

SUPPORTING INFORMATION FOR

Multi-technique Experimental and Computational Approach to Study of Hydration/Dehydration  
Processes in the Crystals of Endomorphin Opioid Peptide Derivative.

by

Marta K. Dudek, Tomasz Pawlak, Piotr Paluch, Agata Jeziorna and Marek J. Potrzebowski

Polish Academy of Sciences, Centre of Molecular and Macromolecular Studies, Sienkiewicza 112, 90-  
363 Lodz, Poland.

**Table 1S.** Experimental NMR chemical shift tensors [in ppm] for structure **1**.

Atom	$\delta_{\text{iso}}$	$\delta_{11}^*$	$\delta_{22}^*$	$\delta_{33}^*$	$\delta_{\text{CSA}}$	$\eta_{\text{CSA}}$
<b>Tyr (N1)</b>	39.6/43.3					
<b>Pro (N2)</b>	139.3					
<b>Phe (N3)</b>	115.1					
<b>Phe (N4)</b>	117.6/124.0					
<b>C-16</b>	155.7	240.5	165.6	61.5	-107.1±8.7	0.67±0.05
<b>C-10</b>	165.8	236.6	171.8	89.9	-77.9±5.6	0.80±0.06
<b>C-20</b>	165.8	236.6	171.8	89.9	-77.9±5.6	0.80±0.06
<b>C-30</b>	170.7	242.3	180.5	90.0	-83.9±4.3	0.67±0.03
<b>C-40</b>	176.2	233.9	186.4	108.4	-68.7±5.4	0.81±0.06
<b>C-40'</b>	178.2	233.8	199.1	102.7	-81.1±6.7	0.60±0.05

$\delta_{\text{iso}} = (\delta_{11} + \delta_{22} + \delta_{33})/3$ ;  $\delta_{11} > \delta_{22} > \delta_{33}$ ; anisotropy  $\delta_{\text{CSA}} = \delta_{33} - \delta_{\text{iso}}$ ;  $\eta_{\text{CSA}} = (\delta_{22} - \delta_{11})/\delta_{\text{CSA}}$

**Table 2S.** Experimental NMR chemical shift tensors [in ppm] for structure **2** (EM2OH after  $\text{P}_2\text{O}_5$ ).

Atom	$\delta_{\text{iso}}$	$\delta_{11}$	$\delta_{22}$	$\delta_{33}$	$\delta_{\text{CSA}}$	$\eta_{\text{CSA}}$
<b>Tyr (N1)</b>	38.4					
<b>Pro (N2)</b>	133.7					
<b>Phe (N3)</b>	109.1/112.4					
<b>Phe (N4)</b>	122.9/123.9					
<b>C-16</b>	155.8	236.1	166.3	66.4	-85.7±6.4	0.90±0.07
<b>C-10</b>	167.9	235.8	179.4	89.4	-84.2±2.9	0.76±0.03
<b>C-20</b>	170.2	245.0	173.2	94.4	-81.5±5.4	0.84±0.06
<b>C-30</b>	171.4	237.8	181.6	96.1	-77.8±3.6	0.87±0.04
<b>C-40</b>	175.4	235.2	184.4	108.2	-71.1±3.8	0.93±0.05

$\delta_{\text{iso}} = (\delta_{11} + \delta_{22} + \delta_{33})/3$ ;  $\delta_{11} > \delta_{22} > \delta_{33}$ ; anisotropy  $\delta_{\text{CSA}} = \delta_{33} - \delta_{\text{iso}}$ ;  $\eta_{\text{CSA}} = (\delta_{22} - \delta_{11})/\delta_{\text{CSA}}$

**Table 3S.** CASTEP calculations.  $^{15}\text{N}$  NMR shielding constants and  $^{13}\text{C}$  NMR nuclear shielding tensors [in ppm] for chosen atoms of structure **1** (molecule ‘A’ and ‘B’) calculated using PBE0 functional with OTGF ultrasoft pseudopotential and GIPAW approach. Geometry was optimized (all atomic positions) with PBE0 functional and OTGF ultrasoft pseudopotential (571.4 eV cut-off energy).

Atom	$\delta_{\text{iso}}$	$\delta_{11}$	$\delta_{22}$	$\delta_{33}$
<b>Tyr (N1)</b>	183.1			
<b>Pro (N2)</b>	73.0			
<b>Phe (N3)</b>	99.8			
<b>Phe (N4)</b>	98.1			
<b>Tyr (N1)'</b>	183.9			
<b>Pro (N2)'</b>	72.8			
<b>Phe (N3)'</b>	99.9			
<b>Phe (N4)'</b>	92.2			
<b>C-16</b>	9.5	-73.9	-5.8	108.2
<b>C-16'</b>	9.8	-73.0	-4.8	107.2
<b>C-10</b>	3.2	-66.5	-3.7	79.9
<b>C-10'</b>	3.0	-64.8	-6.6	80.5
<b>C-20</b>	3.4	-77.3	9.4	78.1
<b>C-20'</b>	3.2	-76.7	6.4	80.0
<b>C-30</b>	-3.4	-73.2	-18.7	81.7
<b>C-30'</b>	-1.5	-73.9	-10.9	80.4
<b>C-40</b>	-13.1	-70.2	-34.2	65.2
<b>C-40'</b>	-11.0	-70.6	-23.7	61.2

**Table 4S.** CASTEP calculations.  $^{15}\text{N}$  NMR shielding constants and  $^{13}\text{C}$  NMR nuclear shielding tensors [in ppm] for chosen atoms of the most probable structures (No. 3 and 10) of **2** (molecule ‘A’ and ‘B’) calculated using PBE0 functional with OTGF ultrasoft pseudopotential and GIPAW approach. Geometry was optimized (all atomic positions) with PBE0 functional and OTGF ultrasoft pseudopotential (571.4 eV cut-off energy).

Atom	$\delta_{\text{iso}}$	$\delta_{11}$	$\delta_{22}$	$\delta_{33}$	Atom	$\delta_{\text{iso}}$	$\delta_{11}$	$\delta_{22}$	$\delta_{33}$
<b>structure 3</b>					<b>structure 10</b>				
<b>Tyr (N1)</b>	184.8				<b>Tyr (N1)</b>	181.8			
<b>Pro (N2)</b>	80.9				<b>Pro (N2)</b>	81.1			
<b>Phe (N3)</b>	100.4				<b>Phe (N3)</b>	103.2			
<b>Phe (N4)</b>	98.3				<b>Phe (N4)</b>	94.0			
<b>Tyr (N1)'</b>	187.8				<b>Tyr (N1)'</b>	181.2			
<b>Pro (N2)'</b>	80.0				<b>Pro (N2)'</b>	79.2			
<b>Phe (N3)'</b>	103.2				<b>Phe (N3)'</b>	103.4			
<b>Phe (N4)'</b>	92.4				<b>Phe (N4)'</b>	93.4			
<b>C-16</b>	9.8	-71.7	-8.7	109.8	<b>C-16</b>	9.7	-73.7	-5.6	108.4
<b>C-16'</b>	10.7	-73.0	-2.9	107.9	<b>C-16'</b>	8.7	-73.7	-10.0	109.7
<b>C-10</b>	4.3	-73.3	5.5	80.8	<b>C-10</b>	5.8	-75.8	15.2	78.0
<b>C-10'</b>	4.2	-78.0	12.4	78.2	<b>C-10'</b>	5.2	-73.3	9.5	79.3
<b>C-20</b>	3.2	-76.6	8.8	77.5	<b>C-20</b>	4.1	-77.6	10.7	79.3
<b>C-20'</b>	2.8	-78.2	4.8	81.7	<b>C-20'</b>	3.1	-76.8	5.5	80.7
<b>C-30</b>	-2.6	-71.5	-17.7	81.6	<b>C-30</b>	-1.8	-71.8	-14.6	81.0
<b>C-30'</b>	0.9	-71.9	-6.3	81.0	<b>C-30'</b>	-0.1	-73.4	-7.3	80.5
<b>C-40</b>	-10.5	-72.9	-21.5	62.9	<b>C-40</b>	-10.8	-74.1	-20.3	61.9
<b>C-40'</b>	-8.1	-74.8	-10.2	60.7	<b>C-40'</b>	-12.6	-76.0	-23.3	61.6

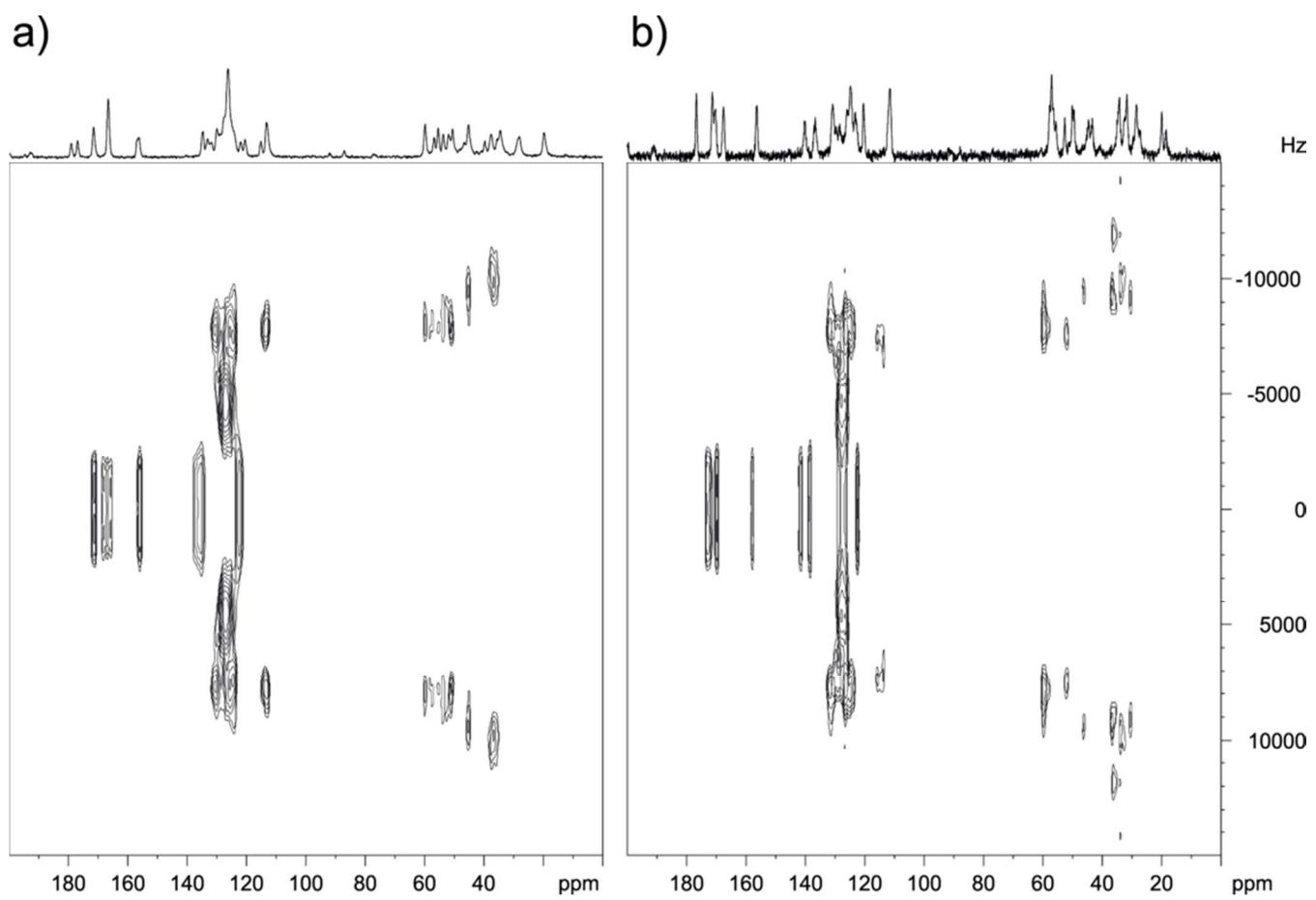


Figure 1S. CP-VC spectra of **1** (a) and **2** (b)

