000	40.568000	145.7168	148.8623	146.2973	145.5200	145.3976
103	C	-5.557000	18.110000	40.565000	143.7360	143.8195	144.5374	144.6139	144.8017
104	C	-6.499000	19.303000	40.450000	1.7003	2.5949	2.3028	2.1958	2.2205
105	O	-7.522000	19.243000	39.720000	10.6510	-11.3504	15.4397	11.6782	6.8520
106	C	-5.889000	17.279000	41.817000	163.2203	161.6393	163.6069	163.4533	163.4513
107	C	-5.269000	15.880000	41.868000	175.4190	173.8825	176.5155	176.1535	176.0441
108	C	-5.388000	15.302000	43.277000	175.2427	175.2805	175.2469	175.0521	175.0123
109	C	-5.888000	14.947000	40.835000	178.8808	178.2716	178.8780	178.8504	178.8463
110	H	-3.555901	18.275218	41.333376	25.8215	28.2078	25.7133	25.7680	25.8362

111	H	-5.706537	17.502182	39.697189	29.5068	29.1648	29.4847	29.4739	29.4599
112	H	-5.557254	17.822953	42.676627	31.7213	31.8855	31.7598	31.8202	31.8563
113	H	-6.952297	17.175557	41.876994	32.3464	31.9573	32.3191	32.2899	32.2743
114	H	-4.231587	15.969938	41.621858	33.3586	31.9667	33.3230	33.3111	33.3231
115	H	-4.951691	14.325265	43.299858	32.3404	32.0678	32.3388	32.3158	32.3029
116	H	-4.875110	15.938001	43.967903	32.8221	32.1539	32.8187	32.8346	32.8365
117	H	-6.420552	15.237874	43.550173	32.7701	32.3886	32.7999	32.7754	32.7584
118	H	-5.428213	13.983285	40.903919	32.3934	32.1355	32.3929	32.3824	32.3703
119	H	-6.937768	14.855444	41.020754	32.9222	32.6162	32.9374	32.9209	32.9055
120	H	-5.732790	15.346953	39.854772	32.2947	31.8863	32.3154	32.3067	32.2958
121	N	-6.166000	20.371000	41.167000	143.7543	150.6621	146.4197	145.3062	145.1027
122	C	-6.954000	21.602000	41.149000	144.1227	144.4255	144.0350	143.9670	143.9707
123	C	-6.878000	22.263000	39.781000	7.5160	7.4569	6.9243	7.0046	7.0548
124	O	-7.867000	22.816000	39.297000	-9.3604	-24.3752	-17.7047	-21.2507	-21.4591
125	C	-6.469000	22.585000	42.215000	161.8951	161.0498	161.7138	161.5162	161.4368
126	C	-6.889000	22.195000	43.638000	11.3999	12.2964	11.4148	11.5181	11.6360
127	O	-7.720000	21.278000	43.836000	46.5354	40.6461	46.7536	46.3373	45.7626
128	O	-6.359000	22.835000	44.572000	41.1031	32.1883	41.8409	41.1858	40.4051
129	H	-5.355182	20.331572	41.733674	26.6575	27.9869	26.5748	26.6393	26.7518

130	H	-7.969030	21.338500	41.361558	28.9876	28.7245	28.9880	28.9662	28.9449
131	H	-5.400935	22.634975	42.174502	30.7992	31.3576	30.8017	30.8635	30.9263
132	H	-6.866014	23.553702	41.993877	31.2544	30.9937	31.3131	31.2870	31.2528
133	N	-5.698000	22.219000	39.158000	148.9241	151.0415	150.2979	149.5245	149.2013
134	C	-5.460000	22.958000	37.912000	140.3548	141.4201	140.2489	140.2673	140.3219
135	C	-6.229000	22.301000	36.779000	7.5596	8.7249	7.4769	7.6638	7.6806
136	O	-6.916000	22.973000	36.000000	-23.7404	-40.8674	-34.4373	-35.3554	-34.1141
137	C	-3.967000	22.922000	37.575000	163.8926	163.5117	164.1821	163.7739	163.7039
138	C	-3.543000	23.771000	36.385000	59.0153	61.4696	59.0067	59.1698	59.4448
139	C	-3.438000	25.159000	36.490000	55.7818	55.5025	55.8384	55.7746	55.7530
140	C	-3.195000	23.179000	35.171000	55.1209	54.8833	55.2395	55.2953	55.2814
141	C	-3.033000	25.935000	35.412000	77.0694	76.9268	77.0641	76.9813	76.9477
142	C	-2.769000	23.950000	34.085000	78.0239	77.9348	77.9698	78.0377	78.0260
143	C	-2.692000	25.325000	34.211000	34.3328	33.6330	34.3147	34.2309	34.1515
144	O	-2.289000	26.117000	33.146000	254.1933	252.9334	254.1844	253.9761	253.8410
145	H	-4.966675	21.675529	39.545173	26.5909	28.2596	26.8681	26.8518	26.9444
146	H	-5.783646	23.970331	38.035856	29.4812	29.3824	29.4853	29.4842	29.4890
147	H	-3.421951	23.253751	38.433931	30.1345	30.4906	30.1040	30.1023	30.1043
148	H	-3.693134	21.906888	37.376394	30.5533	31.1184	30.5673	30.6215	30.6856

149	H	-3.674165	25.634199	37.419146	25.2049	25.1861	25.2236	25.2135	25.2109
150	H	-3.255096	22.115586	35.068829	28.3464	28.4361	28.3777	28.3996	28.4087
151	H	-2.983652	26.999727	35.505919	25.7361	25.7207	25.7443	25.7344	25.7306
152	H	-2.504075	23.478709	33.161637	26.2713	26.2847	26.2773	26.2820	26.2794
153	H	-2.119484	25.501412	32.442568	28.8296	28.7799	28.8169	28.8207	28.8144
154	N	-6.089000	20.988000	36.681000	158.7634	159.0500	160.4412	159.7286	159.5541
155	C	-6.664000	20.229000	35.574000	141.3393	141.4801	141.2131	141.2137	141.2200
156	C	-8.087000	19.746000	35.835000	9.6447	9.6615	8.7538	9.2537	9.2116
157	O	-8.818000	19.448000	34.886000	17.7732	4.4674	14.4781	11.2605	11.5118
158	C	-5.748000	19.059000	35.199000	163.7282	162.4088	163.8392	163.6997	163.6536
159	C	-4.448000	19.514000	34.566000	55.2580	55.8927	55.3849	55.5062	55.6083
160	C	-3.227000	19.335000	35.222000	54.2547	55.4759	54.2088	54.3149	54.3902
161	C	-4.437000	20.143000	33.318000	54.8976	54.8391	54.8506	54.7840	54.7595
162	C	-2.043000	19.775000	34.662000	76.6764	76.3609	76.6347	76.6748	76.6730
163	C	-3.251000	20.584000	32.739000	75.0549	74.1769	75.0373	75.0112	74.9588
164	C	-2.042000	20.370000	33.415000	32.3691	31.9899	32.2733	32.2034	32.1800
165	O	-0.840000	20.792000	32.877000	251.0724	249.8839	250.8143	250.7209	250.6409
166	H	-5.578980	20.506240	37.379489	26.3631	28.5509	26.5169	26.5695	26.6413
167	H	-6.734635	20.905267	34.747820	29.1364	29.0435	29.1523	29.1462	29.1459

168	H	-5.524084	18.498951	36.082803	30.5505	30.7360	30.5059	30.5416	30.5606
169	H	-6.263943	18.423988	34.509462	30.1007	29.9218	30.1071	30.0883	30.0805
170	H	-3.208773	18.848561	36.174861	24.8563	25.0615	24.8011	24.8285	24.8586
171	H	-5.360042	20.288532	32.796739	24.8329	24.7883	24.8123	24.8113	24.8149
172	H	-1.123594	19.654534	35.195929	25.7808	25.8376	25.7487	25.7613	25.7663
173	H	-3.261855	21.079644	31.790781	25.3158	25.2510	25.2961	25.2932	25.2915
174	H	-0.192831	20.567094	33.535096	28.5229	28.5022	28.5234	28.5034	28.5010
175	N	-8.469000	19.673000	37.111000	149.1073	155.7660	148.6669	149.3835	150.2528
176	C	-9.821000	19.275000	37.528000	154.7655	154.1793	154.6897	154.7286	154.8908
177	C	-10.830000	20.410000	37.466000	15.9898	16.5313	15.8483	16.0034	16.0538
178	O	-10.652000	21.343000	36.673000	45.3683	44.2496	45.5573	45.2384	45.1379
179	O	-11.825000	20.405000	38.202000	58.4916	56.2033	58.1805	58.0597	57.9229
180	H	-7.808167	19.898387	37.812855	26.8883	28.1811	27.0861	27.1308	27.1836
181	H	-10.156624	18.483107	36.891477	29.5825	29.4153	29.5875	29.5824	29.5920
182	H	-9.776223	18.910956	38.533170	29.9635	30.3137	30.0373	30.0251	30.0327

Table 6: Cartesian coordinates and isotropic shielding constants (in ppm) for 3FOD

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	3.555000	8.370000	-12.979000	229.6537	229.6342	229.6503	229.6714	229.6693
2	C	2.780000	7.134000	-13.278000	146.7842	146.7744	146.7748	146.7886	146.7836
3	C	3.470000	5.907000	-12.700000	14.5229	14.5374	14.5580	14.5545	14.5478
4	O	4.700000	5.830000	-12.678000	-0.6980	-0.5115	-0.6557	-0.6370	-0.6408
5	C	2.595000	6.973000	-14.779000	180.2535	180.2290	180.2630	180.2479	180.2557
6	H	3.088028	9.153514	-13.363893	28.9731	28.9658	28.9768	28.9723	28.9697
7	H	3.633200	8.481351	-11.998395	28.7387	28.7315	28.7416	28.7461	28.7433
8	H	4.458981	8.296810	-13.375941	28.5857	28.5748	28.5875	28.5880	28.5851
9	H	1.817798	7.226803	-12.819246	29.2311	29.2147	29.2368	29.2349	29.2331
10	H	2.037071	6.081482	-14.976005	31.4390	31.4217	31.4474	31.4372	31.4375
11	H	2.064975	7.818230	-15.165731	31.4500	31.4449	31.4513	31.4520	31.4506
12	H	3.552801	6.906020	-15.251262	31.6288	31.6150	31.6338	31.6321	31.6310
13	N	2.669000	4.953000	-12.234000	151.6110	151.3445	151.4199	151.3947	151.3482
14	C	3.179000	3.696000	-11.700000	140.8302	140.7592	140.7747	140.8477	141.0520
15	C	2.536000	2.529000	-12.441000	12.3891	11.9655	11.9610	12.0386	12.0899

16	O	1.323000	2.517000	-12.659000	10.0132	11.1845	11.5917	10.9369	10.9652
17	C	2.887000	3.555000	-10.190000	162.0747	162.0394	162.0533	162.0627	162.1100
18	C	3.559000	4.685000	-9.406000	173.1059	173.0596	173.0810	173.1231	173.2313
19	C	3.376000	2.208000	-9.676000	182.5764	182.4646	182.4730	182.4889	182.5073
20	C	3.271000	4.651000	-7.916000	185.5698	185.5524	185.5790	185.5659	185.5569
21	H	1.690409	5.101968	-12.250359	27.9004	27.8687	27.8976	27.8883	27.8847
22	H	4.239983	3.689934	-11.838485	29.1437	29.1256	29.1383	29.1407	29.1336
23	H	1.828345	3.616647	-10.047347	31.9516	31.9471	31.9451	31.9527	31.9549
24	H	4.617083	4.618268	-9.550594	32.4636	32.4506	32.4718	32.4712	32.4761
25	H	3.219454	5.620978	-9.797859	31.7350	31.7211	31.7388	31.7359	31.7268
26	H	3.165814	2.127756	-8.629920	31.7847	31.7826	31.7902	31.7948	31.7934
27	H	2.874846	1.422320	-10.201787	32.4749	32.4589	32.4720	32.4674	32.4560
28	H	4.431026	2.127206	-9.835036	32.8538	32.8308	32.8519	32.8473	32.8404
29	H	3.771476	5.466637	-7.437293	32.0630	32.0485	32.0629	32.0602	32.0550
30	H	2.216620	4.735296	-7.754517	32.5427	32.5215	32.5370	32.5361	32.5317
31	H	3.621895	3.727101	-7.505899	32.0289	32.0058	32.0228	32.0217	32.0153
32	N	3.360000	1.564000	-12.840000	146.5666	144.8373	144.8258	145.6008	145.9020
33	C	2.883000	0.331000	-13.460000	150.4764	150.3733	150.4441	150.5609	150.6350
34	C	3.488000	-0.842000	-12.707000	10.8131	10.5594	10.5750	10.6286	10.6515

35	O	4.709000	-0.939000	-12.589000	2.9810	3.1903	3.3148	2.7852	2.5598
36	C	3.281000	0.279000	-14.941000	161.5953	161.6686	161.6733	161.5369	161.5709
37	C	2.823000	-0.907000	-15.809000	172.3772	172.4961	172.5059	172.5128	172.5291
38	C	3.659000	-2.156000	-15.554000	175.6718	176.1616	175.8574	175.8393	175.8670
39	C	1.343000	-1.204000	-15.611000	179.0207	179.1009	179.0246	179.0293	179.0384
40	H	4.333984	1.686439	-12.711692	27.9576	27.8885	27.9007	27.9395	27.9534
41	H	1.814936	0.289156	-13.411127	28.8149	28.8731	28.8858	28.8773	28.8694
42	H	2.913656	1.172165	-15.401667	31.5821	31.5731	31.5929	31.5790	31.5817
43	H	4.349522	0.313193	-14.985637	31.4662	31.4811	31.5024	31.4902	31.4919
44	H	2.972400	-0.618203	-16.828400	31.6490	31.6836	31.6602	31.6526	31.6482
45	H	3.308087	-2.953107	-16.175595	32.4046	32.4794	32.4295	32.4238	32.4230
46	H	4.684373	-1.951403	-15.781268	32.2501	32.2903	32.2799	32.2737	32.2733
47	H	3.571325	-2.440158	-14.526154	32.6021	32.6435	32.5464	32.5566	32.5391
48	H	1.059657	-2.031357	-16.227520	32.1700	32.2424	32.1711	32.1742	32.1742
49	H	1.161929	-1.445643	-14.584490	32.4030	32.4639	32.3657	32.3859	32.3856
50	H	0.767240	-0.343738	-15.881831	31.9942	32.0269	31.9875	31.9952	31.9964
51	N	2.630000	-1.714000	-12.183000	152.8346	152.3129	152.1530	152.2455	152.0950
52	C	3.070000	-2.916000	-11.485000	147.4694	147.6211	147.4364	147.4593	147.4732
53	C	2.466000	-4.149000	-12.145000	12.7081	12.1647	12.2920	12.4083	12.4461