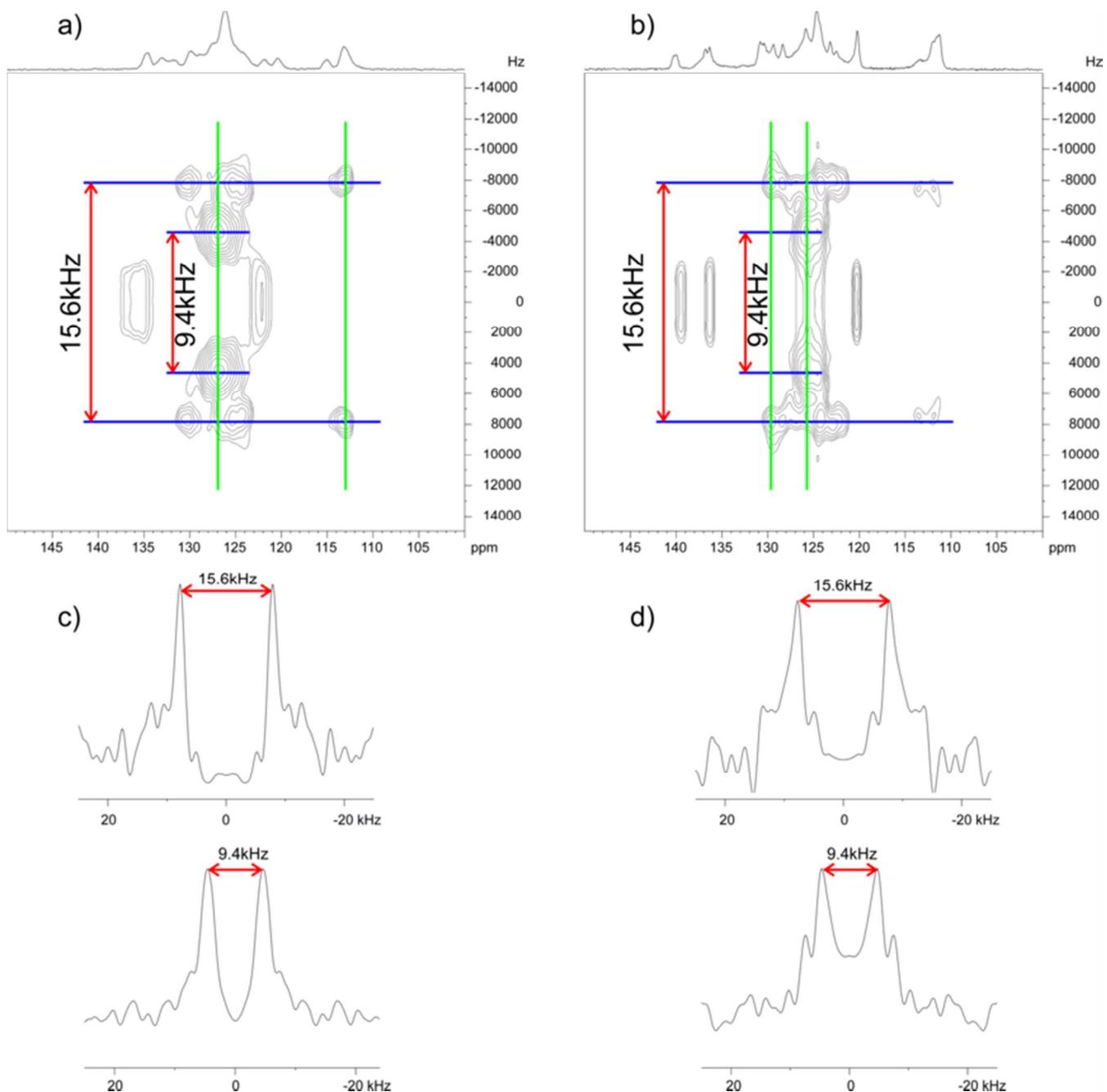


Figure 2S. CPVC VF MAS 2D NMR aromatic part of spectra of EM2-OH **1** (a) and **2** (b) together with the extracted 1D slices (c and d, respectively). Errors of the determined splitting values can be roughly estimated to 1kHz using FID resolution.

## GIPAW coordinates and calculated NMR parameters for structure 1

xx

x	Element	Atom	Fractional coordinates of atoms				x
x		Number	u	v	w	x	x-----x
x H		1	0.898667	0.589547	0.170929	x	
x H		2	0.914902	0.568524	0.232807	x	
x H		3	0.974331	-0.032530	0.172702	x	
x H		4	0.910730	0.097198	0.193341	x	
x H		5	0.975638	0.227459	0.174061	x	
x H		6	0.865699	0.234926	0.107561	x	
x H		7	0.977358	0.297008	0.082397	x	
x H		8	0.996569	0.029627	0.084774	x	
x H		9	0.940110	-0.205322	0.015492	x	
x H		10	0.888687	-0.247672	-0.080310	x	
x H		11	0.853045	0.404453	-0.093432	x	
x H		12	0.903400	0.445442	0.002118	x	
x H		13	0.823271	0.171049	-0.164180	x	
x H		14	0.795113	0.194872	0.034238	x	
x H		15	0.675495	0.066121	-0.025880	x	
x H		16	0.756176	-0.032380	-0.037093	x	
x H		17	0.693502	-0.351793	-0.023629	x	
x H		18	0.659338	-0.237825	0.028001	x	
x H		19	0.757909	-0.391806	0.082174	x	
x H		20	0.806837	-0.389386	0.031095	x	
x H		21	0.732253	-0.052315	0.133581	x	
x H		22	0.629619	0.286614	0.130885	x	
x H		23	0.641608	-0.117509	0.193479	x	
x H		24	0.580448	0.080759	0.195043	x	
x H		25	0.625782	-0.368618	0.124998	x	
x H		26	0.548244	-0.533524	0.049388	x	
x H		27	0.439854	-0.354400	0.004762	x	
x H		28	0.411293	-0.011538	0.036002	x	
x H		29	0.490037	0.155946	0.111805	x	
x H		30	0.760489	0.001299	0.219262	x	
x H		31	0.786701	0.381076	0.285247	x	
x H		32	0.783217	-0.058718	0.328131	x	
x H		33	0.803835	0.169869	0.365794	x	
x H		34	0.665476	-0.163062	0.297889	x	
x H		35	0.540257	-0.109578	0.296330	x	
x H		36	0.499339	0.224358	0.327602	x	
x H		37	0.584007	0.497886	0.361139	x	
x H		38	0.709602	0.444180	0.361921	x	
x H		39	0.042647	-0.226323	0.311777	x	
x H		40	0.079024	0.005092	0.307547	x	
x H		41	0.127580	-0.216486	0.304757	x	
x H		42	0.151581	-0.005546	0.387714	x	
x H		43	0.025210	0.051695	0.386285	x	
x H		44	0.015212	-0.214844	0.397689	x	
x H		45	0.049092	-0.361710	0.485022	x	
x H		46	0.077865	-0.302865	0.581639	x	

x H	47	0.124624	0.330639	0.555278	x
x H	48	0.094647	0.271484	0.458124	x
x H	49	0.109330	-0.074911	0.647591	x
x H	50	0.205369	-0.041045	0.468570	x
x H	51	0.323208	-0.155261	0.533803	x
x H	52	0.242980	-0.269695	0.540373	x
x H	53	0.314212	-0.573933	0.529156	x
x H	54	0.349665	-0.447027	0.479783	x
x H	55	0.256435	-0.618535	0.422038	x
x H	56	0.204107	-0.623353	0.470860	x
x H	57	0.261950	-0.206437	0.363623	x
x H	58	0.374546	0.104203	0.380502	x
x H	59	0.354461	-0.270403	0.306530	x
x H	60	0.420972	-0.081644	0.310251	x
x H	61	0.363267	-0.541332	0.371227	x
x H	62	0.436722	-0.733845	0.444687	x
x H	63	0.548724	-0.584219	0.491648	x
x H	64	0.584864	-0.240405	0.466509	x
x H	65	0.510632	-0.044505	0.394146	x
x H	66	0.329730	-0.024564	0.253038	x
x H	67	0.234730	0.330842	0.225292	x
x H	68	0.309579	0.060583	0.157136	x
x H	69	0.253289	0.270502	0.134817	x
x H	70	0.427131	0.128596	0.214518	x
x H	71	0.527106	0.368642	0.231581	x
x H	72	0.511718	0.732718	0.202515	x
x H	73	0.395875	0.857391	0.157761	x
x H	74	0.294273	0.619951	0.143756	x
x H	75	0.808675	-0.327616	0.194221	x
x H	76	0.730725	-0.355023	0.196786	x
x H	77	0.933576	-0.327157	0.323693	x
x H	78	0.933536	-0.162138	0.279224	x
x H	79	0.049338	0.353862	0.238202	x
x H	80	0.086303	0.326051	0.189802	x
x H	81	0.072701	0.360142	0.329273	x
x H	82	0.222253	-0.484644	0.302694	x
x H	83	0.215659	-0.288402	0.264350	x
x H	84	0.080158	-0.112363	0.191388	x
x H	85	0.045995	-0.331726	0.198307	x
x H	86	1.000888	0.761488	0.692695	x
x H	87	-0.898667	1.089547	-0.170929	x
x H	88	-0.914902	1.068524	-0.232807	x
x H	89	-0.974331	0.467470	-0.172702	x
x H	90	-0.910730	0.597198	-0.193341	x
x H	91	-0.975638	0.727459	-0.174061	x
x H	92	-0.865699	0.734926	-0.107561	x
x H	93	-0.977358	0.797008	-0.082397	x
x H	94	-0.996569	0.529627	-0.084774	x
x H	95	-0.940110	0.294678	-0.015492	x
x H	96	-0.888687	0.252328	0.080310	x
x H	97	-0.853045	0.904453	0.093432	x
x H	98	-0.903400	0.945442	-0.002118	x
x H	99	-0.823271	0.671049	0.164180	x

x H	100	-0.795113	0.694872	-0.034238	x
x H	101	-0.675495	0.566121	0.025880	x
x H	102	-0.756176	0.467620	0.037093	x
x H	103	-0.693502	0.148207	0.023629	x
x H	104	-0.659338	0.262175	-0.028001	x
x H	105	-0.757909	0.108194	-0.082174	x
x H	106	-0.806837	0.110614	-0.031095	x
x H	107	-0.732253	0.447685	-0.133581	x
x H	108	-0.629619	0.786614	-0.130885	x
x H	109	-0.641608	0.382491	-0.193479	x
x H	110	-0.580448	0.580759	-0.195043	x
x H	111	-0.625782	0.131382	-0.124998	x
x H	112	-0.548244	-0.033524	-0.049388	x
x H	113	-0.439854	0.145600	-0.004762	x
x H	114	-0.411293	0.488462	-0.036002	x
x H	115	-0.490037	0.655946	-0.111805	x
x H	116	-0.760489	0.501299	-0.219262	x
x H	117	-0.786701	0.881076	-0.285247	x
x H	118	-0.783217	0.441282	-0.328131	x
x H	119	-0.803835	0.669869	-0.365794	x
x H	120	-0.665476	0.336938	-0.297889	x
x H	121	-0.540257	0.390422	-0.296330	x
x H	122	-0.499339	0.724358	-0.327602	x
x H	123	-0.584007	0.997886	-0.361139	x
x H	124	-0.709602	0.944180	-0.361921	x
x H	125	-0.042647	0.273677	-0.311777	x
x H	126	-0.079024	0.505092	-0.307547	x
x H	127	-0.127580	0.283514	-0.304757	x
x H	128	-0.151581	0.494454	-0.387714	x
x H	129	-0.025210	0.551695	-0.386285	x
x H	130	-0.015212	0.285156	-0.397689	x
x H	131	-0.049092	0.138290	-0.485022	x
x H	132	-0.077865	0.197135	-0.581639	x
x H	133	-0.124624	0.830639	-0.555278	x
x H	134	-0.094647	0.771484	-0.458124	x
x H	135	-0.109330	0.425089	-0.647591	x
x H	136	-0.205369	0.458955	-0.468570	x
x H	137	-0.323208	0.344739	-0.533803	x
x H	138	-0.242980	0.230305	-0.540373	x
x H	139	-0.314212	-0.073933	-0.529156	x
x H	140	-0.349665	0.052973	-0.479783	x
x H	141	-0.256435	-0.118535	-0.422038	x
x H	142	-0.204107	-0.123353	-0.470860	x
x H	143	-0.261950	0.293563	-0.363623	x
x H	144	-0.374546	0.604203	-0.380502	x
x H	145	-0.354461	0.229597	-0.306530	x
x H	146	-0.420972	0.418356	-0.310251	x
x H	147	-0.363267	-0.041332	-0.371227	x
x H	148	-0.436722	-0.233845	-0.444687	x
x H	149	-0.548724	-0.084219	-0.491648	x
x H	150	-0.584864	0.259595	-0.466509	x
x H	151	-0.510632	0.455495	-0.394146	x
x H	152	-0.329730	0.475436	-0.253038	x

x H	153	-0.234730	0.830842	-0.225292	x
x H	154	-0.309579	0.560583	-0.157136	x
x H	155	-0.253289	0.770502	-0.134817	x
x H	156	-0.427131	0.628596	-0.214518	x
x H	157	-0.527106	0.868642	-0.231581	x
x H	158	-0.511718	1.232718	-0.202515	x
x H	159	-0.395875	1.357391	-0.157761	x
x H	160	-0.294273	1.119951	-0.143756	x
x H	161	-0.808675	0.172384	-0.194221	x
x H	162	-0.730725	0.144977	-0.196786	x
x H	163	-0.933576	0.172843	-0.323693	x
x H	164	-0.933536	0.337862	-0.279224	x
x H	165	-0.049338	0.853862	-0.238202	x
x H	166	-0.086303	0.826051	-0.189802	x
x H	167	-0.072701	0.860142	-0.329273	x
x H	168	-0.222253	0.015356	-0.302694	x
x H	169	-0.215659	0.211598	-0.264350	x
x H	170	-0.080158	0.387637	-0.191388	x
x H	171	-0.045995	0.168274	-0.198307	x
x H	172	-1.000888	1.261488	-0.692695	x
x C	1	0.902523	0.106896	0.110291	x
x C	2	0.954695	0.143283	0.073639	x
x C	3	0.924154	0.122292	0.015785	x
x C	4	0.919780	-0.071955	-0.008225	x
x C	5	0.891306	-0.097033	-0.061498	x
x C	6	0.866512	0.074421	-0.092654	x
x C	7	0.870769	0.270313	-0.069171	x
x C	8	0.899360	0.292236	-0.015593	x
x C	9	0.866077	-0.100585	0.097701	x
x C	10	0.761093	0.070949	0.042653	x
x C	11	0.721238	-0.025308	-0.008797	x
x C	12	0.704528	-0.241224	0.008927	x
x C	13	0.769530	-0.302199	0.049090	x
x C	14	0.710251	0.167230	0.073995	x
x C	15	0.660135	0.163886	0.153556	x
x C	16	0.610706	0.001720	0.169453	x
x C	17	0.563293	-0.095344	0.123235	x
x C	18	0.578973	-0.289202	0.105186	x
x C	19	0.534795	-0.383183	0.062982	x
x C	20	0.474264	-0.283346	0.038223	x
x C	21	0.458318	-0.089364	0.055824	x
x C	22	0.502684	0.004529	0.097979	x
x C	23	0.701129	0.264413	0.203943	x
x C	24	0.793459	0.214317	0.281746	x
x C	25	0.771502	0.106510	0.329700	x
x C	26	0.695878	0.136841	0.330186	x
x C	27	0.647639	-0.017606	0.311628	x
x C	28	0.577110	0.013026	0.310558	x
x C	29	0.554253	0.198670	0.328202	x
x C	30	0.601955	0.353809	0.346891	x
x C	31	0.672237	0.322784	0.347614	x
x C	32	0.869970	0.164100	0.283816	x
x C	33	0.113884	-0.131757	0.380300	x

x C	34	0.051424	-0.084709	0.406079	x
x C	35	0.070817	-0.049833	0.464697	x
x C	36	0.066938	-0.210193	0.500104	x
x C	37	0.082932	-0.178230	0.554443	x
x C	38	0.103634	0.017437	0.574674	x
x C	39	0.108857	0.178519	0.539553	x
x C	40	0.092199	0.144361	0.485316	x
x C	41	0.147003	-0.337922	0.399576	x
x C	42	0.243223	-0.157211	0.461894	x
x C	43	0.280370	-0.252481	0.514190	x
x C	44	0.302977	-0.462526	0.496824	x
x C	45	0.241553	-0.531167	0.454352	x
x C	46	0.295536	-0.047758	0.434176	x
x C	47	0.341411	-0.001318	0.353298	x
x C	48	0.387521	-0.162388	0.333171	x
x C	49	0.432303	-0.280864	0.377250	x
x C	50	0.412227	-0.475620	0.391877	x
x C	51	0.453783	-0.584631	0.432874	x
x C	52	0.516179	-0.500456	0.459513	x
x C	53	0.536372	-0.305940	0.445386	x
x C	54	0.494475	-0.196501	0.404823	x
x C	55	0.297332	0.136264	0.310765	x
x C	56	0.255987	0.184427	0.214912	x
x C	57	0.292699	0.213630	0.167851	x
x C	58	0.353536	0.358705	0.178455	x
x C	59	0.419553	0.290036	0.203186	x
x C	60	0.476042	0.424129	0.212499	x
x C	61	0.467325	0.629336	0.196780	x
x C	62	0.401946	0.699249	0.171900	x
x C	63	0.345369	0.565372	0.163154	x
x C	64	0.197078	0.026743	0.198181	x
x C	65	-0.902523	0.606896	-0.110291	x
x C	66	-0.954695	0.643283	-0.073639	x
x C	67	-0.924154	0.622292	-0.015785	x
x C	68	-0.919780	0.428045	0.008225	x
x C	69	-0.891306	0.402967	0.061498	x
x C	70	-0.866512	0.574421	0.092654	x
x C	71	-0.870769	0.770313	0.069171	x
x C	72	-0.899360	0.792236	0.015593	x
x C	73	-0.866077	0.399415	-0.097701	x
x C	74	-0.761093	0.570949	-0.042653	x
x C	75	-0.721238	0.474692	0.008797	x
x C	76	-0.704528	0.258776	-0.008927	x
x C	77	-0.769530	0.197801	-0.049090	x
x C	78	-0.710251	0.667230	-0.073995	x
x C	79	-0.660135	0.663886	-0.153556	x
x C	80	-0.610706	0.501720	-0.169453	x
x C	81	-0.563293	0.404656	-0.123235	x
x C	82	-0.578973	0.210798	-0.105186	x
x C	83	-0.534795	0.116817	-0.062982	x
x C	84	-0.474264	0.216654	-0.038223	x
x C	85	-0.458318	0.410636	-0.055824	x
x C	86	-0.502684	0.504529	-0.097979	x

x C	87	-0.701129	0.764413	-0.203943	x
x C	88	-0.793459	0.714317	-0.281746	x
x C	89	-0.771502	0.606510	-0.329700	x
x C	90	-0.695878	0.636841	-0.330186	x
x C	91	-0.647639	0.482394	-0.311628	x
x C	92	-0.577110	0.513026	-0.310558	x
x C	93	-0.554253	0.698670	-0.328202	x
x C	94	-0.601955	0.853809	-0.346891	x
x C	95	-0.672237	0.822784	-0.347614	x
x C	96	-0.869970	0.664100	-0.283816	x
x C	97	-0.113884	0.368243	-0.380300	x
x C	98	-0.051424	0.415291	-0.406079	x
x C	99	-0.070817	0.450167	-0.464697	x
x C	100	-0.066938	0.289807	-0.500104	x
x C	101	-0.082932	0.321770	-0.554443	x
x C	102	-0.103634	0.517437	-0.574674	x
x C	103	-0.108857	0.678519	-0.539553	x
x C	104	-0.092199	0.644361	-0.485316	x
x C	105	-0.147003	0.162078	-0.399576	x
x C	106	-0.243223	0.342789	-0.461894	x
x C	107	-0.280370	0.247519	-0.514190	x
x C	108	-0.302977	0.037474	-0.496824	x
x C	109	-0.241553	-0.031167	-0.454352	x
x C	110	-0.295536	0.452242	-0.434176	x
x C	111	-0.341411	0.498682	-0.353298	x
x C	112	-0.387521	0.337612	-0.333171	x
x C	113	-0.432303	0.219136	-0.377250	x
x C	114	-0.412227	0.024380	-0.391877	x
x C	115	-0.453783	-0.084631	-0.432874	x
x C	116	-0.516179	-0.000456	-0.459513	x
x C	117	-0.536372	0.194060	-0.445386	x
x C	118	-0.494475	0.303499	-0.404823	x
x C	119	-0.297332	0.636264	-0.310765	x
x C	120	-0.255987	0.684427	-0.214912	x
x C	121	-0.292699	0.713630	-0.167851	x
x C	122	-0.353536	0.858705	-0.178455	x
x C	123	-0.419553	0.790036	-0.203186	x
x C	124	-0.476042	0.924129	-0.212499	x
x C	125	-0.467325	1.129336	-0.196780	x
x C	126	-0.401946	1.199249	-0.171900	x
x C	127	-0.345369	1.065372	-0.163154	x
x C	128	-0.197078	0.526743	-0.198181	x
x N	1	0.942254	0.099924	0.165341	x
x N	2	0.801803	-0.103729	0.068101	x
x N	3	0.705056	0.078857	0.120430	x
x N	4	0.751322	0.147479	0.232347	x
x N	5	0.089866	-0.144834	0.321902	x
x N	6	0.207820	-0.335931	0.433844	x
x N	7	0.295311	-0.098642	0.383482	x
x N	8	0.303942	0.104096	0.260585	x
x N	9	-0.942254	0.599924	-0.165341	x
x N	10	-0.801803	0.396271	-0.068101	x
x N	11	-0.705056	0.578857	-0.120430	x