54	O	1.262000	-4.199000	-12.386000	7.5665	14.4919	16.0210	15.1221	15.2270
55	C	2.659000	-2.862000	-10.013000	138.2078	138.1678	138.1546	138.1800	138.1921
56	O	3.031000	-4.051000	-9.331000	340.4446	340.7063	340.4093	340.3608	340.3867
57	H	1.659240	-1.540443	-12.270197	27.8176	27.8241	27.8080	27.8048	27.7968
58	H	4.137098	-2.971590	-11.540791	28.5467	28.5426	28.5258	28.5312	28.5288
59	H	3.136934	-2.026185	-9.546209	29.4397	29.4594	29.4422	29.4393	29.4405
60	H	1.597959	-2.739151	-9.949754	29.4790	29.5022	29.4773	29.4824	29.4832
61	H	2.734476	-3.916037	-8.438611	32.0221	32.0348	32.0236	32.0278	32.0279
62	N	3.314000	-5.131000	-12.439000	152.2866	154.4987	153.8689	153.1805	152.9465
63	C	2.877000	-6.418000	-12.969000	146.4781	146.6276	146.5506	146.3396	146.2287
64	C	3.478000	-7.521000	-12.108000	11.8114	11.7624	11.8246	12.1941	12.2025
65	O	4.696000	-7.578000	-11.939000	20.5353	18.7921	19.0276	15.6129	16.7166
66	C	3.328000	-6.577000	-14.420000	137.5577	137.3183	137.3744	137.4239	137.4261
67	O	2.821000	-7.775000	-14.980000	338.9416	338.9211	338.8815	338.8126	338.7741
68	H	4.281660	-4.982224	-12.292031	27.8518	27.9256	27.9248	27.9010	27.8926
69	H	1.808822	-6.476126	-12.946253	28.5910	28.5950	28.5825	28.5757	28.5716
70	H	2.973579	-5.744596	-14.991305	29.5564	29.5802	29.5525	29.5556	29.5553
71	H	4.397217	-6.597625	-14.455335	29.4150	29.3993	29.4171	29.4100	29.4066
72	H	3.152812	-7.780527	-15.870152	32.0561	32.0510	32.0437	32.0479	32.0480

73	N	2.625000	-8.388000	-11.564000	149.5418	149.2582	149.1456	148.9435	149.0692
74	C	3.061000	-9.433000	-10.635000	142.4076	142.3887	142.3621	142.3906	142.3983
75	C	2.440000	-10.783000	-10.980000	17.0840	17.0643	17.0598	17.0553	17.0547
76	O	1.349000	-10.861000	-11.542000	51.7868	51.7719	52.3383	51.8093	51.8065
77	C	2.701000	-9.068000	-9.179000	131.7486	131.7031	131.6976	131.7103	131.7123
78	O	1.289000	-8.840000	-9.071000	319.6054	319.5881	319.5855	319.6012	319.6046
79	C	3.448000	-7.815000	-8.740000	177.4594	177.4484	177.4348	177.4486	177.4467
80	O	3.024000	-11.832000	-10.711000	46.4653	46.5504	46.2307	46.4440	46.4419
81	H	1.664577	-8.323721	-11.795423	27.6611	27.6165	27.6064	27.5954	27.6066
82	H	4.124326	-9.506677	-10.728861	28.9558	28.9291	28.9177	28.9305	28.9327
83	H	2.985974	-9.881929	-8.545589	29.3586	29.3566	29.3496	29.3535	29.3542
84	H	3.185544	-7.578780	-7.729942	31.9875	31.9858	31.9744	31.9792	31.9783
85	H	4.502087	-7.987498	-8.803595	32.3528	32.3528	32.3430	32.3439	32.3429
86	H	3.181044	-6.998643	-9.378119	31.9395	31.9022	31.9034	31.8990	31.8953
87	H	0.909212	-9.367406	-9.763895	31.7261	31.7172	31.7128	31.7187	31.7201

Table 7: Cartesian coordinates and isotropic shielding constants (in ppm) for 3FPO

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	1.742000	0.539000	-10.091000	233.8189	233.8098	233.7950	233.8186	233.8178
2	C	0.944000	0.193000	-8.877000	144.7069	144.7456	144.8007	144.7237	144.7226
3	C	1.665000	0.652000	-7.616000	15.8576	15.8764	15.8905	15.8419	15.8458
4	O	2.891000	0.739000	-7.594000	-8.4655	-8.4159	-8.2795	-8.5223	-8.5404
5	C	0.691000	-1.315000	-8.802000	170.0749	170.0776	170.1602	170.0924	170.0994
6	C	0.084000	-1.893000	-10.044000	56.9314	56.9580	56.9579	56.9438	56.9175
7	N	-1.028000	-1.351000	-10.652000	-25.3430	-25.2817	-25.4293	-25.3500	-25.3551
8	C	0.427000	-2.973000	-10.785000	73.4531	73.4881	73.4877	73.4618	73.4759
9	C	-1.338000	-2.068000	-11.717000	50.6818	50.6786	50.6760	50.6799	50.6815
10	N	-0.473000	-3.060000	-11.818000	105.8156	105.7856	105.8450	105.7990	105.8056
11	H	1.260247	0.234364	-10.900451	29.1208	29.1322	29.1031	29.1184	29.1153
12	H	1.870505	1.519727	-10.132970	28.8539	28.8608	28.8447	28.8581	28.8561
13	H	2.624247	0.092275	-10.044347	28.8327	28.8460	28.8715	28.8383	28.8353
14	H	0.003273	0.697822	-8.948322	28.4126	28.4320	28.4146	28.4183	28.4146
15	H	1.622703	-1.807699	-8.617402	30.0638	30.0819	30.0884	30.0736	30.0705

16	H	0.034336	-1.509510	-7.979894	29.7685	29.7814	29.7712	29.7779	29.7738
17	H	1.246776	-3.635288	-10.599955	25.5759	25.5960	25.5851	25.5819	25.5803
18	H	-2.152112	-1.877161	-12.384609	24.4960	24.5038	24.4970	24.4980	24.4969
19	H	-0.473251	-3.754003	-12.524017	24.6566	24.6641	24.6603	24.6588	24.6575
20	N	0.902000	0.941000	-6.566000	159.9944	159.9187	159.7954	159.9547	159.9294
21	C	1.492000	1.355000	-5.292000	144.9943	144.9727	144.9886	145.0075	144.9958
22	C	0.777000	0.729000	-4.100000	13.7682	13.7237	13.7452	13.8427	13.8659
23	O	-0.451000	0.622000	-4.082000	-1.8777	-0.8895	-1.0148	-1.7519	-1.7428
24	C	1.500000	2.876000	-5.165000	139.5490	139.5673	139.5469	139.5375	139.5207
25	O	0.208000	3.407000	-5.359000	343.4436	343.4723	343.5432	343.4376	343.4360
26	H	-0.082441	0.874995	-6.647359	27.4257	27.4326	27.4311	27.4291	27.4222
27	H	2.502040	1.001897	-5.285894	28.5959	28.5855	28.5948	28.5942	28.5885
28	H	1.847319	3.145040	-4.189353	29.4492	29.4385	29.4377	29.4444	29.4404
29	H	2.161985	3.286120	-5.898810	29.3058	29.3089	29.3092	29.3027	29.2993
30	H	-0.377443	2.732659	-5.034932	31.8173	31.8183	31.8032	31.8152	31.8110
31	N	1.563000	0.298000	-3.117000	155.0842	155.3101	155.1626	155.5172	155.2381
32	C	1.029000	-0.282000	-1.889000	145.7106	145.5719	145.5476	145.5910	145.4882
33	C	1.571000	0.481000	-0.684000	12.4461	12.8237	12.8708	13.0800	12.9702
34	O	2.730000	0.908000	-0.672000	-6.3401	-7.2818	-7.7875	-11.1352	-9.6651

35	C	1.390000	-1.764000	-1.781000	137.9573	137.6503	137.6530	137.7758	137.8004
36	O	2.792000	-1.937000	-1.742000	345.1880	345.2345	345.3204	345.2556	345.2539
37	H	2.544498	0.373380	-3.222256	27.3278	27.3451	27.3263	27.3521	27.3412
38	H	-0.037810	-0.202166	-1.910055	28.5838	28.5781	28.5814	28.5878	28.5806
39	H	0.960632	-2.166692	-0.887478	29.4648	29.4708	29.4727	29.4665	29.4597
40	H	0.994404	-2.285274	-2.627568	29.4408	29.4701	29.4624	29.4560	29.4439
41	H	3.124110	-1.112812	-1.405970	31.8448	31.8580	31.8749	31.8771	31.8717
42	N	0.718000	0.639000	0.320000	150.6231	149.4969	149.5397	149.6780	150.2599
43	C	1.030000	1.407000	1.520000	149.0925	148.6999	148.7473	148.9111	148.9959
44	C	0.527000	0.639000	2.735000	12.8254	12.6765	12.7845	12.7346	12.7307
45	O	-0.670000	0.343000	2.831000	2.3369	2.9441	2.5203	2.1224	2.1760
46	C	0.370000	2.779000	1.441000	157.7858	158.4390	157.7486	157.9750	158.2472
47	C	0.719000	3.516000	0.161000	12.3733	12.6027	12.3503	12.3470	12.3393
48	O	-0.063121	3.529039	-0.789499	-37.9797	-36.8332	-36.9619	-37.7114	-38.0418
49	N	1.890245	4.151249	0.136504	165.7319	165.9187	165.8073	165.7958	165.8007
50	H	-0.173870	0.214816	0.251186	27.8247	27.7322	27.7208	27.7608	27.7860
51	H	2.087320	1.548696	1.603041	28.8032	28.6162	28.8024	28.8099	28.8203
52	H	-0.691705	2.655787	1.491009	30.5483	30.7109	30.5718	30.5774	30.5735
53	H	0.690122	3.365747	2.276554	30.8180	31.0523	30.8038	30.8350	30.8399

54	H	2.489697	4.114784	0.923541	28.1045	28.1004	28.0916	28.0926	28.0910
55	H	2.160889	4.659627	-0.668731	28.2052	28.2475	28.1887	28.1881	28.1784
56	N	1.442000	0.301000	3.641000	149.1573	149.5219	149.3838	149.3539	149.3705
57	C	1.125000	-0.530000	4.806000	148.5548	148.4189	148.2672	148.3370	148.3477
58	C	1.572000	0.150000	6.098000	14.9903	15.0517	14.8943	14.9290	14.9640
59	O	2.764000	0.395000	6.286000	19.1056	20.9570	19.9234	18.6288	16.5048
60	C	1.802000	-1.890000	4.673000	159.0173	158.9400	158.9294	159.0432	159.1185
61	C	1.442000	-2.592000	3.385000	12.9738	12.9464	12.7525	12.8301	12.8464
62	O	2.276172	-2.738614	2.491706	-34.8135	-36.6876	-33.8961	-34.6342	-35.2227
63	N	0.196346	-3.043175	3.283727	167.6969	168.2078	167.7893	167.7376	167.6628
64	H	2.370832	0.622820	3.523513	28.1886	28.2397	28.2178	28.2135	28.2187
65	H	0.064194	-0.664139	4.845969	28.5739	28.6287	28.5741	28.5722	28.5776
66	H	2.862644	-1.753051	4.707337	30.7340	30.7723	30.7448	30.7323	30.7346
67	H	1.506035	-2.505553	5.496650	30.9528	30.9894	30.9540	30.9591	30.9593
68	H	-0.442693	-2.903418	4.026826	28.1295	28.1520	28.1396	28.1325	28.1227
69	H	-0.092731	-3.519095	2.465170	28.2138	28.2590	28.2418	28.2232	28.2084
70	N	0.607000	0.450000	6.970000	137.7228	137.4897	137.1330	137.0152	136.4180
71	C	0.853000	1.139000	8.241000	145.2828	145.1391	145.0997	145.1285	145.2137
72	C	0.404000	0.265000	9.419000	14.3112	14.1918	14.1981	14.2667	14.2732

73	O	0.046000	-0.909000	9.263000	39.8717	39.8669	40.0236	39.8951	39.8901
74	C	0.094000	2.467000	8.289000	160.5504	160.7397	160.7655	160.6216	160.6566
75	C	0.407000	3.403000	7.151000	47.9596	47.6578	47.4702	47.6460	47.6642
76	C	-0.325000	3.354000	5.968000	59.2970	59.1405	59.2605	59.2522	59.2107
77	C	1.412000	4.353000	7.271000	61.7876	62.1453	61.8585	61.7825	61.7694
78	C	-0.052000	4.224000	4.921000	61.5564	62.3169	61.4980	61.5749	61.6538
79	C	1.694000	5.224000	6.230000	61.3068	61.4814	61.3189	61.3101	61.3092
80	C	0.960000	5.159000	5.051000	65.0715	64.9663	65.1683	65.1174	65.1286
81	O	0.375000	0.720000	10.569000	61.1540	61.7076	61.6241	61.4090	61.3507
82	H	-0.323044	0.194117	6.747197	28.0265	28.0198	28.0340	27.9939	27.9896
83	H	1.903621	1.327719	8.315025	28.8598	28.8931	28.8752	28.8664	28.8759
84	H	-0.955380	2.258272	8.277377	30.7990	30.8389	30.8345	30.8120	30.8161
85	H	0.331370	2.960042	9.208492	29.8248	29.8240	29.8076	29.8024	29.8032
86	H	-1.110262	2.634670	5.863945	25.4848	25.4519	25.4576	25.4514	25.4458
87	H	1.976018	4.413763	8.178244	25.1558	25.1792	25.1482	25.1464	25.1511
88	H	-0.621939	4.171776	4.016930	25.3574	25.2728	25.3218	25.3215	25.3283
89	H	2.476554	5.946301	6.333880	25.1095	25.1349	25.0990	25.1003	25.1060
90	H	1.176964	5.830065	4.246327	25.3233	25.3370	25.3153	25.3143	25.3241

Table 8: Cartesian coordinates and isotropic shielding constants (in ppm) for 3FQP

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	-11.386000	-0.012000	2.349000	233.8854	233.8826	233.8941	233.8887	233.8814
2	C	-10.023000	-0.594000	2.550000	137.7038	137.7108	137.6970	137.7083	137.7056
3	C	-9.364000	0.045000	3.771000	14.2138	14.2244	14.0616	14.0589	13.9739
4	O	-9.294000	1.273000	3.870000	-12.0433	-11.8224	-12.1897	-12.5079	-12.8174
5	C	-9.124000	-0.387000	1.303000	166.8676	166.9285	166.8708	166.8943	166.8808
6	C	-7.705000	-0.889000	1.565000	179.5700	179.7709	179.5811	179.5996	179.6042
7	C	-9.714000	-1.078000	0.073000	179.8268	179.8165	179.7965	179.8373	179.8329
8	H	-11.809276	-0.428767	1.557013	28.6688	28.6730	28.6870	28.6726	28.6712
9	H	-11.940874	-0.186791	3.150039	28.7687	28.7576	28.7682	28.7672	28.7654
10	H	-11.310061	0.964801	2.206900	28.7415	28.7358	28.7181	28.7376	28.7363
11	H	-10.134499	-1.646749	2.705523	29.8437	29.8418	29.8370	29.8345	29.8297
12	H	-9.081899	0.663918	1.106279	31.2535	31.2721	31.2613	31.2674	31.2638
13	H	-7.105534	-0.735582	0.692072	31.8694	31.9010	31.8920	31.8826	31.8792
14	H	-7.282226	-0.350332	2.387191	32.2397	32.2852	32.2400	32.2454	32.2477
15	H	-7.733447	-1.932661	1.799228	32.3514	32.3604	32.3579	32.3526	32.3491