x N	12	-0.751322	0.647479	-0.232347	x
x N	13	-0.089866	0.355166	-0.321902	x
x N	14	-0.207820	0.164069	-0.433844	x
x N	15	-0.295311	0.401358	-0.383482	x
x N	16	-0.303942	0.604096	-0.260585	x
x O	1	0.883889	0.518236	0.200570	x
x O	2	0.839891	0.040958	-0.144146	x
x O	3	0.898450	-0.261414	0.112996	x
x O	4	0.676726	0.319474	0.054990	x
x O	5	0.685702	0.440134	0.217133	x
x O	6	0.914475	0.251199	0.319633	x
x O	7	0.884931	0.030733	0.252499	x
x O	8	0.118366	0.055251	0.627475	x
x O	9	0.116987	-0.501697	0.383571	x
x O	10	0.334195	0.082948	0.459135	x
x O	11	0.258621	0.268922	0.324241	x
x O	12	0.137263	0.087972	0.178030	x
x O	13	0.215374	-0.161771	0.204351	x
x O	14	0.763558	-0.253061	0.187292	x
x O	15	0.956333	-0.292999	0.294253	x
x O	16	0.045972	0.392162	0.200448	x
x O	17	0.047898	0.265769	0.301815	x
x O	18	0.209271	-0.337287	0.299411	x
x O	19	0.042337	-0.182159	0.204741	x
x O	20	-0.883889	1.018236	-0.200570	x
x O	21	-0.839891	0.540958	0.144146	x
x O	22	-0.898450	0.238586	-0.112996	x
x O	23	-0.676726	0.819474	-0.054990	x
x O	24	-0.685702	0.940134	-0.217133	x
x O	25	-0.914475	0.751199	-0.319633	x
x O	26	-0.884931	0.530733	-0.252499	x
x O	27	-0.118366	0.555251	-0.627475	x
x O	28	-0.116987	-0.001697	-0.383571	x
x O	29	-0.334195	0.582948	-0.459135	x
x O	30	-0.258621	0.768922	-0.324241	x
x O	31	-0.137263	0.587972	-0.178030	x
x O	32	-0.215374	0.338229	-0.204351	x
x O	33	-0.763558	0.246939	-0.187292	x
x O	34	-0.956333	0.207001	-0.294253	x
x O	35	-0.045972	0.892162	-0.200448	x
x O	36	-0.047898	0.765769	-0.301815	x
x O	37	-0.209271	0.162713	-0.299411	x
x O	38	-0.042337	0.317841	-0.204741	x

xx

Chemical Shielding and Electric Field Gradient Tensors							
Nucleus	Species	Ion	Shielding tensor Iso(ppm)	Aniso(ppm)	EFG Tensor Asym	Cq(MHz)	Eta
H	1		25.70	24.68	0.02	2.396E-01	0.10

H	2	25.16	25.19	0.17	2.396E-01	0.11
H	3	19.39	26.14	0.13	1.377E-01	0.03
H	4	22.64	23.66	0.02	1.782E-01	0.06
H	5	20.41	26.24	0.06	1.510E-01	0.08
H	6	26.29	-4.95	0.68	1.761E-01	0.05
H	7	27.24	7.03	0.89	1.767E-01	0.03
H	8	27.51	-5.37	0.83	1.743E-01	0.04
H	9	23.86	5.36	0.41	1.878E-01	0.07
H	10	22.85	-3.83	0.78	1.901E-01	0.06
H	11	22.84	-5.12	0.90	1.892E-01	0.09
H	12	23.23	2.81	0.49	1.888E-01	0.06
H	13	17.40	28.46	0.17	1.712E-01	0.16
H	14	26.89	6.70	0.70	1.779E-01	0.05
H	15	29.49	9.55	0.32	1.815E-01	0.00
H	16	30.13	11.78	0.63	1.793E-01	0.02
H	17	29.35	7.86	0.33	1.865E-01	0.01
H	18	29.62	13.31	0.11	1.773E-01	0.01
H	19	26.95	8.74	0.57	1.794E-01	0.03
H	20	27.20	8.45	0.55	1.786E-01	0.06
H	21	20.98	12.69	0.98	2.036E-01	0.18
H	22	26.00	4.34	0.85	1.743E-01	0.02
H	23	27.80	3.78	0.45	1.792E-01	0.03
H	24	28.09	-6.98	0.98	1.788E-01	0.03
H	25	23.37	3.34	0.40	1.879E-01	0.07
H	26	23.93	4.54	0.61	1.891E-01	0.05
H	27	25.65	-4.83	0.19	1.900E-01	0.04
H	28	23.96	3.67	0.52	1.907E-01	0.05
H	29	24.82	-3.48	0.34	1.871E-01	0.07
H	30	19.40	15.45	0.63	1.827E-01	0.22
H	31	25.10	-4.71	0.36	1.746E-01	0.04
H	32	27.55	5.42	0.68	1.766E-01	0.03
H	33	26.78	7.90	0.73	1.796E-01	0.02
H	34	23.31	3.36	0.44	1.873E-01	0.07
H	35	23.45	3.43	0.51	1.895E-01	0.07
H	36	24.26	3.24	0.88	1.913E-01	0.06
H	37	25.21	7.94	0.25	1.880E-01	0.06
H	38	23.60	4.47	0.58	1.891E-01	0.07
H	39	19.70	24.94	0.07	1.455E-01	0.04
H	40	20.79	24.94	0.25	1.600E-01	0.03
H	41	21.53	22.30	0.30	1.686E-01	0.02
H	42	26.37	4.83	0.55	1.735E-01	0.06
H	43	26.65	7.18	0.91	1.763E-01	0.04
H	44	27.53	-6.62	0.69	1.777E-01	0.03
H	45	25.05	5.94	0.54	1.876E-01	0.07
H	46	23.17	4.87	0.77	1.895E-01	0.07
H	47	23.82	-2.14	0.94	1.917E-01	0.07
H	48	22.92	-3.37	0.20	1.825E-01	0.07
H	49	15.82	28.20	0.17	1.393E-01	0.18
H	50	27.26	10.79	0.41	1.745E-01	0.05
H	51	29.43	8.82	0.49	1.826E-01	0.01
H	52	30.47	10.21	0.91	1.812E-01	0.02
H	53	30.01	7.24	0.66	1.858E-01	0.01
H	54	30.20	13.37	0.19	1.773E-01	0.01

H	55	26.83	10.16	0.43	1.752E-01	0.05
H	56	27.32	9.93	0.57	1.788E-01	0.06
H	57	21.47	12.47	0.95	2.117E-01	0.17
H	58	25.55	5.18	0.69	1.721E-01	0.01
H	59	28.50	5.90	0.34	1.758E-01	0.04
H	60	27.53	5.88	0.89	1.785E-01	0.03
H	61	23.85	4.39	0.53	1.851E-01	0.07
H	62	22.93	3.84	0.53	1.853E-01	0.06
H	63	25.36	-5.41	0.35	1.903E-01	0.04
H	64	23.61	3.64	0.93	1.903E-01	0.04
H	65	23.87	-3.94	0.65	1.881E-01	0.07
H	66	23.72	-6.44	0.18	2.417E-01	0.18
H	67	25.68	-4.90	0.78	1.816E-01	0.04
H	68	27.32	-5.61	0.93	1.780E-01	0.02
H	69	26.71	7.05	0.66	1.794E-01	0.04
H	70	23.45	5.19	0.54	1.902E-01	0.07
H	71	24.31	4.95	0.41	1.887E-01	0.06
H	72	24.33	4.98	0.52	1.926E-01	0.06
H	73	23.75	5.10	0.54	1.916E-01	0.06
H	74	23.19	3.66	0.81	1.896E-01	0.07
H	75	23.27	30.00	0.20	2.132E-01	0.13
H	76	25.06	27.71	0.23	2.309E-01	0.13
H	77	25.92	22.74	0.16	2.560E-01	0.09
H	78	22.15	30.87	0.06	1.946E-01	0.12
H	79	22.79	28.78	0.12	2.096E-01	0.11
H	80	23.91	20.89	0.25	2.379E-01	0.11
H	81	22.96	26.39	0.18	2.265E-01	0.10
H	82	23.95	26.52	0.24	2.266E-01	0.12
H	83	24.28	27.79	0.11	2.247E-01	0.13
H	84	23.78	26.02	0.19	2.295E-01	0.11
H	85	23.12	29.84	0.12	2.234E-01	0.12
H	86	22.28	25.44	0.10	2.075E-01	0.12
H	87	25.70	24.68	0.02	2.396E-01	0.10
H	88	25.16	25.19	0.17	2.396E-01	0.11
H	89	19.39	26.14	0.13	1.377E-01	0.03
H	90	22.64	23.66	0.02	1.782E-01	0.06
H	91	20.41	26.24	0.06	1.510E-01	0.08
H	92	26.29	-4.95	0.68	1.761E-01	0.05
H	93	27.24	7.03	0.89	1.767E-01	0.03
H	94	27.51	-5.37	0.83	1.743E-01	0.04
H	95	23.86	5.36	0.41	1.878E-01	0.07
H	96	22.85	-3.83	0.78	1.901E-01	0.06
H	97	22.84	-5.12	0.90	1.892E-01	0.09
H	98	23.23	2.81	0.49	1.888E-01	0.06
H	99	17.40	28.46	0.17	1.712E-01	0.16
H	100	26.89	6.70	0.70	1.779E-01	0.05
H	101	29.49	9.55	0.32	1.815E-01	0.00
H	102	30.13	11.78	0.63	1.793E-01	0.02
H	103	29.35	7.86	0.33	1.865E-01	0.01
H	104	29.62	13.31	0.11	1.773E-01	0.01
H	105	26.95	8.74	0.57	1.794E-01	0.03
H	106	27.20	8.45	0.55	1.786E-01	0.06
H	107	20.98	12.69	0.98	2.036E-01	0.18

H	108	26.00	4.34	0.85	1.743E-01	0.02
H	109	27.80	3.78	0.45	1.792E-01	0.03
H	110	28.09	-6.98	0.98	1.788E-01	0.03
H	111	23.37	3.34	0.40	1.879E-01	0.07
H	112	23.93	4.54	0.61	1.891E-01	0.05
H	113	25.65	-4.83	0.19	1.900E-01	0.04
H	114	23.96	3.67	0.52	1.907E-01	0.05
H	115	24.82	-3.48	0.34	1.871E-01	0.07
H	116	19.40	15.45	0.63	1.827E-01	0.22
H	117	25.10	-4.71	0.36	1.746E-01	0.04
H	118	27.55	5.42	0.68	1.766E-01	0.03
H	119	26.78	7.90	0.73	1.796E-01	0.02
H	120	23.31	3.36	0.44	1.873E-01	0.07
H	121	23.45	3.43	0.51	1.895E-01	0.07
H	122	24.26	3.24	0.88	1.913E-01	0.06
H	123	25.21	7.94	0.25	1.880E-01	0.06
H	124	23.60	4.47	0.58	1.891E-01	0.07
H	125	19.70	24.94	0.07	1.455E-01	0.04
H	126	20.79	24.94	0.25	1.600E-01	0.03
H	127	21.53	22.30	0.30	1.686E-01	0.02
H	128	26.37	4.83	0.55	1.735E-01	0.06
H	129	26.65	7.18	0.91	1.763E-01	0.04
H	130	27.53	-6.62	0.69	1.777E-01	0.03
H	131	25.05	5.94	0.54	1.876E-01	0.07
H	132	23.17	4.87	0.77	1.895E-01	0.07
H	133	23.82	-2.14	0.94	1.917E-01	0.07
H	134	22.92	-3.37	0.20	1.825E-01	0.07
H	135	15.82	28.20	0.17	1.393E-01	0.18
H	136	27.26	10.79	0.41	1.745E-01	0.05
H	137	29.43	8.82	0.49	1.826E-01	0.01
H	138	30.47	10.21	0.91	1.812E-01	0.02
H	139	30.01	7.24	0.66	1.858E-01	0.01
H	140	30.20	13.37	0.19	1.773E-01	0.01
H	141	26.83	10.16	0.43	1.752E-01	0.05
H	142	27.32	9.93	0.57	1.788E-01	0.06
H	143	21.47	12.47	0.95	2.117E-01	0.17
H	144	25.55	5.18	0.69	1.721E-01	0.01
H	145	28.50	5.90	0.34	1.758E-01	0.04
H	146	27.53	5.88	0.89	1.785E-01	0.03
H	147	23.85	4.39	0.53	1.851E-01	0.07
H	148	22.93	3.84	0.53	1.853E-01	0.06
H	149	25.36	-5.41	0.35	1.903E-01	0.04
H	150	23.61	3.64	0.93	1.903E-01	0.04
H	151	23.87	-3.94	0.65	1.881E-01	0.07
H	152	23.72	-6.44	0.18	2.417E-01	0.18
H	153	25.68	-4.90	0.78	1.816E-01	0.04
H	154	27.32	-5.61	0.93	1.780E-01	0.02
H	155	26.71	7.05	0.66	1.794E-01	0.04
H	156	23.45	5.19	0.54	1.902E-01	0.07
H	157	24.31	4.95	0.41	1.887E-01	0.06
H	158	24.33	4.98	0.52	1.926E-01	0.06
H	159	23.75	5.10	0.54	1.916E-01	0.06
H	160	23.19	3.66	0.81	1.896E-01	0.07

H	161	23.27	30.00	0.20	2.132E-01	0.13
H	162	25.06	27.71	0.23	2.309E-01	0.13
H	163	25.92	22.74	0.16	2.560E-01	0.09
H	164	22.15	30.87	0.06	1.946E-01	0.12
H	165	22.79	28.78	0.12	2.096E-01	0.11
H	166	23.91	20.89	0.25	2.379E-01	0.11
H	167	22.96	26.39	0.18	2.265E-01	0.10
H	168	23.95	26.52	0.24	2.266E-01	0.12
H	169	24.28	27.79	0.11	2.247E-01	0.13
H	170	23.78	26.02	0.19	2.295E-01	0.11
H	171	23.12	29.84	0.12	2.234E-01	0.12
H	172	22.28	25.44	0.10	2.075E-01	0.12
C	1	118.85	-24.05	0.93	2.499E+00	0.34
C	2	131.93	28.63	0.69	1.071E+00	0.70
C	3	47.83	176.65	0.62	1.846E+00	0.60
C	4	37.00	175.22	0.77	2.766E+00	0.17
C	5	53.85	151.53	0.70	2.092E+00	0.28
C	6	9.46	148.04	0.69	-3.040E+00	0.34
C	7	55.11	143.23	0.71	1.946E+00	0.24
C	8	38.89	169.33	0.82	2.638E+00	0.22
C	9	3.24	114.99	0.82	2.824E+00	0.31
C	10	106.69	36.25	0.70	2.573E+00	0.33
C	11	142.08	-34.96	0.48	1.172E+00	0.63
C	12	150.39	-31.84	0.15	9.173E-01	0.78
C	13	123.82	47.41	0.80	2.970E+00	0.20
C	14	3.39	-121.09	0.85	3.098E+00	0.41
C	15	113.11	42.03	0.27	2.189E+00	0.71
C	16	130.00	28.07	0.26	8.497E-01	0.62
C	17	33.61	197.20	0.53	2.514E+00	0.46
C	18	38.39	175.89	0.80	2.734E+00	0.19
C	19	37.88	197.79	0.61	3.064E+00	0.04
C	20	43.17	193.90	0.65	2.852E+00	0.12
C	21	38.77	196.20	0.66	2.910E+00	0.11
C	22	42.86	177.41	0.75	2.588E+00	0.21
C	23	-3.41	127.65	0.64	3.280E+00	0.35
C	24	115.01	36.93	0.87	1.947E+00	0.65
C	25	129.29	27.57	0.51	8.721E-01	0.69
C	26	32.49	198.95	0.49	2.538E+00	0.43
C	27	38.10	171.40	0.85	2.647E+00	0.20
C	28	42.26	185.55	0.71	2.728E+00	0.19
C	29	40.65	188.95	0.67	2.702E+00	0.19
C	30	41.14	190.35	0.67	2.908E+00	0.07
C	31	39.15	180.71	0.75	2.624E+00	0.24
C	32	-13.06	117.39	0.46	3.715E+00	0.25
C	33	117.78	20.23	0.70	2.532E+00	0.32
C	34	134.35	30.01	0.31	1.014E+00	0.75
C	35	46.43	178.10	0.61	1.921E+00	0.59
C	36	37.17	172.70	0.77	2.803E+00	0.15
C	37	55.64	147.36	0.69	1.995E+00	0.27
C	38	9.79	146.14	0.70	-3.110E+00	0.21
C	39	55.65	148.83	0.71	2.019E+00	0.31
C	40	35.12	182.29	0.67	2.782E+00	0.09
C	41	3.04	116.24	0.75	2.802E+00	0.29

C	42	107.66	-36.12	0.94	2.615E+00	0.36
C	43	140.56	-34.40	0.60	1.179E+00	0.66
C	44	150.60	-31.22	0.19	9.107E-01	0.77
C	45	123.79	48.21	0.78	3.071E+00	0.20
C	46	3.21	-119.91	0.92	3.147E+00	0.41
C	47	116.34	45.83	0.60	2.065E+00	0.82
C	48	137.09	27.51	0.11	6.321E-01	0.78
C	49	35.12	193.77	0.55	2.435E+00	0.56
C	50	41.50	172.50	0.82	2.641E+00	0.21
C	51	37.75	196.99	0.62	3.014E+00	0.06
C	52	41.20	197.42	0.63	2.967E+00	0.08
C	53	38.53	197.67	0.62	3.024E+00	0.06
C	54	39.54	182.67	0.67	2.719E+00	0.16
C	55	-1.45	122.81	0.77	3.212E+00	0.34
C	56	112.40	33.68	0.64	2.393E+00	0.40
C	57	134.70	26.63	0.26	9.500E-01	0.85
C	58	32.71	195.07	0.51	2.501E+00	0.45
C	59	39.90	172.71	0.83	2.543E+00	0.30
C	60	40.81	192.24	0.65	2.925E+00	0.08
C	61	43.51	194.19	0.68	2.864E+00	0.12
C	62	41.98	187.06	0.73	2.805E+00	0.18
C	63	40.54	174.76	0.74	2.717E+00	0.15
C	64	-11.04	108.32	0.65	3.535E+00	0.20
C	65	118.85	-24.05	0.93	2.499E+00	0.34
C	66	131.93	28.63	0.69	1.071E+00	0.70
C	67	47.83	176.65	0.62	1.846E+00	0.60
C	68	37.00	175.22	0.77	2.766E+00	0.17
C	69	53.85	151.53	0.70	2.092E+00	0.28
C	70	9.46	148.04	0.69	-3.040E+00	0.34
C	71	55.11	143.23	0.71	1.946E+00	0.24
C	72	38.89	169.33	0.82	2.638E+00	0.22
C	73	3.24	114.99	0.82	2.824E+00	0.31
C	74	106.69	36.25	0.70	2.573E+00	0.33
C	75	142.08	-34.96	0.48	1.172E+00	0.63
C	76	150.39	-31.84	0.15	9.173E-01	0.78
C	77	123.82	47.41	0.80	2.970E+00	0.20
C	78	3.39	-121.09	0.85	3.098E+00	0.41
C	79	113.11	42.03	0.27	2.189E+00	0.71
C	80	130.00	28.07	0.26	8.497E-01	0.62
C	81	33.61	197.20	0.53	2.514E+00	0.46
C	82	38.39	175.89	0.80	2.734E+00	0.19
C	83	37.88	197.79	0.61	3.064E+00	0.04
C	84	43.17	193.90	0.65	2.852E+00	0.12
C	85	38.77	196.20	0.66	2.910E+00	0.11
C	86	42.86	177.41	0.75	2.588E+00	0.21
C	87	-3.41	127.65	0.64	3.280E+00	0.35
C	88	115.01	36.93	0.87	1.947E+00	0.65
C	89	129.29	27.57	0.51	8.721E-01	0.69
C	90	32.49	198.95	0.49	2.538E+00	0.43
C	91	38.10	171.40	0.85	2.647E+00	0.20
C	92	42.26	185.55	0.71	2.728E+00	0.19
C	93	40.65	188.95	0.67	2.702E+00	0.19
C	94	41.14	190.35	0.67	2.908E+00	0.07