16	H	-9.072720	-0.917281	-0.768326	31.6770	31.6923	31.6879	31.6795	31.6768
17	H	-9.799866	-2.127922	0.260593	32.2271	32.2388	32.2278	32.2261	32.2229
18	H	-10.682242	-0.672296	-0.133908	32.0945	32.1035	32.1080	32.1049	32.1021
19	N	-8.901000	-0.791000	4.710000	139.8695	139.9804	140.0312	139.9512	139.8298
20	C	-8.169000	-0.297000	5.893000	145.9291	145.8749	145.9332	145.8326	145.7657
21	C	-6.773000	-0.911000	5.954000	12.2947	12.1470	12.2665	12.4519	12.3737
22	O	-6.634000	-2.132000	5.921000	3.2609	1.6491	2.0305	-0.3953	0.1084
23	C	-8.908000	-0.641000	7.202000	168.0871	167.7961	167.8980	167.9212	167.9380
24	C	-8.322000	0.071000	8.436000	166.1895	166.6591	166.2757	166.2485	166.3309
25	C	-8.956000	-0.339000	9.741000	9.4596	9.8006	9.3586	9.3376	9.3805
26	O	-9.011679	-1.534004	10.079854	-0.3018	-0.6174	0.2874	0.3116	0.1512
27	N	-9.471528	0.632782	10.469683	164.0505	164.3643	164.1011	164.0475	164.0280
28	H	-9.053497	-1.763854	4.608025	27.5343	27.5005	27.5040	27.5247	27.5179
29	H	-8.102048	0.766496	5.796083	28.6477	28.6454	28.6647	28.6416	28.6381
30	H	-9.935521	-0.360541	7.099805	31.5411	31.5131	31.5493	31.5451	31.5354
31	H	-8.854817	-1.698172	7.358396	30.9466	30.9259	30.9681	30.9639	30.9555
32	H	-7.274398	-0.141099	8.485428	31.4072	31.4586	31.3659	31.3739	31.3823
33	H	-8.449892	1.126123	8.312476	31.4586	31.4154	31.4575	31.4552	31.4491
34	H	-9.404496	1.571309	10.161828	28.0032	27.9943	27.9961	27.9951	27.9897

35	H	-9.925349	0.423362	11.324252	28.3339	28.3438	28.3322	28.3363	28.3304
36	N	-5.739000	-0.077000	6.041000	147.6060	147.5901	148.0673	147.7127	147.6152
37	C	-4.368000	-0.558000	6.238000	140.5014	140.5564	140.4863	140.5086	140.4945
38	C	-3.822000	0.104000	7.498000	12.3899	12.3133	12.1232	12.0834	12.0306
39	O	-3.826000	1.326000	7.615000	14.6185	13.3899	11.0862	12.4300	11.9490
40	C	-3.453000	-0.236000	5.042000	162.6261	162.1956	162.3221	162.3829	162.3992
41	C	-3.986000	-0.900000	3.768000	173.3848	173.5290	173.3672	173.4030	173.3845
42	C	-2.022000	-0.708000	5.318000	181.3862	183.0590	181.3900	181.4076	181.4221
43	C	-3.133000	-0.646000	2.542000	185.6350	185.5063	185.5629	185.6110	185.6112
44	H	-5.900614	0.897177	5.970571	27.9090	27.8309	27.8917	27.8829	27.8799
45	H	-4.386977	-1.623807	6.330713	29.2185	29.1650	29.1908	29.1854	29.1853
46	H	-3.444194	0.824769	4.902027	31.8587	31.8447	31.8509	31.8523	31.8432
47	H	-4.041710	-1.955938	3.931678	32.5813	32.4482	32.5751	32.5731	32.5638
48	H	-4.972725	-0.531846	3.578957	31.7751	31.7185	31.7566	31.7753	31.7715
49	H	-1.401644	-0.476246	4.477554	31.9277	31.7938	31.9176	31.9204	31.9164
50	H	-1.644317	-0.212017	6.187630	33.0329	32.4898	32.9670	32.9968	33.0021
51	H	-2.020516	-1.765419	5.481596	33.3351	32.8323	33.3051	33.3075	33.3008
52	H	-3.566928	-1.138919	1.697229	32.1219	32.0768	32.1246	32.1266	32.1228
53	H	-3.082918	0.406180	2.354094	32.5230	32.5545	32.5157	32.5160	32.5125

54	H	-2.146702	-1.025868	2.708785	32.0365	32.0542	32.0298	32.0307	32.0275
55	N	-3.375000	-0.712000	8.453000	147.1770	147.6031	147.5035	147.7574	147.4313
56	C	-2.853000	-0.194000	9.719000	140.8175	140.7038	140.7863	140.7861	140.7411
57	C	-1.437000	-0.716000	9.932000	11.6058	11.9227	11.8633	11.7921	11.7163
58	O	-1.206000	-1.925000	9.903000	11.7881	9.2597	8.8897	10.0094	9.3011
59	C	-3.746000	-0.610000	10.910000	166.3037	165.9645	166.0121	166.0834	166.0803
60	C	-3.196000	-0.051000	12.223000	177.1603	179.1623	176.9210	177.0573	177.0433
61	C	-5.170000	-0.135000	10.693000	179.0973	179.6621	179.0030	179.0371	179.0239
62	H	-3.396551	-1.690280	8.302652	28.1369	28.0661	28.1327	28.1433	28.1308
63	H	-2.847217	0.874792	9.668506	29.1669	29.0901	29.1254	29.1387	29.1356
64	H	-3.744338	-1.678195	10.972097	31.6848	31.6635	31.6883	31.6810	31.6726
65	H	-3.829223	-0.351309	13.031544	32.2111	32.1208	32.2258	32.2270	32.2182
66	H	-2.207768	-0.427920	12.384952	32.4305	32.3637	32.4158	32.4114	32.3937
67	H	-3.166208	1.017327	12.171128	32.4822	32.4975	32.4553	32.4610	32.4533
68	H	-5.775080	-0.430143	11.524666	32.3687	32.2864	32.3854	32.3794	32.3698
69	H	-5.180757	0.931296	10.604704	32.6531	32.6195	32.6430	32.6374	32.6301
70	H	-5.558741	-0.571059	9.796544	32.0868	31.9939	32.0284	32.0597	32.0602
71	N	-0.495000	0.209000	10.107000	146.6964	145.3255	145.6456	145.6058	145.5963
72	C	0.897000	-0.131000	10.387000	144.8164	144.5784	144.4802	144.5494	144.5496

73	C	1.240000	0.146000	11.846000	10.9672	10.2216	10.3432	10.3785	10.4682
74	O	1.120000	1.287000	12.310000	22.4994	22.1379	21.9229	22.0362	22.0173
75	C	1.835000	0.713000	9.524000	162.7011	162.7070	162.8420	162.6341	162.5676
76	C	1.741000	0.505000	8.031000	60.2596	60.0992	60.0987	60.1338	60.1339
77	C	0.921000	1.301000	7.245000	55.4370	55.1585	55.5089	55.4675	55.4616
78	C	2.514000	-0.461000	7.400000	57.4571	56.9260	57.5543	57.5268	57.5052
79	C	0.858000	1.124000	5.864000	75.8788	79.1169	75.6848	75.8091	75.8559
80	C	2.452000	-0.649000	6.029000	77.2798	77.4962	77.2950	77.2827	77.2752
81	C	1.634000	0.150000	5.263000	35.8688	35.5984	35.8991	35.9166	35.9021
82	O	1.596000	-0.051000	3.894000	253.0051	252.3926	252.9913	253.0888	253.0569
83	H	-0.748395	1.164001	10.044832	27.7828	27.6666	27.6892	27.7068	27.7052
84	H	1.020551	-1.171600	10.170699	28.7428	28.7653	28.7046	28.7077	28.7077
85	H	1.635302	1.744167	9.728241	30.3974	30.3948	30.4049	30.3870	30.3768
86	H	2.840269	0.504079	9.825141	30.4910	30.4989	30.4871	30.4843	30.4823
87	H	0.327605	2.062740	7.706014	25.2204	25.2116	25.1904	25.1983	25.1956
88	H	3.170133	-1.071840	7.984178	25.1646	25.1487	25.1516	25.1565	25.1537
89	H	0.212534	1.738587	5.271923	25.8030	25.7874	25.7789	25.7864	25.7888
90	H	3.039256	-1.414356	5.566117	25.9155	25.9451	25.9132	25.9106	25.9108
91	H	2.199632	-0.768676	3.742114	28.6582	28.7292	28.6646	28.6597	28.6592

92	N	1.705000	-0.880000	12.554000	142.1523	142.9554	142.6596	142.8642	142.8137
93	C	2.150000	-0.742000	13.951000	146.6732	146.7637	146.6776	146.6494	146.6472
94	C	3.488000	-1.452000	14.196000	14.3400	14.3586	14.2917	14.3160	14.3281
95	O	3.964000	-2.262000	13.395000	53.1083	53.0518	53.8028	53.3463	53.3166
96	C	1.124000	-1.346000	14.895000	164.6020	164.5958	164.5629	164.6394	164.6986
97	C	-0.295000	-0.835000	14.740000	175.2316	175.6916	175.1358	175.1826	175.2063
98	C	-1.163000	-1.395000	15.844000	169.9678	169.9125	169.8904	169.9178	169.9255
99	C	-2.620000	-0.986000	15.706000	153.8787	154.5917	153.8849	153.8674	153.8716
100	N	-3.372000	-1.196000	16.986000	233.4775	233.4734	233.4114	233.4674	233.4651
101	O	4.120000	-1.246000	15.241000	59.5898	59.7167	59.7152	59.7905	59.7374
102	H	1.753745	-1.770878	12.124978	27.7642	27.7648	27.7534	27.7612	27.7646
103	H	2.265788	0.305657	14.135141	28.8605	28.8862	28.8403	28.8473	28.8474
104	H	1.115456	-2.405404	14.745034	31.9754	31.9949	31.9704	31.9663	31.9690
105	H	1.440206	-1.153594	15.898939	31.5454	31.5544	31.5180	31.5250	31.5254
106	H	-0.296128	0.233633	14.794051	32.0448	31.9786	32.0325	32.0368	32.0373
107	H	-0.682588	-1.143596	13.791610	31.9804	31.9191	31.9283	31.9205	31.9238
108	H	-1.100685	-2.463002	15.824286	31.5247	31.5132	31.5308	31.5331	31.5298
109	H	-0.793572	-1.044760	16.785146	31.8761	31.8595	31.8949	31.8898	31.8870
110	H	-2.668783	0.048628	15.437551	29.9969	29.9090	30.0001	30.0068	30.0048

111	H	-3.075261	-1.569539	14.933265	29.6807	29.6650	29.6793	29.6830	29.6809
112	H	-4.315113	-0.920946	16.863594	28.8213	28.8213	28.8271	28.8240	28.8225
113	H	-3.337223	-2.153304	17.235921	29.1117	29.0951	29.1105	29.1170	29.1160
114	H	-2.960204	-0.652411	17.703660	29.2265	29.1988	29.2547	29.2309	29.2294

Table 9: Cartesian coordinates and isotropic shielding constants (in ppm) for 3FTK

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	-8.053000	2.244000	10.035000	233.2123	233.2249	233.2255	233.2211	233.1485
2	C	-7.146000	1.404000	9.189000	145.9431	145.9323	145.9827	145.9849	146.0588
3	C	-5.816000	2.087000	8.950000	13.5650	13.5950	13.4747	13.5811	13.5706
4	O	-5.758000	3.321000	8.852000	-12.0554	-10.3275	-11.5118	-11.9677	-12.6673
5	C	-7.763000	1.152000	7.820000	161.8519	161.9448	161.9579	161.9468	162.0001
6	C	-9.089000	0.451000	7.893000	14.7063	14.8010	14.7751	14.8042	14.8064
7	O	-9.228000	-0.582000	8.550000	-18.8903	-18.7873	-18.8610	-18.9264	-18.9622
8	N	-10.079000	1.000000	7.196000	158.5961	158.5977	158.4739	158.4825	158.5096
9	H	-8.910889	1.769041	10.171166	28.9708	28.9815	28.9720	28.9746	28.9781
10	H	-7.625342	2.410863	10.912135	28.7213	28.7316	28.7405	28.7272	28.7248
11	H	-8.222194	3.107241	9.580810	28.6713	28.6859	28.6881	28.6653	28.6601
12	H	-7.002718	0.487377	9.722077	28.7669	28.7607	28.7663	28.7714	28.7752
13	H	-7.897356	2.091187	7.325251	30.8178	30.8290	30.8454	30.8357	30.8369
14	H	-7.088794	0.553257	7.243933	30.2792	30.2928	30.2622	30.2860	30.2765
15	H	-9.920981	1.831410	6.682300	27.8228	27.8190	27.8137	27.8219	27.8225

16	H	-10.974268	0.577428	7.190647	27.9443	27.9387	27.9383	27.9395	27.9390
17	N	-4.764000	1.287000	8.797000	149.8739	150.0848	149.9940	149.8468	150.0374
18	C	-3.455000	1.811000	8.428000	140.5231	140.2697	140.2654	140.4332	140.4616
19	C	-2.983000	1.191000	7.112000	9.6300	9.2308	9.2489	9.2699	9.2986
20	O	-2.795000	-0.022000	7.021000	-16.8299	-17.0428	-17.0164	-17.1225	-17.4228
21	C	-2.422000	1.556000	9.537000	167.1459	167.2604	167.2593	167.4329	167.5187
22	C	-1.068000	2.099000	9.133000	179.8909	180.0229	180.0089	179.9435	179.9218
23	C	-2.891000	2.193000	10.846000	179.1656	179.0576	179.0700	179.2297	179.2074
24	H	-4.872895	0.313028	8.937071	27.8203	27.8165	27.8110	27.8046	27.7966
25	H	-3.548911	2.868925	8.298096	29.0380	29.0341	29.0189	29.0286	29.0379
26	H	-2.327455	0.500612	9.685719	31.4141	31.4108	31.3999	31.4158	31.4162
27	H	-0.361556	1.913504	9.914939	31.9958	32.0145	32.0036	32.0030	31.9997
28	H	-0.742635	1.614656	8.236090	32.2991	32.3012	32.2918	32.3007	32.2971
29	H	-1.142717	3.152666	8.962399	32.4567	32.4618	32.4538	32.4556	32.4561
30	H	-2.165972	2.010297	11.611411	32.1212	32.1360	32.1213	32.1224	32.1151
31	H	-3.006074	3.247830	10.708190	32.5095	32.4817	32.4762	32.4945	32.4913
32	H	-3.829066	1.766517	11.134174	31.8726	31.9198	31.9095	31.8802	31.8628
33	N	-2.826000	2.026000	6.087000	160.1041	160.4046	160.1607	160.1630	160.1842
34	C	-2.174000	1.597000	4.853000	151.9536	152.1523	151.9958	151.9786	151.9862