C	95	39.15	180.71	0.75	2.624E+00	0.24
C	96	-13.06	117.39	0.46	3.715E+00	0.25
C	97	117.78	20.23	0.70	2.532E+00	0.32
C	98	134.35	30.01	0.31	1.014E+00	0.75
C	99	46.43	178.10	0.61	1.921E+00	0.59
C	100	37.17	172.70	0.77	2.803E+00	0.15
C	101	55.64	147.36	0.69	1.995E+00	0.27
C	102	9.79	146.14	0.70	-3.110E+00	0.21
C	103	55.65	148.83	0.71	2.019E+00	0.31
C	104	35.12	182.29	0.67	2.782E+00	0.09
C	105	3.04	116.24	0.75	2.802E+00	0.29
C	106	107.66	-36.12	0.94	2.615E+00	0.36
C	107	140.56	-34.40	0.60	1.179E+00	0.66
C	108	150.60	-31.22	0.19	9.107E-01	0.77
C	109	123.79	48.21	0.78	3.071E+00	0.20
C	110	3.21	-119.91	0.92	3.147E+00	0.41
C	111	116.34	45.83	0.60	2.065E+00	0.82
C	112	137.09	27.51	0.11	6.321E-01	0.78
C	113	35.12	193.77	0.55	2.435E+00	0.56
C	114	41.50	172.50	0.82	2.641E+00	0.21
C	115	37.75	196.99	0.62	3.014E+00	0.06
C	116	41.20	197.42	0.63	2.967E+00	0.08
C	117	38.53	197.67	0.62	3.024E+00	0.06
C	118	39.54	182.67	0.67	2.719E+00	0.16
C	119	-1.45	122.81	0.77	3.212E+00	0.34
C	120	112.40	33.68	0.64	2.393E+00	0.40
C	121	134.70	26.63	0.26	9.500E-01	0.85
C	122	32.71	195.07	0.51	2.501E+00	0.45
C	123	39.90	172.71	0.83	2.543E+00	0.30
C	124	40.81	192.24	0.65	2.925E+00	0.08
C	125	43.51	194.19	0.68	2.864E+00	0.12
C	126	41.98	187.06	0.73	2.805E+00	0.18
C	127	40.54	174.76	0.74	2.717E+00	0.15
C	128	-11.04	108.32	0.65	3.535E+00	0.20
N	1	183.05	17.76	0.59	1.593E+00	0.24
N	2	72.95	-165.72	0.49	-3.564E+00	0.14
N	3	99.79	-176.84	0.03	-3.419E+00	0.44
N	4	98.08	-160.70	0.10	-3.264E+00	0.51
N	5	183.91	18.88	0.82	1.594E+00	0.22
N	6	72.80	-163.51	0.53	-3.510E+00	0.15
N	7	99.90	-165.82	0.10	-3.581E+00	0.43
N	8	92.18	-169.44	0.14	-3.403E+00	0.22
N	9	183.05	17.76	0.59	1.593E+00	0.24
N	10	72.95	-165.72	0.49	-3.564E+00	0.14
N	11	99.79	-176.84	0.03	-3.419E+00	0.44
N	12	98.08	-160.70	0.10	-3.264E+00	0.51
N	13	183.91	18.88	0.82	1.594E+00	0.22
N	14	72.80	-163.51	0.53	-3.510E+00	0.15
N	15	99.90	-165.82	0.10	-3.581E+00	0.43
N	16	92.18	-169.44	0.14	-3.403E+00	0.22
O	1	270.65	38.14	0.62	7.644E+00	0.90
O	2	153.85	108.33	0.58	-8.804E+00	0.50
O	3	-43.13	550.11	0.42	8.866E+00	0.35

O	4	-49.73	570.35	0.40	8.503E+00	0.26
O	5	-28.36	505.34	0.39	9.039E+00	0.32
O	6	-19.02	304.83	0.55	6.317E+00	0.83
O	7	-18.33	376.55	0.50	8.342E+00	0.39
O	8	163.46	101.51	0.80	-8.556E+00	0.53
O	9	-32.54	517.12	0.39	8.533E+00	0.45
O	10	-47.89	567.93	0.39	8.426E+00	0.26
O	11	-27.53	524.00	0.30	8.326E+00	0.42
O	12	-63.23	385.78	0.39	7.802E+00	0.36
O	13	-2.42	318.93	0.53	7.589E+00	0.61
O	14	250.65	-33.98	0.65	7.755E+00	0.76
O	15	246.68	-21.84	0.32	7.339E+00	0.90
O	16	249.34	-21.10	0.72	7.179E+00	0.90
O	17	254.60	20.07	0.30	7.236E+00	0.85
O	18	263.50	-28.29	0.74	7.834E+00	0.82
O	19	257.60	41.37	0.81	7.545E+00	0.88
O	20	270.65	38.14	0.62	7.644E+00	0.90
O	21	153.85	108.33	0.58	-8.804E+00	0.50
O	22	-43.13	550.11	0.42	8.866E+00	0.35
O	23	-49.73	570.35	0.40	8.503E+00	0.26
O	24	-28.36	505.34	0.39	9.039E+00	0.32
O	25	-19.02	304.83	0.55	6.317E+00	0.83
O	26	-18.33	376.55	0.50	8.342E+00	0.39
O	27	163.46	101.51	0.80	-8.556E+00	0.53
O	28	-32.54	517.12	0.39	8.533E+00	0.45
O	29	-47.89	567.93	0.39	8.426E+00	0.26
O	30	-27.53	524.00	0.30	8.326E+00	0.42
O	31	-63.23	385.78	0.39	7.802E+00	0.36
O	32	-2.42	318.93	0.53	7.589E+00	0.61
O	33	250.65	-33.98	0.65	7.755E+00	0.76
O	34	246.68	-21.84	0.32	7.339E+00	0.90
O	35	249.34	-21.10	0.72	7.179E+00	0.90
O	36	254.60	20.07	0.30	7.236E+00	0.85
O	37	263.50	-28.29	0.74	7.834E+00	0.82
O	38	257.60	41.37	0.81	7.545E+00	0.88

=====

GIPAW coordinates and calculated NMR parameters for 2 (structure 1)

xx						
x	Element	Atom	Fractional coordinates of atoms x			
x		Number	u	v	w	
x-----x	x	x	x	x	x	
x H		1	0.977171	-0.010734	0.167694	x
x H		2	0.911034	0.054671	0.194863	x
x H		3	0.964488	0.243798	0.179714	x
x H		4	0.859730	0.236242	0.111363	x
x H		5	0.967369	0.321307	0.084978	x
x H		6	0.992840	0.060150	0.086028	x
x H		7	0.936355	-0.182469	0.014953	x
x H		8	0.901905	-0.213878	-0.082279	x
x H		9	0.870926	0.439474	-0.095007	x
x H		10	0.906016	0.470642	0.002198	x
x H		11	0.859059	0.204074	-0.170508	x
x H		12	0.793771	0.202084	0.031543	x
x H		13	0.673580	0.075155	-0.028891	x
x H		14	0.754206	-0.010516	-0.042097	x
x H		15	0.697046	-0.339403	-0.032332	x
x H		16	0.659617	-0.242405	0.019608	x
x H		17	0.757538	-0.393314	0.073940	x
x H		18	0.808472	-0.379888	0.024456	x
x H		19	0.736604	-0.055990	0.130253	x
x H		20	0.641067	0.293269	0.136107	x
x H		21	0.649843	-0.118723	0.195439	x
x H		22	0.592941	0.085895	0.200619	x
x H		23	0.627734	-0.360574	0.125158	x
x H		24	0.544871	-0.512839	0.050650	x
x H		25	0.437340	-0.320886	0.010349	x
x H		26	0.414178	0.020171	0.045817	x
x H		27	0.497415	0.173304	0.120574	x
x H		28	0.770847	-0.020603	0.219776	x
x H		29	0.802289	0.346662	0.289280	x
x H		30	0.787298	-0.094549	0.328113	x
x H		31	0.811681	0.125695	0.367848	x
x H		32	0.668708	-0.184248	0.301832	x
x H		33	0.544363	-0.103499	0.294843	x
x H		34	0.508335	0.247123	0.319214	x
x H		35	0.597682	0.510331	0.351250	x
x H		36	0.722315	0.430239	0.356935	x
x H		37	0.053383	-0.209943	0.309081	x
x H		38	0.085059	0.030402	0.303607	x
x H		39	0.134619	-0.169004	0.298480	x
x H		40	0.165070	0.010670	0.385315	x
x H		41	0.044247	0.113761	0.386448	x
x H		42	0.019457	-0.146102	0.389889	x
x H		43	0.060091	-0.348778	0.474672	x
x H		44	0.075993	-0.323748	0.571462	x
x H		45	0.110491	0.326888	0.563105	x
x H		46	0.090999	0.302080	0.465216	x

x H	47	0.093516	-0.114416	0.643740	x
x H	48	0.209622	-0.047247	0.472003	x
x H	49	0.324360	-0.189985	0.536629	x
x H	50	0.241269	-0.282977	0.542225	x
x H	51	0.302072	-0.604425	0.529359	x
x H	52	0.343302	-0.487860	0.481997	x
x H	53	0.247048	-0.632221	0.421760	x
x H	54	0.192734	-0.622774	0.469085	x
x H	55	0.273122	-0.256895	0.374248	x
x H	56	0.378603	0.071277	0.381560	x
x H	57	0.350028	-0.296024	0.305179	x
x H	58	0.413837	-0.104130	0.304573	x
x H	59	0.366127	-0.566239	0.370544	x
x H	60	0.442559	-0.747622	0.444037	x
x H	61	0.554763	-0.589793	0.487652	x
x H	62	0.588397	-0.249525	0.458393	x
x H	63	0.511029	-0.063580	0.386155	x
x H	64	0.298938	-0.061208	0.254270	x
x H	65	0.220308	0.331279	0.244470	x
x H	66	0.265098	0.054451	0.161051	x
x H	67	0.210506	0.272951	0.146858	x
x H	68	0.392085	0.114192	0.211011	x
x H	69	0.493125	0.345137	0.218224	x
x H	70	0.477346	0.706942	0.186524	x
x H	71	0.358801	0.837423	0.150486	x
x H	72	0.256587	0.610128	0.147603	x
x H	73	0.820628	-0.309124	0.172873	x
x H	74	0.752869	-0.380638	0.193104	x
x H	75	0.962773	-0.393087	0.316887	x
x H	76	0.945875	-0.207247	0.276606	x
x H	77	-0.002823	0.510526	0.233304	x
x H	78	0.053196	0.379685	0.210601	x
x H	79	-0.977171	0.489266	-0.167694	x
x H	80	-0.911034	0.554671	-0.194863	x
x H	81	-0.964488	0.743798	-0.179714	x
x H	82	-0.859730	0.736242	-0.111363	x
x H	83	-0.967369	0.821307	-0.084978	x
x H	84	-0.992840	0.560150	-0.086028	x
x H	85	-0.936355	0.317531	-0.014953	x
x H	86	-0.901905	0.286122	0.082279	x
x H	87	-0.870926	0.939474	0.095007	x
x H	88	-0.906016	0.970642	-0.002198	x
x H	89	-0.859059	0.704074	0.170508	x
x H	90	-0.793771	0.702084	-0.031543	x
x H	91	-0.673580	0.575155	0.028891	x
x H	92	-0.754206	0.489484	0.042097	x
x H	93	-0.697046	0.160597	0.032332	x
x H	94	-0.659617	0.257595	-0.019608	x
x H	95	-0.757538	0.106686	-0.073940	x
x H	96	-0.808472	0.120112	-0.024456	x
x H	97	-0.736604	0.444010	-0.130253	x
x H	98	-0.641067	0.793269	-0.136107	x
x H	99	-0.649843	0.381277	-0.195439	x

x H	100	-0.592941	0.585895	-0.200619	x
x H	101	-0.627734	0.139426	-0.125158	x
x H	102	-0.544871	-0.012839	-0.050650	x
x H	103	-0.437340	0.179114	-0.010349	x
x H	104	-0.414178	0.520171	-0.045817	x
x H	105	-0.497415	0.673304	-0.120574	x
x H	106	-0.770847	0.479397	-0.219776	x
x H	107	-0.802289	0.846662	-0.289280	x
x H	108	-0.787298	0.405451	-0.328113	x
x H	109	-0.811681	0.625695	-0.367848	x
x H	110	-0.668708	0.315752	-0.301832	x
x H	111	-0.544363	0.396501	-0.294843	x
x H	112	-0.508335	0.747123	-0.319214	x
x H	113	-0.597682	1.010331	-0.351250	x
x H	114	-0.722315	0.930239	-0.356935	x
x H	115	-0.053383	0.290057	-0.309081	x
x H	116	-0.085059	0.530402	-0.303607	x
x H	117	-0.134619	0.330996	-0.298480	x
x H	118	-0.165070	0.510670	-0.385315	x
x H	119	-0.044247	0.613761	-0.386448	x
x H	120	-0.019457	0.353898	-0.389889	x
x H	121	-0.060091	0.151222	-0.474672	x
x H	122	-0.075993	0.176252	-0.571462	x
x H	123	-0.110491	0.826888	-0.563105	x
x H	124	-0.090999	0.802080	-0.465216	x
x H	125	-0.093516	0.385584	-0.643740	x
x H	126	-0.209622	0.452753	-0.472003	x
x H	127	-0.324360	0.310015	-0.536629	x
x H	128	-0.241269	0.217023	-0.542225	x
x H	129	-0.302072	-0.104425	-0.529359	x
x H	130	-0.343302	0.012140	-0.481997	x
x H	131	-0.247048	-0.132221	-0.421760	x
x H	132	-0.192734	-0.122774	-0.469085	x
x H	133	-0.273122	0.243105	-0.374248	x
x H	134	-0.378603	0.571277	-0.381560	x
x H	135	-0.350028	0.203976	-0.305179	x
x H	136	-0.413837	0.395870	-0.304573	x
x H	137	-0.366127	-0.066239	-0.370544	x
x H	138	-0.442559	-0.247622	-0.444037	x
x H	139	-0.554763	-0.089793	-0.487652	x
x H	140	-0.588397	0.250475	-0.458393	x
x H	141	-0.511029	0.436420	-0.386155	x
x H	142	-0.298938	0.438792	-0.254270	x
x H	143	-0.220308	0.831279	-0.244470	x
x H	144	-0.265098	0.554451	-0.161051	x
x H	145	-0.210506	0.772951	-0.146858	x
x H	146	-0.392085	0.614192	-0.211011	x
x H	147	-0.493125	0.845137	-0.218224	x
x H	148	-0.477346	1.206942	-0.186524	x
x H	149	-0.358801	1.337423	-0.150486	x
x H	150	-0.256587	1.110128	-0.147603	x
x H	151	-0.820628	0.190876	-0.172873	x
x H	152	-0.752869	0.119362	-0.193104	x

x H	153	-0.962773	0.106913	-0.316887	x
x H	154	-0.945875	0.292753	-0.276606	x
x H	155	0.002823	1.010526	-0.233304	x
x H	156	-0.053196	0.879685	-0.210601	x
x C	1	0.897385	0.111620	0.111671	x
x C	2	0.948269	0.164811	0.074832	x
x C	3	0.922399	0.146506	0.016124	x
x C	4	0.920740	-0.045522	-0.008822	x
x C	5	0.901963	-0.064495	-0.063220	x
x C	6	0.884685	0.109696	-0.095382	x
x C	7	0.885011	0.302685	-0.070859	x
x C	8	0.904006	0.318861	-0.016038	x
x C	9	0.861551	-0.096615	0.098180	x
x C	10	0.759997	0.075929	0.039062	x
x C	11	0.720284	-0.013916	-0.013108	x
x C	12	0.705719	-0.235406	0.001684	x
x C	13	0.770073	-0.297417	0.042292	x
x C	14	0.710894	0.168363	0.072504	x
x C	15	0.670513	0.163689	0.156393	x
x C	16	0.619988	0.006267	0.173057	x
x C	17	0.568665	-0.083080	0.127796	x
x C	18	0.580910	-0.276350	0.107624	x
x C	19	0.533976	-0.362731	0.065810	x
x C	20	0.473903	-0.255932	0.043506	x
x C	21	0.461044	-0.063283	0.063381	x
x C	22	0.508063	0.022821	0.105196	x
x C	23	0.717542	0.253811	0.205903	x
x C	24	0.806048	0.179421	0.284769	x
x C	25	0.779200	0.072265	0.330712	x
x C	26	0.703988	0.117547	0.329675	x
x C	27	0.653221	-0.031368	0.312629	x
x C	28	0.583090	0.014619	0.308555	x
x C	29	0.562961	0.209835	0.322068	x
x C	30	0.613291	0.358763	0.339897	x
x C	31	0.683152	0.312776	0.343461	x
x C	32	0.882179	0.117480	0.288654	x
x C	33	0.123467	-0.104146	0.377891	x
x C	34	0.062035	-0.036862	0.403098	x
x C	35	0.076821	-0.025532	0.462621	x
x C	36	0.073010	-0.200174	0.493653	x
x C	37	0.082007	-0.187288	0.548322	x
x C	38	0.095248	0.003141	0.573956	x
x C	39	0.100575	0.178469	0.543464	x
x C	40	0.090463	0.163185	0.488761	x
x C	41	0.148815	-0.321407	0.395801	x
x C	42	0.245011	-0.169284	0.464495	x
x C	43	0.279005	-0.275317	0.516133	x
x C	44	0.295417	-0.489834	0.497755	x
x C	45	0.233452	-0.540998	0.453889	x
x C	46	0.298862	-0.065204	0.437725	x
x C	47	0.342583	-0.029345	0.355119	x
x C	48	0.384751	-0.187011	0.330267	x
x C	49	0.433687	-0.303955	0.372440	x

x C	50	0.415427	-0.497215	0.389193	x
x C	51	0.458600	-0.600014	0.430448	x
x C	52	0.521054	-0.511382	0.455162	x
x C	53	0.539796	-0.318857	0.438738	x
x C	54	0.496214	-0.215394	0.397968	x
x C	55	0.293640	0.117174	0.318131	x
x C	56	0.229535	0.180921	0.228011	x
x C	57	0.253990	0.208109	0.175314	x
x C	58	0.316602	0.346041	0.179143	x
x C	59	0.383966	0.274334	0.198842	x
x C	60	0.441266	0.403869	0.202469	x
x C	61	0.432528	0.607362	0.185437	x
x C	62	0.365878	0.680353	0.165379	x
x C	63	0.308565	0.551775	0.162881	x
x C	64	0.161651	0.051931	0.220877	x
x C	65	-0.897385	0.611620	-0.111671	x
x C	66	-0.948269	0.664811	-0.074832	x
x C	67	-0.922399	0.646506	-0.016124	x
x C	68	-0.920740	0.454478	0.008822	x
x C	69	-0.901963	0.435505	0.063220	x
x C	70	-0.884685	0.609696	0.095382	x
x C	71	-0.885011	0.802685	0.070859	x
x C	72	-0.904006	0.818861	0.016038	x
x C	73	-0.861551	0.403385	-0.098180	x
x C	74	-0.759997	0.575929	-0.039062	x
x C	75	-0.720284	0.486084	0.013108	x
x C	76	-0.705719	0.264594	-0.001684	x
x C	77	-0.770073	0.202583	-0.042292	x
x C	78	-0.710894	0.668363	-0.072504	x
x C	79	-0.670513	0.663689	-0.156393	x
x C	80	-0.619988	0.506267	-0.173057	x
x C	81	-0.568665	0.416920	-0.127796	x
x C	82	-0.580910	0.223650	-0.107624	x
x C	83	-0.533976	0.137269	-0.065810	x
x C	84	-0.473903	0.244068	-0.043506	x
x C	85	-0.461044	0.436717	-0.063381	x
x C	86	-0.508063	0.522821	-0.105196	x
x C	87	-0.717542	0.753811	-0.205903	x
x C	88	-0.806048	0.679421	-0.284769	x
x C	89	-0.779200	0.572265	-0.330712	x
x C	90	-0.703988	0.617547	-0.329675	x
x C	91	-0.653221	0.468632	-0.312629	x
x C	92	-0.583090	0.514619	-0.308555	x
x C	93	-0.562961	0.709835	-0.322068	x
x C	94	-0.613291	0.858763	-0.339897	x
x C	95	-0.683152	0.812776	-0.343461	x
x C	96	-0.882179	0.617480	-0.288654	x
x C	97	-0.123467	0.395854	-0.377891	x
x C	98	-0.062035	0.463138	-0.403098	x
x C	99	-0.076821	0.474468	-0.462621	x
x C	100	-0.073010	0.299826	-0.493653	x
x C	101	-0.082007	0.312712	-0.548322	x
x C	102	-0.095248	0.503141	-0.573956	x

x C	103	-0.100575	0.678469	-0.543464	x
x C	104	-0.090463	0.663185	-0.488761	x
x C	105	-0.148815	0.178593	-0.395801	x
x C	106	-0.245011	0.330716	-0.464495	x
x C	107	-0.279005	0.224683	-0.516133	x
x C	108	-0.295417	0.010166	-0.497755	x
x C	109	-0.233452	-0.040998	-0.453889	x
x C	110	-0.298862	0.434796	-0.437725	x
x C	111	-0.342583	0.470655	-0.355119	x
x C	112	-0.384751	0.312989	-0.330267	x
x C	113	-0.433687	0.196045	-0.372440	x
x C	114	-0.415427	0.002785	-0.389193	x
x C	115	-0.458600	-0.100014	-0.430448	x
x C	116	-0.521054	-0.011382	-0.455162	x
x C	117	-0.539796	0.181143	-0.438738	x
x C	118	-0.496214	0.284606	-0.397968	x
x C	119	-0.293640	0.617174	-0.318131	x
x C	120	-0.229535	0.680921	-0.228011	x
x C	121	-0.253990	0.708109	-0.175314	x
x C	122	-0.316602	0.846041	-0.179143	x
x C	123	-0.383966	0.774334	-0.198842	x
x C	124	-0.441266	0.903869	-0.202469	x
x C	125	-0.432528	1.107362	-0.185437	x
x C	126	-0.365878	1.180353	-0.165379	x
x C	127	-0.308565	1.051775	-0.162881	x
x C	128	-0.161651	0.551931	-0.220877	x
x N	1	0.939184	0.099147	0.166245	x
x N	2	0.800854	-0.099999	0.063328	x
x N	3	0.710570	0.079245	0.119790	x
x N	4	0.764110	0.124670	0.234005	x
x N	5	0.098387	-0.113477	0.319054	x
x N	6	0.206673	-0.337391	0.433791	x
x N	7	0.301122	-0.130380	0.388295	x
x N	8	0.282949	0.076815	0.266015	x
x N	9	-0.939184	0.599147	-0.166245	x
x N	10	-0.800854	0.400001	-0.063328	x
x N	11	-0.710570	0.579245	-0.119790	x
x N	12	-0.764110	0.624670	-0.234005	x
x N	13	-0.098387	0.386523	-0.319054	x
x N	14	-0.206673	0.162609	-0.433791	x
x N	15	-0.301122	0.369620	-0.388295	x
x N	16	-0.282949	0.576815	-0.266015	x
x O	1	0.868631	0.077597	-0.147702	x
x O	2	0.890200	-0.255955	0.118518	x
x O	3	0.676160	0.320814	0.055477	x
x O	4	0.710193	0.435953	0.219029	x
x O	5	0.926616	0.195920	0.325018	x
x O	6	0.894920	-0.017789	0.256155	x
x O	7	0.101724	0.023622	0.626977	x
x O	8	0.115722	-0.472323	0.375140	x
x O	9	0.335384	0.073286	0.460828	x
x O	10	0.265733	0.261971	0.337090	x
x O	11	0.104511	0.142437	0.217714	x