35	C	-2.913000	0.559000	4.022000	13.6019	13.6075	13.5939	13.6023	13.5419
36	O	-2.283000	-0.300000	3.409000	-21.8499	-13.4332	-16.8124	-18.6762	-20.6955
37	H	-3.157715	2.955675	6.162961	27.6444	27.6364	27.6480	27.6385	27.6363
38	H	-2.019916	2.461758	4.241975	29.5900	29.6286	29.6035	29.5951	29.5942
39	H	-1.215090	1.196057	5.107236	29.1817	29.2382	29.2183	29.1881	29.1884
40	N	-4.242000	0.605000	4.010000	157.7069	157.4100	157.2611	157.4215	157.4086
41	C	-5.004000	-0.260000	3.112000	146.6222	146.6360	146.5274	146.5713	146.5440
42	C	-5.207000	0.519000	1.821000	13.4468	13.3668	13.4890	13.4945	13.5103
43	O	-6.098000	1.372000	1.732000	8.2774	8.1808	8.7748	7.9777	7.5152
44	C	-6.344000	-0.675000	3.720000	138.8873	138.6524	138.8586	138.8761	138.8663
45	O	-6.162000	-1.618000	4.772000	339.9516	338.3856	339.5714	339.7333	339.7122
46	H	-4.718076	1.229166	4.613215	27.8418	27.7297	27.8268	27.8339	27.8337
47	H	-4.470190	-1.169917	2.933120	28.5158	28.5458	28.4812	28.4795	28.4732
48	H	-6.836569	0.192113	4.107803	29.4222	29.3475	29.4493	29.4414	29.4304
49	H	-6.953999	-1.113297	2.957965	29.5110	29.5005	29.5247	29.5230	29.5148
50	H	-7.041705	-1.807215	5.076657	32.0577	31.9850	32.0894	32.0723	32.0603
51	N	-4.357000	0.245000	0.834000	147.9724	148.0866	147.6523	147.9033	147.9310
52	C	-4.364000	0.983000	-0.422000	149.6615	149.8682	150.3741	150.4052	150.5800
53	C	-5.130000	0.236000	-1.501000	12.7113	12.7752	12.7382	12.6922	12.5899

54	O	-5.216000	-0.988000	-1.466000	-6.8159	-7.0886	-7.3672	-7.9389	-8.6647
55	C	-2.934000	1.234000	-0.903000	158.5767	158.2009	158.5926	158.6294	158.6331
56	C	-2.073000	1.921000	0.141000	12.2844	12.2489	12.3589	12.3833	12.4685
57	O	-2.183000	3.133000	0.348000	-11.0229	-18.7497	-10.2923	-11.0492	-11.6247
58	N	-1.198000	1.156000	0.790000	156.0711	161.9872	155.3155	155.4533	155.4624
59	H	-3.698658	-0.484001	0.957466	27.7568	27.8593	27.8015	27.7805	27.7718
60	H	-4.852177	1.917596	-0.240028	28.8206	28.8214	28.8377	28.8365	28.8398
61	H	-2.485943	0.295841	-1.155988	30.9310	30.8665	30.9166	30.9161	30.9241
62	H	-2.967880	1.847063	-1.779303	31.2315	31.1824	31.2197	31.2204	31.2188
63	H	-1.144342	0.187595	0.591472	28.0518	28.1413	28.0745	28.0637	28.0664
64	H	-0.600922	1.555475	1.471188	28.2109	28.1492	28.2020	28.1962	28.1886
65	N	-5.665000	0.966000	-2.474000	163.4781	164.1062	164.1098	163.8880	163.7218
66	C	-6.325000	0.330000	-3.613000	142.6159	142.5394	142.5240	142.4901	142.3954
67	C	-5.649000	0.745000	-4.907000	11.3136	11.4009	11.4770	11.5612	11.4369
68	O	-5.265000	1.911000	-5.077000	15.3523	13.5979	14.9352	12.2895	13.5053
69	C	-7.836000	0.647000	-3.670000	133.8185	133.6825	133.7328	133.7410	133.7010
70	O	-8.045000	2.009000	-4.079000	319.0074	318.9794	319.0215	319.0460	319.0368
71	C	-8.475000	0.415000	-2.313000	178.9220	178.8765	178.9314	178.9364	178.9054
72	H	-5.615999	1.953668	-2.426978	28.2042	28.1999	28.2413	28.2303	28.2176

73	H	-6.230956	-0.728164	-3.485154	28.6371	28.6431	28.6420	28.6453	28.6475
74	H	-8.291512	-0.005412	-4.385379	29.2519	29.2401	29.2664	29.2553	29.2484
75	H	-9.519984	0.638353	-2.367969	31.8467	31.8080	31.8486	31.8517	31.8495
76	H	-8.343416	-0.607625	-2.026952	32.4521	32.4131	32.4524	32.4573	32.4510
77	H	-8.012086	1.050715	-1.587413	31.9937	31.9116	31.9971	31.9996	31.9941
78	H	-7.221823	2.266820	-4.477006	31.2699	31.3003	31.3303	31.3152	31.3026
79	N	-5.476000	-0.225000	-5.798000	134.0966	133.0601	133.0668	132.7941	132.5795
80	C	-4.867000	0.008000	-7.094000	147.9492	147.6320	147.6641	147.7630	147.8902
81	C	-5.813000	-0.526000	-8.165000	15.6593	15.4745	15.4841	15.5542	15.5656
82	O	-7.019000	-0.262000	-8.088000	50.3378	50.1285	50.0592	50.1215	50.0589
83	C	-3.489000	-0.658000	-7.153000	160.7087	160.7667	160.7906	160.7116	160.7532
84	C	-2.565000	-0.266000	-6.006000	55.3666	55.0602	54.9162	55.0430	55.0764
85	C	-2.629000	-0.917000	-4.774000	52.8690	53.0176	52.8554	52.8506	52.8399
86	C	-1.640000	0.763000	-6.152000	56.3334	56.8235	56.3942	56.3221	56.3145
87	C	-1.775000	-0.564000	-3.720000	76.1827	75.2304	76.1166	76.2266	76.2551
88	C	-0.794000	1.129000	-5.105000	78.0060	78.1374	78.0301	77.9991	77.9802
89	C	-0.875000	0.472000	-3.894000	36.3205	36.2382	36.3440	36.3490	36.3440
90	O	-0.043000	0.839000	-2.857000	254.5863	254.9237	254.6139	254.6670	254.6725
91	O	-5.434000	-1.204000	-9.116000	46.1935	46.6439	46.6073	46.5769	46.5202

92	H	-5.773737	-1.141004	-5.569112	27.9117	27.8113	27.8229	27.8231	27.8399
93	H	-4.712005	1.053168	-7.262818	28.9136	28.9076	28.9143	28.9251	28.9422
94	H	-3.622493	-1.719496	-7.135535	30.6427	30.6671	30.6742	30.6507	30.6515
95	H	-3.019575	-0.388699	-8.076048	30.3284	30.3129	30.3142	30.3127	30.3112
96	H	-3.343430	-1.700575	-4.630822	25.3278	25.2627	25.2900	25.2817	25.2724
97	H	-1.576367	1.283325	-7.084798	25.1720	25.1656	25.1572	25.1595	25.1612
98	H	-1.818838	-1.090856	-2.789731	25.8818	25.7471	25.8558	25.8580	25.8615
99	H	-0.083626	1.917609	-5.240519	25.9879	25.9638	25.9772	25.9754	25.9732
100	H	0.481049	1.547496	-3.211832	28.8182	28.8080	28.8122	28.8093	28.8097

Table 10: Cartesian coordinates and isotropic shielding constants (in ppm) for 3FVA

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	-6.702000	-0.246000	-0.738000	231.3718	231.3290	231.2714	231.3813	231.3811
2	C	-7.086000	-0.456000	-2.167000	147.2167	147.1591	147.1351	147.2331	147.2351
3	C	-6.105000	0.245000	-3.087000	18.0685	18.0370	18.0392	18.0517	18.0485
4	O	-6.086000	1.471000	-3.179000	-22.0112	-20.9008	-21.2933	-21.9700	-21.9743
5	C	-8.507000	0.053000	-2.450000	163.5682	163.4902	163.4931	163.5706	163.5749
6	C	-9.595000	-0.823000	-1.836000	11.1721	11.0630	11.0774	11.1443	11.1379
7	O	-9.322000	-1.820000	-1.146000	-6.1628	-6.1261	-5.9561	-6.3095	-6.3170
8	N	-10.845000	-0.455000	-2.097000	165.7197	165.7769	165.8206	165.7497	165.7502
9	H	-7.350701	-0.708794	-0.150540	28.2389	28.2241	28.2438	28.2350	28.2325
10	H	-5.795758	-0.612929	-0.582471	28.8168	28.8023	28.8284	28.8191	28.8166
11	H	-6.705172	0.722831	-0.534392	29.0052	29.0060	29.0059	29.0075	29.0054
12	H	-7.061716	-1.509366	-2.353359	29.0541	29.0266	29.0624	29.0513	29.0490
13	H	-8.601272	1.043419	-2.056195	30.4151	30.3958	30.3982	30.4147	30.4137
14	H	-8.653477	0.089766	-3.509289	30.5537	30.5242	30.5550	30.5525	30.5508
15	H	-11.019559	0.346420	-2.651397	28.0118	27.9944	28.0082	28.0106	28.0080

16	H	-11.601644	-0.982273	-1.737038	27.8870	27.8800	27.8971	27.8863	27.8846
17	N	-5.305000	-0.560000	-3.780000	144.8593	144.6244	144.6738	144.8568	144.9487
18	C	-4.238000	-0.059000	-4.637000	148.8616	148.6737	148.6509	148.8151	148.8771
19	C	-4.339000	-0.686000	-6.017000	14.3702	14.2094	14.2587	14.1939	14.2583
20	O	-4.460000	-1.902000	-6.140000	4.1100	2.8091	2.5579	1.5701	1.1851
21	C	-2.891000	-0.381000	-3.992000	157.9954	157.9720	157.9636	158.0470	158.1043
22	C	-2.771000	0.218000	-2.611000	11.5691	11.4967	11.5133	11.5919	11.5523
23	O	-2.502456	-0.499109	-1.638413	-43.0366	-43.1239	-43.2026	-43.6078	-43.8778
24	N	-2.893780	1.541306	-2.519178	165.6955	165.7163	165.7146	165.6731	165.6364
25	H	-5.439551	-1.538387	-3.711039	27.5058	27.5021	27.5128	27.4905	27.4944
26	H	-4.329030	1.001264	-4.748592	28.6379	28.6206	28.6505	28.6299	28.6272
27	H	-2.784050	-1.443282	-3.921163	30.6205	30.5908	30.6184	30.6164	30.6154
28	H	-2.107870	0.007314	-4.609105	30.7866	30.7585	30.7749	30.7918	30.7873
29	H	-3.109741	2.075442	-3.324261	28.1044	28.0814	28.1006	28.0987	28.0925
30	H	-2.769064	1.990590	-1.645857	28.1087	28.0873	28.1045	28.0972	28.0906
31	N	-4.312000	0.157000	-7.046000	151.0598	150.2445	150.4116	150.9141	150.7988
32	C	-4.492000	-0.300000	-8.432000	146.8024	146.5382	146.5879	146.7975	146.7373
33	C	-3.406000	0.301000	-9.310000	13.8081	13.5830	13.7036	13.6696	13.7136
34	O	-3.213000	1.513000	-9.314000	4.1126	3.5209	3.4856	3.3451	3.1241

35	C	-5.873000	0.128000	-8.959000	168.5656	168.5666	168.5997	168.7769	168.7987
36	C	-7.049000	-0.532000	-8.226000	166.9530	166.7304	166.7395	166.8875	166.8747
37	C	-8.384000	0.084000	-8.604000	10.0731	10.1085	10.0885	10.0350	10.0215
38	O	-8.538000	1.308000	-8.617000	-7.4984	-5.1688	-5.2824	-7.3539	-7.4754
39	N	-9.375000	-0.766000	-8.883000	165.3926	165.5657	165.5445	165.4432	165.4453
40	H	-4.166349	1.120885	-6.873339	27.7429	27.6561	27.7175	27.7356	27.7295
41	H	-4.426149	-1.367690	-8.456522	28.9352	28.9228	28.9698	28.9682	28.9700
42	H	-5.961819	1.189634	-8.859281	31.1750	31.1408	31.2003	31.2030	31.2010
43	H	-5.934393	-0.123125	-9.997300	31.7825	31.7506	31.8170	31.8124	31.8117
44	H	-7.067334	-1.574011	-8.468441	31.4257	31.4038	31.4143	31.4291	31.4257
45	H	-6.904099	-0.424299	-7.171342	31.2994	31.2745	31.3358	31.3082	31.3032
46	H	-9.210682	-1.742037	-8.861743	28.1098	28.0598	28.1157	28.1108	28.1117
47	H	-10.274176	-0.420265	-9.111145	28.4141	28.3866	28.4323	28.4169	28.4169
48	N	-2.688000	-0.550000	-10.038000	153.4237	153.4564	153.3635	153.3937	153.4196
49	C	-1.748000	-0.074000	-11.048000	148.4024	148.6759	148.6566	148.7109	148.8530
50	C	-2.009000	-0.747000	-12.390000	13.2108	13.3590	13.1600	13.3139	13.4797
51	O	-2.262000	-1.949000	-12.450000	0.4031	-0.4609	-2.0660	-0.7239	0.3467
52	C	-0.299000	-0.363000	-10.629000	158.7369	158.7484	158.7904	158.9258	159.0631
53	C	0.697000	0.175000	-11.625000	15.8196	15.4783	15.9287	16.0183	16.0500

54	O	0.899000	1.379000	-11.723000	-11.4635	-12.9061	-11.4279	-12.1558	-12.6380
55	N	1.318000	-0.718000	-12.380000	158.5581	164.1087	158.3397	158.1755	158.1210
56	H	-2.793141	-1.523528	-9.892094	27.7440	27.7241	27.7501	27.7537	27.7506
57	H	-1.889645	0.982499	-11.140982	28.6085	28.6299	28.6201	28.6367	28.6441
58	H	-0.116216	0.088696	-9.676392	30.8417	30.8060	30.8355	30.8416	30.8430
59	H	-0.166877	-1.421298	-10.542693	31.2309	31.2070	31.2416	31.2368	31.2580
60	H	1.124135	-1.682241	-12.267058	28.6403	28.2848	28.6282	28.6179	28.6097
61	H	1.976189	-0.421459	-13.057459	29.9928	28.5242	29.9710	29.9875	30.0108
62	N	-1.942000	0.035000	-13.461000	154.7648	156.4592	156.3348	155.9386	155.4995
63	C	-1.937000	-0.543000	-14.799000	142.5854	142.6166	142.5832	142.5482	142.4015
64	C	-0.871000	0.104000	-15.676000	13.3681	13.9219	13.9913	14.0999	14.1212
65	O	-0.674000	1.318000	-15.627000	-11.9517	-12.8078	-11.9383	-14.7813	-14.5914
66	C	-3.322000	-0.437000	-15.495000	135.0983	135.1186	135.1150	135.1203	135.1144
67	O	-3.203000	-0.912000	-16.838000	298.6618	300.3354	300.1960	299.7523	299.5372
68	C	-3.844000	0.981000	-15.511000	179.2859	179.3333	179.3466	179.3374	179.3246
69	H	-1.895108	1.017631	-13.349922	28.0749	28.1456	28.1571	28.1312	28.1122
70	H	-1.708617	-1.581097	-14.676132	28.5487	28.5209	28.5278	28.5299	28.5333
71	H	-4.017423	-1.031435	-14.940081	29.4679	29.4796	29.4877	29.4825	29.4794
72	H	-4.796298	1.005025	-15.998289	31.9733	31.9683	31.9799	31.9804	31.9791

73	H	-3.948442	1.333976	-14.506311	32.3438	32.3344	32.3546	32.3551	32.3513
74	H	-3.156881	1.608067	-16.039729	32.0802	32.0971	32.1036	32.0933	32.0854
75	H	-2.468720	-0.428017	-17.197294	30.4726	30.3673	30.3936	30.3760	30.3670
76	N	-0.187000	-0.710000	-16.472000	135.7648	134.4190	134.6250	134.2154	133.5632
77	C	0.767000	-0.200000	-17.457000	141.2413	141.0097	141.0664	141.1942	141.4975
78	C	0.043000	0.142000	-18.765000	13.2238	13.0765	13.0862	13.1105	13.1074
79	O	-1.185000	-0.034000	-18.875000	51.7041	51.3563	51.9107	51.7942	51.9267
80	C	1.920000	-1.196000	-17.666000	163.0948	163.2099	163.2130	163.0942	163.1565
81	C	2.818000	-1.298000	-16.478000	47.2655	47.2728	46.7999	46.9070	47.0129
82	C	2.559000	-2.231000	-15.482000	59.4495	59.8435	59.4606	59.4820	59.4249
83	C	3.889000	-0.428000	-16.318000	62.3616	63.1918	62.4875	62.4450	62.4191
84	C	3.379000	-2.309000	-14.355000	60.2566	60.5840	60.1681	60.2649	60.2996
85	C	4.703000	-0.496000	-15.202000	60.9732	61.5175	61.0051	61.0069	61.0063
86	C	4.446000	-1.433000	-14.213000	64.2947	64.6546	64.4276	64.4381	64.4058
87	O	0.644000	0.627000	-19.730000	57.4767	58.3755	57.9615	58.2755	58.1707
88	H	-0.326337	-1.687259	-16.396837	28.0507	27.9834	27.9875	27.9864	27.9820
89	H	1.204750	0.703994	-17.088123	29.2173	29.2481	29.2216	29.2236	29.2408
90	H	1.508216	-2.162095	-17.870925	30.8005	30.8235	30.8101	30.8052	30.8153
91	H	2.498466	-0.881749	-18.509518	29.8645	29.8747	29.8503	29.8550	29.8670

92	H	1.725194	-2.894471	-15.579331	25.3345	25.3110	25.2981	25.3115	25.3129
93	H	4.087398	0.306581	-17.070282	25.0534	25.1390	25.0497	25.0530	25.0540
94	H	3.185089	-3.043424	-13.601395	25.2172	25.1228	25.1998	25.2085	25.2088
95	H	5.530926	0.174383	-15.101880	25.0002	25.0695	24.9933	24.9969	24.9976
96	H	5.067904	-1.480578	-13.343591	25.2416	25.2529	25.2455	25.2443	25.2394

Table 11: Cartesian coordinates and isotropic shielding constants (in ppm) for 3G03

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	-22.242000	-6.689000	-26.925000	226.2211	226.3221	226.3367	226.2820	226.2538
2	C	-21.106000	-6.292000	-26.039000	147.4086	147.4608	147.7324	147.2880	147.3602
3	C	-21.644000	-6.122000	-24.644000	12.6737	12.8814	12.8018	12.6344	12.5658
4	O	-22.613000	-5.386000	-24.429000	-1.2590	2.9455	5.8200	0.9466	0.8583
5	C	-20.462000	-4.996000	-26.521000	165.8914	163.8828	166.2386	165.7087	165.7144
6	C	-19.096000	-5.108000	-27.207000	176.8268	174.4914	177.0394	176.3897	176.2404
7	C	-18.932000	-3.957000	-28.216000	174.0862	173.3349	174.1553	173.9959	173.9737
8	C	-18.936000	-6.416000	-27.956000	179.8552	179.0822	179.8380	179.8483	179.8401
9	H	-21.912521	-6.807262	-27.851044	29.0926	28.9545	29.0889	29.1023	29.0959
10	H	-22.630700	-7.540208	-26.601800	28.9322	28.8716	28.9409	28.9191	28.9159
11	H	-22.935370	-5.982540	-26.909124	28.5635	28.5300	28.5414	28.5490	28.5467
12	H	-20.350302	-7.049252	-26.058724	29.3299	28.9254	29.3365	29.3297	29.3278
13	H	-21.137096	-4.529090	-27.207397	32.3222	32.0191	32.3215	32.3047	32.2982
14	H	-20.353142	-4.349007	-25.675749	31.2928	30.9328	31.3334	31.3092	31.3208
15	H	-18.352710	-5.061836	-26.438698	32.3931	31.4937	32.3737	32.4130	32.4226

16	H	-17.978282	-4.035511	-28.694704	32.5306	31.9505	32.5413	32.5108	32.5086
17	H	-19.706398	-4.014927	-28.952106	32.7659	32.4470	32.7736	32.7409	32.7381
18	H	-18.997328	-3.020534	-27.702518	31.8782	31.8523	31.8529	31.8777	31.8695
19	H	-17.970584	-6.447642	-28.416293	32.7784	31.8266	32.7714	32.7586	32.7566
20	H	-19.031783	-7.232922	-27.271628	32.5892	31.7961	32.5639	32.5563	32.5533
21	H	-19.692685	-6.490788	-28.708817	33.0869	32.6515	33.0926	33.0748	33.0729
22	N	-21.024000	-6.825000	-23.704000	149.9430	150.9563	149.5932	150.1403	150.0724
23	C	-21.556000	-6.934000	-22.362000	141.8336	141.9123	141.3720	141.5198	141.5710
24	C	-20.889000	-5.919000	-21.454000	8.5057	9.5238	8.4958	8.6814	8.4382
25	O	-19.778000	-5.445000	-21.731000	-20.0907	-38.2841	-26.2184	-20.8636	-18.3772
26	C	-21.301000	-8.318000	-21.753000	132.4459	132.3136	132.7213	132.6216	132.4170
27	O	-19.886000	-8.554000	-21.691000	302.7397	307.6755	303.4565	303.6910	304.0608
28	C	-21.987000	-9.411000	-22.580000	175.7385	175.5086	175.5995	175.5864	175.5790
29	H	-20.176674	-7.286251	-23.926230	27.4568	27.3249	27.2895	27.3813	27.3897
30	H	-22.609623	-6.763085	-22.436610	28.7500	28.9429	28.6983	28.7121	28.7069
31	H	-21.711716	-8.345723	-20.765355	28.5214	28.9936	28.5543	28.5435	28.5414
32	H	-21.795786	-10.366153	-22.137259	31.8611	31.8594	31.8781	31.8602	31.8517
33	H	-23.041813	-9.232682	-22.601722	32.0562	32.0974	32.0479	32.0434	32.0308
34	H	-21.602307	-9.397203	-23.578359	31.6543	31.6285	31.6262	31.6399	31.6348

35	H	-19.805781	-9.419541	-21.307719	31.8758	31.9331	31.9434	31.9058	31.8896
36	N	-21.577000	-5.602000	-20.367000	149.6023	152.8183	150.1876	149.3829	148.9401
37	C	-21.010000	-4.726000	-19.364000	141.0836	141.2889	140.7904	140.8721	140.7973
38	C	-19.562000	-5.125000	-19.110000	9.1177	9.9983	9.9512	9.7144	10.0525
39	O	-18.668000	-4.289000	-19.162000	-10.7705	-32.9178	-10.5581	-3.3330	3.8696
40	C	-21.805000	-4.750000	-18.055000	165.2771	164.6579	165.1010	165.0769	164.9523
41	C	-21.160000	-3.944000	-16.978000	55.8437	55.4257	55.9042	55.9443	56.1210
42	C	-21.292000	-2.576000	-16.948000	60.9638	61.1946	60.9257	60.9027	60.8569
43	C	-20.361000	-4.549000	-16.023000	62.1780	62.6416	62.8949	62.8398	62.9692
44	C	-20.652000	-1.820000	-15.960000	60.7527	60.5803	60.5473	60.5000	60.4200
45	C	-19.714000	-3.797000	-15.064000	65.5724	65.3992	65.4937	65.4807	65.4330
46	C	-19.863000	-2.449000	-15.019000	64.5139	66.6187	64.4632	64.5099	64.4526
47	H	-22.488003	-5.967968	-20.239556	27.2858	27.6813	27.2418	27.2119	27.1979
48	H	-21.055163	-3.724020	-19.736687	28.6709	29.0770	28.6300	28.6262	28.6202
49	H	-22.784527	-4.360436	-18.238487	29.8407	29.9019	29.8601	29.8426	29.7972
50	H	-21.892838	-5.763277	-17.722655	30.1603	30.4871	30.1759	30.1829	30.1921
51	H	-21.889772	-2.084845	-17.687145	24.9777	25.1029	24.9695	24.9629	24.9469
52	H	-20.243769	-5.612544	-16.028619	25.4621	25.4333	25.5108	25.5123	25.5301
53	H	-20.774022	-0.757293	-15.934202	25.0143	25.0486	24.9865	24.9798	24.9653

54	H	-19.086574	-4.283123	-14.346420	25.8783	25.3409	25.8985	25.8961	25.8944
55	H	-19.372007	-1.877816	-14.259016	26.2932	25.2784	26.2956	26.2976	26.2900
56	N	-19.301000	-6.407000	-18.857000	142.7774	147.1938	143.9200	142.3941	141.3645
57	C	-17.905000	-6.787000	-18.576000	138.6117	138.9289	138.8983	138.8456	138.8708
58	C	-16.961000	-6.377000	-19.687000	6.2799	6.7732	6.5664	6.6546	6.8656
59	O	-15.842000	-5.912000	-19.422000	13.2981	-0.0883	29.4662	31.9040	38.2786
60	C	-17.752000	-8.276000	-18.285000	174.3247	173.9414	174.3679	174.5105	174.4740
61	C	-18.508000	-8.703000	-17.077000	163.5975	163.6792	163.7177	163.7243	163.8040
62	C	-19.902000	-9.164000	-17.431000	7.9395	8.3914	8.0927	8.0901	8.1294
63	O	-20.302000	-10.229000	-16.924000	3.2303	8.4550	5.4413	4.3767	3.6148
64	O	-20.594000	-8.488000	-18.231000	72.9878	70.1662	77.7452	78.8921	78.8120
65	H	-20.023301	-7.084038	-18.857765	21.2223	21.5609	21.2544	21.1945	21.1638
66	H	-17.635655	-6.247260	-17.692238	29.5424	29.7325	29.5830	29.5866	29.5924
67	H	-18.106352	-8.831015	-19.128382	31.6945	31.7927	31.7101	31.7413	31.7420
68	H	-16.714846	-8.494601	-18.138625	31.4951	31.6142	31.5849	31.5625	31.5371
69	H	-17.984099	-9.506434	-16.602741	30.8957	30.9625	30.9327	30.9347	30.9257
70	H	-18.574368	-7.879486	-16.397059	31.1249	31.1857	31.1541	31.1551	31.1612
71	N	-17.403000	-6.525000	-20.931000	146.9475	148.6077	147.2291	146.0168	145.2524
72	C	-16.576000	-6.097000	-22.055000	142.1700	142.5621	141.9515	141.9848	141.9703

73	C	-16.200000	-4.624000	-21.931000	7.2903	7.4534	7.9093	7.8873	7.9666
74	O	-15.027000	-4.252000	-22.056000	-21.1537	-47.6946	-19.0143	-18.5758	-18.2364
75	C	-17.276000	-6.319000	-23.402000	174.9308	173.6650	175.0071	174.7702	174.6907
76	C	-16.535000	-5.709000	-24.551000	63.8947	65.0740	63.5195	63.6283	63.8691
77	N	-15.587000	-6.403000	-25.276000	99.5892	99.9126	99.6962	99.4232	99.4423
78	C	-16.566000	-4.458000	-25.073000	60.8813	63.1013	61.1781	61.3675	61.3102
79	C	-15.079000	-5.610000	-26.204000	53.2375	52.8847	53.3685	53.1116	53.0264
80	N	-15.655000	-4.425000	-26.103000	-37.1239	-28.1436	-37.1744	-36.5016	-36.5061
81	H	-18.293243	-6.925558	-21.095684	26.7129	27.8634	26.8614	26.8595	26.8515
82	H	-15.691480	-6.698335	-22.024653	29.2836	29.3275	29.2736	29.2820	29.2779
83	H	-17.369496	-7.371229	-23.572215	30.6655	30.4899	30.6744	30.6548	30.6333
84	H	-18.254830	-5.889220	-23.356382	29.5500	30.9560	29.4422	29.5676	29.5858
85	H	-17.183545	-3.648063	-24.745067	26.6683	26.6875	26.7030	26.7295	26.7226
86	H	-14.328340	-5.881823	-26.916406	24.8429	24.8197	24.8453	24.8315	24.8266
87	H	-15.328154	-7.346515	-25.124745	24.9806	25.0206	25.0098	24.9842	24.9799
88	N	-17.203000	-3.785000	-21.705000	152.7923	151.9414	155.8113	154.3658	153.7613
89	C	-16.969000	-2.355000	-21.612000	140.6111	140.4932	140.8709	140.7565	140.7948
90	C	-16.112000	-1.982000	-20.403000	8.9481	10.4769	9.1308	9.1548	9.0606
91	O	-15.236000	-1.129000	-20.494000	2.0652	-17.2637	4.0289	4.9219	6.3454

92	C	-18.279000	-1.586000	-21.550000	165.1994	163.9972	165.1772	165.0920	165.0172
93	C	-19.005000	-1.566000	-22.868000	59.3526	60.1592	59.5855	59.5708	59.7943
94	C	-20.215000	-2.236000	-23.019000	55.7162	56.7180	55.3986	55.5109	55.4356
95	C	-18.481000	-0.888000	-23.961000	56.0343	56.6299	56.0861	56.1152	56.1176
96	C	-20.890000	-2.228000	-24.226000	77.1470	78.7093	77.2486	77.0856	77.0601
97	C	-19.157000	-0.862000	-25.171000	77.0536	76.9517	77.1409	77.0705	77.0669
98	C	-20.361000	-1.542000	-25.291000	35.9745	35.2011	35.7827	35.8871	35.7851
99	O	-21.039000	-1.546000	-26.490000	247.5246	251.1628	247.3579	247.5797	247.4037
100	H	-18.121680	-4.138262	-21.598547	26.3884	28.0576	26.4914	26.5844	26.5599
101	H	-16.435386	-2.083655	-22.498864	29.2352	29.0813	29.2733	29.2966	29.2916
102	H	-18.910741	-2.039567	-20.815099	30.2632	30.5808	30.1980	30.2587	30.2593
103	H	-18.073806	-0.578457	-21.253940	30.1706	29.9266	30.1970	30.1724	30.1389
104	H	-20.630164	-2.766227	-22.187496	25.1980	25.1104	25.0949	25.1254	25.0978
105	H	-17.544134	-0.379540	-23.867996	24.6482	24.6929	24.6427	24.6536	24.6450
106	H	-21.817071	-2.752250	-24.328963	25.9521	25.8494	25.9444	25.9043	25.8914
107	H	-18.754873	-0.323447	-26.003559	25.3702	25.3510	25.3461	25.3447	25.3354
108	H	-21.811632	-2.073428	-26.324597	28.7312	28.5909	28.6875	28.6884	28.6755
109	N	-16.375000	-2.625000	-19.272000	148.3406	152.9472	149.2107	149.4674	150.0880
110	C	-15.680000	-2.284000	-18.026000	142.5735	142.8323	142.8190	142.6244	142.5326

111	C	-14.217000	-2.677000	-18.127000	4.8255	6.1363	4.3588	4.4960	4.6115
112	O	-13.335000	-1.969000	-17.631000	-14.2451	-19.2087	-15.9128	-16.5594	-18.1700
113	C	-16.363000	-2.964000	-16.838000	173.5434	172.9996	173.6919	173.6702	173.7923
114	C	-15.897000	-2.417000	-15.548000	81.3365	82.7348	80.8340	81.0420	81.3036
115	C	-14.985000	-2.972000	-14.704000	62.2834	61.1003	62.2834	62.1566	61.9811
116	C	-16.266000	-1.161000	-14.973000	63.7120	65.0243	63.6188	63.7146	63.7908
117	N	-14.775000	-2.143000	-13.634000	144.6544	143.8075	144.8004	144.4694	144.2028
118	C	-15.562000	-1.033000	-13.766000	52.4917	53.2375	52.4967	52.4545	52.4485
119	C	-17.148000	-0.143000	-15.350000	63.5796	68.2677	63.5426	63.7410	63.7961
120	C	-15.701000	0.075000	-12.926000	81.4570	81.2245	81.5490	81.3833	81.3356
121	C	-17.287000	0.964000	-14.506000	71.2714	71.7314	71.2728	71.2134	71.1068
122	C	-16.557000	1.068000	-13.322000	68.1630	68.5550	68.1793	68.1260	68.0422
123	H	-17.052013	-3.347320	-19.269292	25.3854	28.0185	25.6358	25.6974	25.7690
124	H	-15.728995	-1.226779	-17.868575	29.3751	29.0646	29.3977	29.3839	29.3815
125	H	-17.420445	-2.820067	-16.915412	31.2668	30.0204	31.2546	31.2747	31.2802
126	H	-16.151336	-4.012419	-16.868272	30.6240	30.1260	30.6733	30.6556	30.6749
127	H	-14.503538	-3.915717	-14.853976	25.3165	25.2223	25.2875	25.2815	25.2674
128	H	-14.152600	-2.319508	-12.884624	25.6175	25.5714	25.6186	25.5944	25.5810
129	H	-17.703220	-0.209350	-16.262265	24.7658	24.5858	24.7044	24.7289	24.7288

130	H	-15.158227	0.145084	-12.006552	25.1521	25.1197	25.1439	25.1333	25.1296
131	H	-17.966417	1.745999	-14.773899	25.2791	25.3111	25.2582	25.2603	25.2506
132	H	-16.667863	1.939885	-12.711732	25.1361	25.1368	25.1182	25.1204	25.1138
133	N	-13.960000	-3.798000	-18.800000	148.0442	149.2973	148.7893	148.6924	148.6174
134	C	-12.600000	-4.286000	-18.991000	147.8666	148.1725	147.8867	147.9061	147.9852
135	C	-11.769000	-3.313000	-19.812000	8.0655	10.2605	9.1125	9.0530	9.0658
136	O	-10.547000	-3.324000	-19.735000	8.0721	-9.8656	5.7871	6.4316	4.2795
137	C	-12.600000	-5.648000	-19.625000	182.9795	182.4978	183.0499	183.0717	183.1313
138	H	-14.714143	-4.313935	-19.181024	25.8231	27.7294	25.8986	25.9811	25.9954
139	H	-12.149977	-4.365449	-18.023494	29.3106	29.0879	29.2915	29.2853	29.2813
140	H	-11.591487	-5.981610	-19.753478	31.8864	31.4652	31.8902	31.8694	31.8587
141	H	-13.125309	-6.334804	-18.994722	31.7027	31.6281	31.7154	31.7211	31.7184
142	H	-13.083203	-5.597638	-20.578351	31.8101	32.0291	31.8398	31.8700	31.8704
143	N	-12.430000	-2.472000	-20.600000	155.0183	159.7632	155.1472	155.9846	156.4242
144	C	-11.714000	-1.458000	-21.355000	147.0247	146.9071	146.9250	147.2223	147.3337
145	C	-11.248000	-0.277000	-20.504000	9.6334	9.9174	9.3316	9.5040	9.6961
146	O	-10.603000	0.627000	-21.024000	3.7203	-1.5567	2.9562	2.0967	1.1932
147	C	-12.524000	-0.995000	-22.562000	176.0354	174.0339	176.0847	176.0871	176.0202
148	C	-12.419000	-1.946000	-23.724000	169.3481	168.8836	168.9660	169.2874	169.3362

149	C	-13.571000	-1.830000	-24.674000	12.6491	11.6057	12.3584	12.2706	12.3839
150	O	-14.442000	-0.976000	-24.510000	4.1695	-15.0416	11.0678	10.4380	11.2164
151	N	-13.590000	-2.694000	-25.687000	149.8580	171.9573	149.5441	149.9586	149.8126
152	H	-13.415185	-2.536581	-20.673074	27.3819	28.0253	27.5210	27.5731	27.6388
153	H	-10.820566	-1.928107	-21.709508	29.6679	29.4037	29.6351	29.6505	29.6364
154	H	-13.551721	-0.909412	-22.276758	30.6793	31.5321	30.6835	30.7032	30.7096
155	H	-12.168854	-0.033398	-22.868744	31.3877	31.0693	31.3231	31.3336	31.3175
156	H	-11.512458	-1.742972	-24.254906	31.1692	30.7976	31.1066	31.1227	31.1084
157	H	-12.381589	-2.947060	-23.347996	31.7091	31.2850	31.6215	31.6339	31.6253
158	H	-12.867484	-3.364479	-25.779351	28.5851	28.2514	28.5225	28.5282	28.5233
159	H	-14.326642	-2.665900	-26.347809	27.1132	28.3341	27.0592	27.0483	27.0494
160	N	-11.554000	-0.282000	-19.202000	150.5634	146.4230	150.5885	150.3037	150.4507
161	C	-11.026000	0.750000	-18.302000	147.0315	146.7803	147.1503	147.0565	146.9450
162	C	-9.625000	0.392000	-17.854000	9.1285	10.7337	10.1540	10.0318	9.9422
163	O	-8.898000	1.247000	-17.338000	27.3065	22.9745	25.6980	23.1721	20.3080
164	C	-11.927000	0.979000	-17.080000	163.4488	159.9835	163.5580	163.5021	163.4974
165	C	-13.156000	1.864000	-17.255000	174.2591	173.8015	174.5150	174.4175	174.3277
166	C	-14.214000	1.489000	-16.235000	176.1711	174.1384	176.0490	175.9569	175.9008
167	C	-12.802000	3.345000	-17.135000	176.3757	176.3346	176.2911	176.3168	176.3462

168	H	-12.143822	-0.990447	-18.841012	26.6039	26.5502	26.4941	26.5112	26.5650
169	H	-11.001559	1.665108	-18.855968	29.2610	28.9087	29.2656	29.2649	29.2564
170	H	-12.261286	0.021755	-16.738188	31.8802	32.0779	31.9205	31.9180	31.9295
171	H	-11.324252	1.408253	-16.307125	32.6434	31.7828	32.5719	32.6111	32.6043
172	H	-13.542943	1.702716	-18.239460	32.6000	32.0179	32.6260	32.6235	32.6101
173	H	-15.072303	2.114565	-16.364941	33.4247	32.1289	33.3614	33.3640	33.3541
174	H	-14.494559	0.465556	-16.371927	33.7817	32.1971	33.6931	33.7402	33.7734
175	H	-13.821533	1.622325	-15.248545	34.1458	32.3846	34.1113	34.1074	34.0913
176	H	-13.685813	3.934456	-17.262731	32.5439	32.1386	32.5177	32.5189	32.5077
177	H	-12.383462	3.534510	-16.168661	33.0186	32.5508	32.9841	32.9903	32.9797
178	H	-12.088741	3.603501	-17.889546	32.0949	31.8056	32.1007	32.0959	32.0873
179	N	-9.248000	-0.870000	-18.039000	147.3486	148.2195	148.0135	148.0164	147.8128
180	C	-7.904000	-1.332000	-17.710000	144.9922	144.7978	145.0734	144.9671	144.9442
181	C	-7.126000	-1.648000	-18.986000	14.4148	14.5323	14.3752	14.4561	14.4923
182	O	-6.893000	-0.771000	-19.830000	49.8115	48.4651	49.8770	49.8879	49.6423
183	C	-7.938000	-2.611000	-16.848000	131.4934	131.2307	131.5487	131.4911	131.4397
184	O	-8.899000	-2.465000	-15.794000	307.2611	306.9038	307.0267	307.2153	307.1994
185	C	-6.546000	-2.909000	-16.253000	172.9265	172.8748	172.9290	172.9302	172.9287
186	O	-6.726000	-2.806000	-19.169000	37.2147	36.4077	37.0576	36.9902	36.7564

187	H	-9.899531	-1.515679	-18.411434	27.3994	27.5249	27.2727	27.3664	27.4483
188	H	-7.429455	-0.545667	-17.161013	29.2631	29.1127	29.2892	29.2754	29.2623
189	H	-8.220635	-3.431920	-17.473385	29.0472	29.0920	29.0859	29.0782	29.0831
190	H	-6.594417	-3.798604	-15.660412	32.1544	32.1149	32.1610	32.1644	32.1596
191	H	-5.841127	-3.046709	-17.046152	31.0939	31.0667	31.1199	31.1036	31.1012
192	H	-6.237096	-2.088352	-15.639800	32.4067	32.3323	32.4140	32.4141	32.4101
193	H	-8.856305	-3.285914	-15.317789	32.7093	32.6288	32.7417	32.7225	32.7147

Table 12: Cartesian coordinates and isotropic shielding constants (in ppm) for 3HYD

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	1.149000	1.920000	3.550000	228.7748	228.9682	228.9846	228.9269	228.8847
2	C	2.138000	2.288000	4.580000	146.5205	147.0576	146.9667	146.1765	146.2213
3	C	3.461000	1.638000	4.282000	11.5349	11.6406	11.5642	11.6964	11.6860
4	O	3.527000	0.405000	4.165000	-14.4314	-6.3486	-5.9751	-18.2822	-15.7912
5	C	1.635000	1.889000	5.948000	162.3480	162.8640	162.7964	162.2341	162.2907
6	C	2.444000	2.344000	7.182000	173.6455	173.8296	173.8481	173.4488	173.4118
7	C	1.603000	2.227000	8.438000	174.4721	174.3244	174.3562	174.5109	174.4801
8	C	3.699000	1.583000	7.375000	177.2855	176.7870	176.9021	177.3162	177.2273
9	H	0.282421	2.352516	3.755110	28.9020	28.8959	28.8725	28.9053	28.9081
10	H	1.467604	2.223551	2.663181	28.6993	28.6776	28.7292	28.6824	28.6807
11	H	1.032992	0.936869	3.540200	28.5416	28.5567	28.5691	28.5519	28.5488
12	H	2.276883	3.348904	4.570343	29.5784	29.6059	29.5995	29.5769	29.5725
13	H	0.640978	2.270949	6.052569	31.6953	31.7174	31.6988	31.6984	31.6992
14	H	1.576787	0.820894	5.973724	31.7692	31.7952	31.8142	31.7671	31.7690
15	H	2.709815	3.364024	6.998172	31.8969	31.8247	31.8376	31.9055	31.8949

16	H	2.177288	2.545611	9.282737	32.1163	32.0981	32.1066	32.1172	32.1180
17	H	0.734034	2.844248	8.344173	32.0932	32.0713	32.0869	32.0938	32.0940
18	H	1.304128	1.208566	8.573532	32.3224	32.3062	32.3165	32.3240	32.3254
19	H	4.207402	1.947754	8.242976	32.2639	32.2369	32.2504	32.2625	32.2615
20	H	3.470755	0.545730	7.504906	32.7124	32.7009	32.7109	32.7024	32.7015
21	H	4.325968	1.705459	6.516621	32.2244	32.1103	32.1434	32.2799	32.2714
22	N	4.521000	2.434000	4.230000	143.9091	144.3744	144.2906	144.3418	144.1712
23	C	5.866000	1.930000	4.058000	141.6920	141.7482	141.7583	141.7604	141.7255
24	C	6.790000	2.592000	5.064000	7.4039	7.7744	7.7149	7.6219	7.5973
25	O	6.806000	3.837000	5.179000	2.6043	-0.6385	-0.1196	-0.3065	-1.5277
26	C	6.425000	2.168000	2.650000	166.8603	166.3539	166.2651	166.2277	166.2400
27	C	7.834000	1.667000	2.541000	179.2194	179.9440	179.2793	179.2884	179.2908
28	C	5.522000	1.554000	1.584000	178.9809	178.9230	178.9062	178.9170	178.9015
29	H	4.386265	3.411344	4.312133	27.4035	27.4023	27.3888	27.3843	27.3821
30	H	5.817050	0.872223	4.211663	29.1436	29.1086	29.1154	29.1286	29.1250
31	H	6.444584	3.223587	2.476069	31.5652	31.5970	31.5607	31.5463	31.5422
32	H	8.200095	1.844477	1.551366	32.0254	32.0864	32.0399	32.0285	32.0254
33	H	8.451246	2.181833	3.247296	32.3194	32.2848	32.2876	32.2949	32.2943
34	H	7.856157	0.617163	2.746553	32.4775	32.4662	32.4528	32.4541	32.4482

35	H	5.938370	1.736783	0.615431	32.1603	32.1959	32.1790	32.1679	32.1643
36	H	5.445309	0.499115	1.745977	32.4384	32.4354	32.4261	32.4292	32.4218
37	H	4.549167	1.995585	1.643148	31.9448	31.9668	31.9544	31.9487	31.9435
38	N	7.567000	1.777000	5.771000	141.4312	140.4288	140.9293	141.0679	141.0619
39	C	8.674000	2.248000	6.587000	146.9734	147.2032	147.2543	147.2295	147.1732
40	C	9.920000	1.636000	5.964000	11.2836	10.7492	11.0361	11.0942	11.1174
41	O	10.041000	0.405000	5.901000	19.2837	19.9020	19.7107	19.1092	19.3021
42	C	8.541000	1.813000	8.049000	167.6608	167.6762	167.7027	167.6869	167.7071
43	C	9.625000	2.367000	8.970000	166.0593	165.5634	165.5334	165.5707	165.5056
44	C	9.581000	1.798000	10.378000	14.6333	14.6050	14.6435	14.6325	14.6313
45	O	9.326000	0.609000	10.555000	57.6587	58.1076	57.9203	57.8509	57.8545
46	O	9.823000	2.595000	11.317000	35.6060	35.7529	35.5414	35.7911	35.7908
47	H	7.383192	0.804698	5.740289	27.7241	27.6565	27.6595	27.6827	27.6875
48	H	8.705223	3.317411	6.603865	28.8556	28.8612	28.8690	28.8713	28.8688
49	H	7.588343	2.136001	8.413712	31.8691	31.8500	31.8751	31.8737	31.8739
50	H	8.575140	0.744308	8.089401	31.1346	31.1259	31.1541	31.1570	31.1586
51	H	10.581002	2.146965	8.542747	31.9348	31.9526	31.8974	31.8945	31.8986
52	H	9.513434	3.429601	9.027724	31.5884	31.5709	31.5403	31.5472	31.5522
53	N	10.842000	2.465000	5.490000	147.3115	147.3299	147.3763	147.2823	147.2677

54	C	12.006000	2.016000	4.750000	151.5353	151.6880	151.6987	151.6999	151.7245
55	C	13.270000	2.689000	5.248000	11.7593	11.8440	11.8956	11.8828	11.9445
56	O	13.284000	3.899000	5.529000	17.4874	20.2753	19.6984	19.7366	19.1493
57	C	11.833000	2.220000	3.258000	176.3025	178.0484	176.4829	176.5095	176.5489
58	H	10.729906	3.435687	5.649064	27.8235	27.7944	27.7991	27.7966	27.8072
59	H	12.104133	0.964565	4.922497	29.0177	28.8331	29.0398	29.0310	29.0337
60	H	12.708939	1.878157	2.747340	32.2483	32.1297	32.2620	32.2546	32.2558
61	H	10.983051	1.665768	2.918420	31.7742	31.8398	31.7933	31.7977	31.7967
62	H	11.684888	3.260080	3.055030	31.7956	31.9089	31.8378	31.8297	31.8306
63	N	14.334000	1.918000	5.332000	150.6611	149.0460	149.3983	149.7646	149.9869
64	C	15.634000	2.369000	5.796000	149.5147	149.7281	149.6284	149.6049	149.5591
65	C	16.689000	1.821000	4.849000	9.5480	9.2784	9.3019	9.4354	9.3885
66	O	16.716000	0.605000	4.614000	7.3266	7.2545	7.0802	6.5144	6.2928
67	C	15.875000	1.877000	7.209000	159.0663	158.9518	159.1069	159.0490	159.1028
68	C	17.250000	2.151000	7.852000	176.3554	175.2699	176.3113	176.1289	176.0111
69	C	17.789000	3.495000	7.677000	179.2387	179.1234	179.2088	179.2084	179.2133
70	C	17.128000	1.821000	9.337000	174.2677	173.9946	174.2869	174.2199	174.2018
71	H	14.241844	0.970138	5.061511	28.4377	28.3568	28.3951	28.4052	28.4075
72	H	15.679186	3.437989	5.806972	28.9404	28.9611	28.9571	28.9535	28.9498

73	H	15.129511	2.317712	7.837426	32.1559	32.1702	32.1808	32.1569	32.1595
74	H	15.719478	0.818378	7.214740	31.5710	31.5708	31.6123	31.5926	31.5901
75	H	17.956504	1.531697	7.339930	32.1398	32.1735	32.1352	32.1456	32.1633
76	H	18.739684	3.564111	8.163132	32.1190	32.2132	32.1079	32.1229	32.1345
77	H	17.906468	3.699058	6.633227	32.1182	32.2147	32.0838	32.0940	32.1040
78	H	17.116251	4.207770	8.106263	32.4960	32.5751	32.5025	32.5092	32.5102
79	H	18.065943	1.999075	9.820169	32.3465	32.2852	32.3524	32.3535	32.3516
80	H	16.375716	2.440129	9.779321	32.5454	32.5147	32.5533	32.5501	32.5491
81	H	16.856804	0.792424	9.452688	32.1915	32.0974	32.2048	32.1942	32.1902
82	N	17.519000	2.699000	4.281000	145.4488	144.8338	144.9162	144.5035	144.3863
83	C	18.548000	2.342000	3.321000	148.3295	148.2969	148.2453	148.2654	148.4399
84	C	19.876000	2.878000	3.804000	14.4804	13.5293	13.9194	13.7845	13.6201
85	O	20.024000	4.082000	3.994000	22.8278	28.0623	31.1352	30.7536	29.4966
86	C	18.275000	2.935000	1.947000	164.0806	163.9577	163.9745	163.9877	163.9940
87	C	16.873000	2.775000	1.400000	60.2181	59.8281	59.8707	60.0149	60.1458
88	C	15.855000	3.614000	1.819000	53.2995	52.5109	53.1568	53.1452	53.1800
89	C	16.556000	1.796000	0.450000	56.1640	56.0486	56.2620	56.1698	56.1078
90	C	14.558000	3.509000	1.303000	78.2575	80.1277	78.2810	78.3186	78.3182
91	C	15.281000	1.695000	-0.071000	77.6150	77.8753	77.7200	77.6981	77.6536

92	C	14.283000	2.550000	0.357000	36.1953	36.1541	36.2421	36.2304	36.1811
93	O	13.017000	2.418000	-0.175000	253.0885	253.1400	253.2062	253.2135	253.1368
94	H	17.427102	3.652787	4.529888	27.7929	27.7982	27.8153	27.8120	27.8206
95	H	18.558258	1.275316	3.237451	28.6306	28.6233	28.6336	28.6202	28.6303
96	H	18.494582	3.981341	1.990049	30.3033	30.2887	30.2954	30.2907	30.2966
97	H	18.953078	2.484211	1.252810	30.5103	30.4974	30.4969	30.4995	30.4957
98	H	16.064622	4.361316	2.555531	25.2191	25.1000	25.2121	25.2040	25.2064
99	H	17.313869	1.115318	0.122576	25.1847	25.1425	25.1792	25.1656	25.1530
100	H	13.787300	4.169367	1.641876	25.8547	25.7222	25.8489	25.8416	25.8347
101	H	15.064798	0.951410	-0.809398	25.9986	25.9926	26.0017	25.9940	25.9833
102	H	13.090811	1.696345	-0.788405	28.7139	28.7216	28.7164	28.7105	28.7007
103	N	20.857000	2.006000	3.973000	139.5133	140.3734	140.1852	139.9762	139.7745
104	C	22.208000	2.473000	4.312000	147.6502	147.8937	147.8570	147.7960	147.8493
105	C	23.293000	1.644000	3.744000	15.9347	15.8455	15.8731	15.9079	15.9201
106	O	23.018000	0.697000	3.000000	45.4600	45.4608	45.4511	45.3267	45.2435
107	C	22.356000	2.753000	5.793000	163.2310	163.3032	163.4204	163.3332	163.2815
108	C	22.263000	1.578000	6.717000	174.6178	174.7579	174.7189	174.6681	174.6209
109	C	22.913000	1.965000	8.038000	172.1967	172.1622	172.1834	172.1712	172.1443
110	C	20.853000	1.118000	7.009000	173.9296	174.6211	173.9413	173.9513	173.9345

111	O	24.470000	1.913000	3.995000	75.2325	75.5526	75.3580	75.4894	75.4588
112	H	20.680150	1.037300	3.870804	27.4882	27.5258	27.5096	27.5109	27.5135
113	H	22.327841	3.415007	3.818886	29.2193	29.2519	29.2402	29.2246	29.2166
114	H	23.307042	3.218576	5.946812	31.5202	31.5248	31.4975	31.5115	31.5092
115	H	21.597175	3.453372	6.073293	31.8531	31.9210	31.8501	31.8505	31.8447
116	H	22.754387	0.764587	6.225271	32.0965	32.0960	32.1141	32.1122	32.1127
117	H	22.859259	1.139927	8.717166	32.3173	32.3323	32.3303	32.3259	32.3234
118	H	23.937901	2.222013	7.869411	32.2613	32.2687	32.2690	32.2634	32.2601
119	H	22.398723	2.805081	8.455950	32.4655	32.5066	32.4760	32.4730	32.4712
120	H	20.881704	0.279566	7.673157	32.3647	32.3639	32.3944	32.3841	32.3776
121	H	20.304841	1.915726	7.465130	32.8262	32.9006	32.7926	32.8185	32.8397
122	H	20.374380	0.833095	6.095407	31.7334	31.6806	31.6961	31.6956	31.6747

Table 13: Cartesian coordinates and isotropic shielding constants (in ppm) for 3NHC

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	5.026000	6.111000	-8.432000	241.2227	241.2423	241.2450	241.2295	241.2288
2	C	4.844000	5.322000	-7.179000	155.0055	155.0113	155.0435	155.0379	155.0330
3	C	4.312000	6.127000	-6.016000	21.8626	21.8561	21.8826	21.8548	21.8383
4	O	4.152000	7.327000	-6.123000	-9.1299	-8.9192	-9.1553	-9.2742	-9.4114
5	H	5.375274	5.520687	-9.145890	28.7822	28.7899	28.7897	28.7898	28.7875
6	H	4.155406	6.489320	-8.713140	28.6893	28.6930	28.7025	28.6952	28.6939
7	H	5.668095	6.846574	-8.268461	28.6196	28.6283	28.6238	28.6219	28.6205
8	H	4.163370	4.520615	-7.377556	29.1377	29.1408	29.1478	29.1454	29.1427
9	H	5.788775	4.904489	-6.899743	29.1582	29.1662	29.1720	29.1707	29.1690
10	N	4.028000	5.449000	-4.904000	159.9482	159.4749	159.5794	159.6943	159.7861
11	C	3.436000	6.090000	-3.714000	143.6400	143.6194	143.5962	143.6094	143.5223
12	C	3.970000	5.420000	-2.444000	7.6889	7.4613	7.4644	7.4495	7.4204
13	O	4.327000	4.227000	-2.488000	-25.3783	-27.6476	-29.1525	-28.3612	-28.1028
14	C	1.926000	5.971000	-3.763000	163.6840	163.7072	163.6861	163.7347	163.7567
15	C	1.409000	4.566000	-3.776000	63.3959	63.3559	63.4393	63.4833	63.4894

16	C	1.108000	3.924000	-4.961000	55.7225	55.7104	55.7068	55.7024	55.7206
17	C	1.217000	3.864000	-2.584000	56.2418	56.1955	56.2320	56.3157	56.3838
18	C	0.623000	2.609000	-4.967000	81.3122	81.3907	81.3697	81.3123	81.3036
19	C	0.775000	2.586000	-2.583000	80.9004	80.9396	80.9124	80.9068	80.9128
20	C	0.467000	1.952000	-3.773000	35.8553	35.8567	35.8317	35.8229	35.7985
21	O	0.005000	0.653000	-3.725000	254.2776	254.2917	254.1983	254.2374	254.2114
22	H	4.221609	4.478537	-4.875425	28.3023	28.2865	28.3076	28.3200	28.3126
23	H	3.704788	7.125635	-3.703339	28.3783	28.3718	28.3708	28.3658	28.3595
24	H	1.519917	6.472326	-2.909379	30.4536	30.4603	30.4688	30.4583	30.4594
25	H	1.576587	6.467523	-4.644065	30.2396	30.2150	30.2174	30.2205	30.2179
26	H	1.247172	4.438360	-5.888882	25.3315	25.3099	25.3175	25.3165	25.3131
27	H	1.423946	4.347465	-1.652155	25.5409	25.4786	25.4993	25.5103	25.5029
28	H	0.378080	2.124812	-5.889213	26.0212	26.0164	26.0259	26.0168	26.0149
29	H	0.662939	2.062436	-1.656597	25.8783	25.8722	25.8806	25.8813	25.8792
30	H	-0.139457	0.418174	-4.634114	28.7394	28.7392	28.7468	28.7374	28.7350
31	N	4.021000	6.179000	-1.343000	151.7801	151.3345	151.3469	151.6404	151.7301
32	C	4.519000	5.696000	-0.038000	144.8300	144.5730	144.5707	144.6842	144.6796
33	C	3.728000	6.308000	1.134000	15.8969	15.9342	15.9248	15.9223	15.8831
34	O	3.395000	7.480000	1.108000	5.4555	2.9856	2.8140	3.0531	3.8887

35	C	5.988000	6.115000	0.154000	159.6881	159.3175	159.3841	159.5040	159.5165
36	C	7.018000	5.486000	-0.756000	170.8965	170.8377	170.8856	170.9056	170.8987
37	S	8.539000	6.448000	-0.666000	609.7814	610.0315	609.9058	609.6756	609.5704
38	C	9.131000	6.042000	0.979000	183.4123	183.3826	183.4032	183.3941	183.3893
39	H	3.707766	7.116014	-1.406162	27.5909	27.5975	27.5976	27.6027	27.6100
40	H	4.408120	4.631764	-0.040573	28.9265	28.8799	28.8814	28.8907	28.8832
41	H	6.044602	7.176032	0.027875	31.6072	31.6001	31.5902	31.5855	31.5807
42	H	6.262843	5.890532	1.163443	31.2278	31.1975	31.2009	31.1968	31.1929
43	H	7.209518	4.481512	-0.441002	31.0580	31.0412	31.0370	31.0331	31.0311
44	H	6.654052	5.483353	-1.762198	31.1581	31.1239	31.1254	31.1323	31.1323
45	H	10.049217	6.558805	1.165253	31.3022	31.2855	31.3021	31.2951	31.2927
46	H	8.401659	6.338200	1.703726	31.1148	31.0803	31.1089	31.1000	31.0968
47	H	9.295053	4.986952	1.048713	31.3214	31.2919	31.3177	31.3141	31.3106
48	N	3.454000	5.513000	2.172000	153.1002	151.4942	151.4404	152.0031	152.2855
49	C	2.825000	5.950000	3.426000	144.3788	144.2564	144.2736	144.3097	144.2805
50	C	3.607000	5.308000	4.598000	11.9004	11.6648	11.6151	11.7343	11.7988
51	O	3.838000	4.100000	4.611000	7.9772	8.3921	8.6278	7.9545	7.8324
52	C	1.347000	5.515000	3.444000	158.2669	158.3345	158.3171	158.2066	158.2854
53	C	0.511000	5.815000	4.692000	171.3112	171.4252	171.2254	171.2453	171.2795

54	C	-1.016000	5.827000	4.366000	174.6011	174.7170	174.6164	174.6020	174.6158
55	C	0.846000	4.835000	5.849000	175.8415	176.4501	176.0955	176.0454	176.0035
56	H	3.693112	4.555809	2.090076	28.1551	28.0558	28.0628	28.0967	28.1127
57	H	2.852991	7.015768	3.516863	28.9339	28.9282	28.9321	28.9300	28.9208
58	H	0.862957	5.980966	2.611247	31.4624	31.4452	31.4572	31.4497	31.4489
59	H	1.319526	4.457492	3.283309	31.7142	31.7089	31.7184	31.7124	31.7150
60	H	0.770639	6.797819	5.025997	31.8930	32.0022	31.8670	31.8814	31.8820
61	H	-1.569270	6.038926	5.257000	32.1352	32.2003	32.1225	32.1267	32.1252
62	H	-1.218311	6.579785	3.633002	32.1101	32.1577	32.1028	32.1041	32.1021
63	H	-1.306807	4.870512	3.984604	32.3051	32.3726	32.3035	32.3035	32.3001
64	H	0.245885	5.072344	6.702481	32.3177	32.4937	32.3182	32.3222	32.3154
65	H	0.641852	3.831992	5.537232	32.6625	32.7824	32.6766	32.6734	32.6639
66	H	1.881100	4.925380	6.104536	32.1514	32.3519	32.1197	32.1396	32.1575
67	N	4.022000	6.101000	5.571000	160.4256	160.2202	160.1820	160.0241	159.6811
68	C	4.675000	5.573000	6.753000	156.2864	156.4770	156.2052	156.1793	156.1660
69	C	4.081000	6.166000	8.007000	9.9603	9.7222	9.7474	9.7763	9.7492
70	O	3.779000	7.376000	8.065000	-2.5484	4.1812	0.3374	-0.3068	-1.0213
71	H	3.883701	7.077998	5.490703	27.6222	27.6440	27.6142	27.6059	27.5980
72	H	4.554829	4.510013	6.775755	28.5956	28.6304	28.5785	28.5808	28.5729

73	H	5.718093	5.808061	6.712945	29.6197	29.6625	29.6261	29.6232	29.6230
74	N	3.964000	5.325000	9.035000	148.5006	149.2424	149.0042	148.7905	148.4715
75	C	3.223000	5.678000	10.254000	145.6802	145.7719	145.6936	145.7084	145.6993
76	C	3.813000	5.010000	11.466000	17.8668	17.8316	17.8141	17.8511	17.8482
77	O	4.393000	3.934000	11.382000	53.7168	53.7274	53.8372	53.7013	53.6885
78	C	1.758000	5.265000	10.132000	137.5921	137.2907	137.6019	137.6105	137.6007
79	O	1.644000	3.867000	9.884000	344.0716	343.5740	343.8032	344.0015	344.0337
80	O	3.684000	5.548000	12.570000	46.7393	46.8735	46.6999	46.6491	46.6509
81	H	4.390302	4.433494	8.975134	27.6283	27.6855	27.6527	27.6339	27.6116
82	H	3.293047	6.739454	10.369362	28.9141	28.9369	28.9127	28.9122	28.9092
83	H	1.248378	5.503469	11.042120	29.6056	29.6026	29.6097	29.6047	29.6040
84	H	1.306851	5.803344	9.324813	29.6830	29.7219	29.6773	29.6838	29.6836
85	H	2.431933	3.493509	10.261048	31.9812	31.9944	32.0050	31.9791	31.9753

Table 14: Cartesian coordinates and isotropic shielding constants (in ppm) for 3NVG

Atom No	Proton	Coordinates			Chemical shifts				
					Full	Bonded	No field	Iterated charge	Iterated dipole
1	N	-13.617000	-1.968000	0.011000	230.3051	230.3573	230.3655	230.2841	230.2732
2	C	-12.315000	-2.459000	0.552000	144.7777	144.7885	144.8314	144.7470	144.7318
3	C	-12.059000	-1.849000	1.902000	14.2323	14.3195	14.2548	14.1883	14.2057
4	O	-12.171000	-0.636000	2.069000	-14.1303	-13.4955	-13.7699	-13.9833	-14.2932
5	C	-11.146000	-2.105000	-0.377000	168.5333	168.4477	168.5204	168.4979	168.5054
6	C	-9.830000	-2.625000	0.151000	170.8281	170.6065	170.9580	170.9104	170.8900
7	S	-8.355000	-2.030000	-0.725000	622.1891	623.8157	622.3558	621.6629	621.5252
8	C	-8.673000	-2.736000	-2.319000	185.0801	185.0445	185.0538	185.0286	185.0317
9	H	-13.779092	-2.373404	-0.877523	28.8929	28.9373	28.9168	28.8947	28.8932
10	H	-14.347923	-2.222694	0.628238	28.7000	28.7368	28.6633	28.7075	28.7087
11	H	-13.587351	-0.982316	-0.076456	28.5270	28.5578	28.5420	28.5309	28.5304
12	H	-12.381177	-3.524173	0.628982	29.4780	29.5509	29.5098	29.4932	29.4887
13	H	-11.326740	-2.531069	-1.341727	30.9129	30.9478	30.8978	30.8963	30.8939
14	H	-11.086849	-1.040870	-0.472015	31.4374	31.4616	31.4349	31.4271	31.4277
15	H	-9.746048	-2.342953	1.179738	31.3878	31.4288	31.4216	31.4101	31.3992

16	H	-9.844883	-3.693482	0.096009	30.9001	30.9557	30.8976	30.8918	30.8892
17	H	-7.878251	-2.479184	-2.987819	31.2675	31.2175	31.2710	31.2574	31.2553
18	H	-8.735568	-3.800581	-2.231524	31.3389	31.3180	31.3374	31.3247	31.3233
19	H	-9.597189	-2.354516	-2.700111	31.1426	31.1115	31.1440	31.1266	31.1275
20	N	-11.728000	-2.702000	2.865000	142.1807	142.5313	142.5066	142.3275	142.2886
21	C	-11.159000	-2.241000	4.126000	141.7261	141.4506	141.3591	141.6201	141.6208
22	C	-9.762000	-2.813000	4.206000	14.6002	14.2021	14.3874	14.4412	14.5423
23	O	-9.594000	-4.018000	4.139000	17.7861	16.8170	17.8917	17.2908	17.0946
24	C	-11.992000	-2.696000	5.318000	161.8862	162.0687	161.8585	161.9536	161.9769
25	C	-13.366000	-2.028000	5.283000	172.9460	172.7366	172.6828	172.8681	172.7878
26	C	-11.198000	-2.434000	6.631000	181.0942	182.5508	181.4057	181.3448	181.3368
27	C	-14.404000	-2.700000	6.223000	184.2478	184.3469	184.2528	184.2049	184.1903
28	H	-11.870659	-3.671406	2.723578	27.6038	27.6723	27.6449	27.6193	27.6091
29	H	-11.145271	-1.171561	4.157816	29.0291	29.1002	29.0194	29.0326	29.0435
30	H	-12.175659	-3.749175	5.273373	31.7223	31.8394	31.7341	31.7234	31.7179
31	H	-13.255993	-1.003440	5.571228	32.1589	32.2755	32.1302	32.1494	32.1479
32	H	-13.738502	-2.063531	4.280563	31.6200	31.7177	31.6455	31.6250	31.6326
33	H	-11.780797	-2.752678	7.469863	31.6540	31.9138	31.6877	31.6742	31.6678
34	H	-10.278640	-2.980903	6.607017	31.9904	32.3936	31.9801	31.9987	32.0056

35	H	-10.988775	-1.388323	6.718662	32.2686	32.7443	32.2823	32.2827	32.2861
36	H	-15.338634	-2.184376	6.148900	31.9680	32.0409	31.9692	31.9668	31.9670
37	H	-14.536682	-3.721998	5.935224	32.3829	32.4510	32.3829	32.3859	32.3854
38	H	-14.051733	-2.656547	7.232416	31.9665	32.0755	31.9764	31.9663	31.9670
39	N	-8.768000	-1.929000	4.308000	146.0394	145.4709	144.9742	144.9777	144.8441
40	C	-7.384000	-2.326000	4.238000	147.9137	148.3699	148.1529	148.1757	148.1370
41	C	-6.660000	-1.746000	5.429000	15.8346	16.1904	16.1126	16.0047	15.9932
42	O	-6.635000	-0.540000	5.590000	16.3658	16.1827	14.3769	12.7019	12.0446
43	C	-6.737000	-1.786000	2.965000	166.9019	167.4126	167.2227	167.1840	167.1958
44	C	-5.252000	-1.929000	2.975000	53.6469	53.8559	54.4558	54.5808	54.7052
45	N	-4.397000	-0.861000	3.112000	-33.7432	-35.8613	-33.4967	-33.7071	-33.9260
46	C	-4.475000	-3.030000	2.985000	77.7115	77.0240	77.6946	77.5566	77.4219
47	C	-3.148000	-1.294000	3.130000	53.5619	53.3338	53.2628	53.2817	53.3217
48	N	-3.169000	-2.611000	3.059000	97.1371	107.8263	97.1098	97.0522	96.9103
49	H	-8.987381	-0.972074	4.435535	27.6652	27.6439	27.6486	27.6555	27.6743
50	H	-7.324196	-3.394321	4.234158	28.4868	28.5444	28.5397	28.5244	28.5226
51	H	-7.130133	-2.318688	2.124411	30.0190	30.1363	30.0381	30.0329	30.0307
52	H	-6.984037	-0.749801	2.864178	30.3641	30.3218	30.3874	30.3824	30.3841
53	H	-4.813278	-4.044251	2.943009	25.8894	25.7934	25.9352	25.9117	25.8910

54	H	-2.272201	-0.682367	3.191483	25.0888	24.8051	25.1324	25.1251	25.1416
55	H	-2.373830	-3.200750	3.059042	22.9792	24.8807	22.9872	22.9704	22.9376
56	N	-6.075000	-2.619000	6.240000	144.5346	144.4206	144.4103	144.2776	143.9174
57	C	-5.226000	-2.214000	7.359000	146.2235	145.8579	145.8070	145.9515	145.9344
58	C	-3.870000	-2.851000	7.171000	17.4390	17.1829	17.2326	17.2792	17.2595
59	O	-3.775000	-4.060000	7.186000	21.1461	20.2212	19.8848	19.8570	19.9512
60	C	-5.812000	-2.697000	8.686000	161.3938	161.4686	161.5697	161.3752	161.3159
61	C	-6.853000	-1.798000	9.248000	50.0821	49.8247	49.8058	49.9337	49.9335
62	C	-6.588000	-1.011000	10.365000	64.2087	64.2647	64.2299	64.2195	64.2070
63	C	-8.094000	-1.704000	8.644000	61.8355	61.7748	61.7313	61.9119	61.9772
64	C	-7.541000	-0.174000	10.882000	63.7554	63.7919	63.7723	63.7041	63.6802
65	C	-9.065000	-0.858000	9.168000	61.3026	61.4669	61.2608	61.2807	61.2812
66	C	-8.784000	-0.094000	10.286000	65.3497	65.2568	65.3483	65.3463	65.3441
67	H	-6.219798	-3.585240	6.080270	27.9377	27.8407	27.8540	27.8414	27.8255
68	H	-5.156589	-1.146506	7.382197	29.3697	29.3778	29.3745	29.3644	29.3523
69	H	-6.242831	-3.664850	8.535833	30.2182	30.2296	30.2140	30.1908	30.1795
70	H	-5.017505	-2.784546	9.397347	30.7804	30.7839	30.7798	30.7669	30.7617
71	H	-5.624284	-1.060651	10.827263	25.4689	25.4467	25.4446	25.4450	25.4441
72	H	-8.307318	-2.284272	7.770684	25.2263	25.2005	25.1807	25.1854	25.1781

73	H	-7.322536	0.417167	11.746694	25.2271	25.2151	25.2142	25.2112	25.2103
74	H	-10.028624	-0.798110	8.706761	25.2131	25.2020	25.1877	25.1992	25.2041
75	H	-9.529668	0.558991	10.689090	25.3215	25.3209	25.3089	25.3089	25.3094
76	N	-2.823000	-2.047000	7.017000	166.4662	165.9806	165.7888	165.8963	165.7035
77	C	-1.473000	-2.574000	6.924000	156.8417	156.7832	156.7308	156.7373	156.6340
78	C	-0.761000	-1.935000	5.765000	18.0452	19.2114	17.8793	17.8145	17.5172
79	O	-0.738000	-0.721000	5.670000	14.9613	24.7068	19.5038	19.5716	17.2711
80	H	-2.966349	-1.068835	6.964615	28.4721	28.4735	28.4127	28.4115	28.3985
81	H	-0.943878	-2.359813	7.829016	29.9991	29.9102	30.0060	30.0028	29.9802
82	H	-1.513395	-3.633103	6.777136	29.0766	28.9450	29.0722	29.0681	29.0479
83	N	-0.195000	-2.765000	4.894000	144.2408	142.8391	143.5436	143.1739	143.8651
84	C	0.520000	-2.292000	3.702000	149.7123	149.8159	149.3626	149.5018	149.7236
85	C	-0.002000	-2.991000	2.467000	16.3771	19.0892	15.8154	15.9934	16.0963
86	O	0.322000	-2.567000	1.363000	42.9741	68.3323	45.8049	44.8919	44.3922
87	C	2.009000	-2.594000	3.809000	158.4166	158.3219	158.5876	158.6656	158.9855
88	C	2.617000	-2.053000	5.053000	11.1716	10.6944	10.8086	10.7214	10.8280
89	O	2.993000	-2.813000	5.962000	-21.4771	-19.0020	-19.8194	-20.4307	-21.5910
90	N	2.707000	-0.752000	5.135000	169.3742	169.8095	169.5066	169.5619	169.4802
91	O	-0.712000	-3.989000	2.558000	69.1506	59.2654	69.7671	69.5048	69.4106

92	H	-0.258117	-3.739704	5.055458	27.8562	27.9933	27.7113	27.7140	27.7547
93	H	0.363695	-1.235809	3.631793	28.4257	28.7764	28.3868	28.3981	28.4279
94	H	2.148062	-3.654757	3.790127	31.0645	31.2265	31.0713	31.0729	31.0910
95	H	2.509358	-2.165444	2.965862	30.5754	30.6907	30.5976	30.5927	30.5952
96	H	2.394420	-0.185963	4.385336	28.0540	28.1197	28.0362	28.0448	28.0449
97	H	3.087767	-0.332344	5.946791	28.2268	28.2932	28.2333	28.2322	28.2118