x O	12	0.169924	-0.142542	0.220476	x
x O	13	0.775438	-0.263134	0.178448	x
x O	14	0.978914	-0.325543	0.287744	x
x O	15	0.006431	0.441193	0.201499	x
x O	16	-0.868631	0.577597	0.147702	x
x O	17	-0.890200	0.244045	-0.118518	x
x O	18	-0.676160	0.820814	-0.055477	x
x O	19	-0.710193	0.935953	-0.219029	x
x O	20	-0.926616	0.695920	-0.325018	x
x O	21	-0.894920	0.482211	-0.256155	x
x O	22	-0.101724	0.523622	-0.626977	x
x O	23	-0.115722	0.027677	-0.375140	x
x O	24	-0.335384	0.573286	-0.460828	x
x O	25	-0.265733	0.761971	-0.337090	x
x O	26	-0.104511	0.642437	-0.217714	x
x O	27	-0.169924	0.357458	-0.220476	x
x O	28	-0.775438	0.236866	-0.178448	x
x O	29	-0.978914	0.174457	-0.287744	x
x O	30	-0.006431	0.941193	-0.201499	x

xx

---

| Chemical Shielding and Electric Field Gradient Tensors |

---

Nucleus	Shielding tensor			EFG Tensor		
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
H	1	26.06	9.28	0.30	2.193E-01	0.08
H	2	21.89	27.22	0.13	1.649E-01	0.03
H	3	15.84	36.30	0.12	9.306E-02	0.02
H	4	26.44	4.31	0.81	1.769E-01	0.07
H	5	26.96	7.30	0.87	1.764E-01	0.04
H	6	27.78	-5.80	0.79	1.746E-01	0.05
H	7	24.19	5.75	0.24	1.890E-01	0.07
H	8	23.22	-2.66	0.89	1.942E-01	0.06
H	9	23.23	-4.10	0.41	1.926E-01	0.08
H	10	23.45	2.52	0.70	1.910E-01	0.06
H	11	18.65	27.17	0.15	1.861E-01	0.14
H	12	26.99	6.66	0.82	1.778E-01	0.05
H	13	29.72	9.64	0.34	1.833E-01	0.00
H	14	30.31	10.78	0.73	1.811E-01	0.02
H	15	29.67	7.83	0.37	1.862E-01	0.01
H	16	29.77	12.15	0.19	1.789E-01	0.01
H	17	26.85	9.49	0.52	1.801E-01	0.04
H	18	27.36	9.76	0.48	1.801E-01	0.06
H	19	21.16	-12.84	0.95	2.065E-01	0.18
H	20	25.91	4.54	0.73	1.746E-01	0.02
H	21	27.96	4.01	0.53	1.796E-01	0.04
H	22	28.40	8.57	0.91	1.797E-01	0.03
H	23	23.38	3.86	0.48	1.892E-01	0.07
H	24	23.94	3.67	0.71	1.900E-01	0.05
H	25	25.25	-4.24	0.45	1.903E-01	0.04
H	26	24.14	3.34	0.86	1.926E-01	0.05
H	27	24.33	3.05	0.96	1.882E-01	0.07

H	28	20.27	13.54	0.72	1.960E-01	0.20
H	29	24.90	-5.50	0.38	1.743E-01	0.04
H	30	27.59	5.11	0.67	1.777E-01	0.03
H	31	26.66	7.97	0.58	1.807E-01	0.02
H	32	23.44	3.17	0.63	1.878E-01	0.07
H	33	23.59	3.69	0.06	1.911E-01	0.06
H	34	24.46	3.32	0.88	1.909E-01	0.06
H	35	24.76	6.83	0.31	1.897E-01	0.06
H	36	23.55	4.19	0.45	1.894E-01	0.07
H	37	17.42	30.95	0.11	1.150E-01	0.06
H	38	25.23	14.58	0.34	2.146E-01	0.02
H	39	24.76	17.36	0.16	2.035E-01	0.02
H	40	26.22	5.97	0.41	1.736E-01	0.07
H	41	26.54	7.02	0.77	1.753E-01	0.07
H	42	27.28	-5.71	0.98	1.776E-01	0.05
H	43	24.46	5.97	0.15	1.897E-01	0.07
H	44	23.41	3.66	0.76	1.912E-01	0.08
H	45	23.76	-1.89	0.52	1.934E-01	0.07
H	46	23.21	-3.08	0.07	1.882E-01	0.06
H	47	16.29	27.61	0.16	1.464E-01	0.18
H	48	27.54	10.06	0.45	1.750E-01	0.04
H	49	29.86	9.33	0.45	1.829E-01	0.00
H	50	30.35	10.00	0.85	1.819E-01	0.02
H	51	29.96	6.80	0.60	1.869E-01	0.02
H	52	30.18	12.11	0.19	1.795E-01	0.01
H	53	26.33	10.92	0.32	1.725E-01	0.06
H	54	27.08	11.89	0.45	1.806E-01	0.06
H	55	24.80	-7.24	0.72	2.449E-01	0.17
H	56	25.91	-4.66	0.95	1.731E-01	0.02
H	57	29.06	7.51	0.60	1.762E-01	0.03
H	58	27.77	5.24	0.79	1.815E-01	0.02
H	59	23.60	5.12	0.46	1.817E-01	0.07
H	60	23.38	3.25	0.66	1.865E-01	0.06
H	61	25.44	-4.85	0.69	1.914E-01	0.04
H	62	23.94	-3.78	0.93	1.916E-01	0.04
H	63	24.06	3.76	0.88	1.895E-01	0.07
H	64	24.11	-6.88	0.44	2.443E-01	0.18
H	65	25.47	-3.88	0.38	1.773E-01	0.03
H	66	27.38	5.99	0.53	1.794E-01	0.02
H	67	26.45	8.47	0.59	1.811E-01	0.04
H	68	23.28	4.72	0.60	1.919E-01	0.07
H	69	23.84	3.01	0.71	1.902E-01	0.06
H	70	25.04	6.61	0.40	1.905E-01	0.06
H	71	23.67	-3.80	1.00	1.912E-01	0.06
H	72	22.75	3.81	0.94	1.898E-01	0.07
H	73	27.98	17.10	0.32	2.781E-01	0.12
H	74	23.81	32.45	0.08	2.151E-01	0.15
H	75	26.38	20.07	0.12	2.731E-01	0.07
H	76	20.40	33.22	0.04	1.766E-01	0.14
H	77	23.89	28.81	0.04	2.407E-01	0.11
H	78	23.52	22.03	0.16	2.358E-01	0.13
H	79	26.06	9.28	0.30	2.193E-01	0.08
H	80	21.89	27.22	0.13	1.649E-01	0.03

H	81	15.84	36.30	0.12	9.306E-02	0.02
H	82	26.44	4.31	0.81	1.769E-01	0.07
H	83	26.96	7.30	0.87	1.764E-01	0.04
H	84	27.78	-5.80	0.79	1.746E-01	0.05
H	85	24.19	5.75	0.24	1.890E-01	0.07
H	86	23.22	-2.66	0.89	1.942E-01	0.06
H	87	23.23	-4.10	0.41	1.926E-01	0.08
H	88	23.45	2.52	0.70	1.910E-01	0.06
H	89	18.65	27.17	0.15	1.861E-01	0.14
H	90	26.99	6.66	0.82	1.778E-01	0.05
H	91	29.72	9.64	0.34	1.833E-01	0.00
H	92	30.31	10.78	0.73	1.811E-01	0.02
H	93	29.67	7.83	0.37	1.862E-01	0.01
H	94	29.77	12.15	0.19	1.789E-01	0.01
H	95	26.85	9.49	0.52	1.801E-01	0.04
H	96	27.36	9.76	0.48	1.801E-01	0.06
H	97	21.16	-12.84	0.95	2.065E-01	0.18
H	98	25.91	4.54	0.73	1.746E-01	0.02
H	99	27.96	4.01	0.53	1.796E-01	0.04
H	100	28.40	8.57	0.91	1.797E-01	0.03
H	101	23.38	3.86	0.48	1.892E-01	0.07
H	102	23.94	3.67	0.71	1.900E-01	0.05
H	103	25.25	-4.24	0.45	1.903E-01	0.04
H	104	24.14	3.34	0.86	1.926E-01	0.05
H	105	24.33	3.05	0.96	1.882E-01	0.07
H	106	20.27	13.54	0.72	1.960E-01	0.20
H	107	24.90	-5.50	0.38	1.743E-01	0.04
H	108	27.59	5.11	0.67	1.777E-01	0.03
H	109	26.66	7.97	0.58	1.807E-01	0.02
H	110	23.44	3.17	0.63	1.878E-01	0.07
H	111	23.59	3.69	0.06	1.911E-01	0.06
H	112	24.46	3.32	0.88	1.909E-01	0.06
H	113	24.76	6.83	0.31	1.897E-01	0.06
H	114	23.55	4.19	0.45	1.894E-01	0.07
H	115	17.42	30.95	0.11	1.150E-01	0.06
H	116	25.23	14.58	0.34	2.146E-01	0.02
H	117	24.76	17.36	0.16	2.035E-01	0.02
H	118	26.22	5.97	0.41	1.736E-01	0.07
H	119	26.54	7.02	0.77	1.753E-01	0.07
H	120	27.28	-5.71	0.98	1.776E-01	0.05
H	121	24.46	5.97	0.15	1.897E-01	0.07
H	122	23.41	3.66	0.76	1.912E-01	0.08
H	123	23.76	-1.89	0.52	1.934E-01	0.07
H	124	23.21	-3.08	0.07	1.882E-01	0.06
H	125	16.29	27.61	0.16	1.464E-01	0.18
H	126	27.54	10.06	0.45	1.750E-01	0.04
H	127	29.86	9.33	0.45	1.829E-01	0.00
H	128	30.35	10.00	0.85	1.819E-01	0.02
H	129	29.96	6.80	0.60	1.869E-01	0.02
H	130	30.18	12.11	0.19	1.795E-01	0.01
H	131	26.33	10.92	0.32	1.725E-01	0.06
H	132	27.08	11.89	0.45	1.806E-01	0.06
H	133	24.80	-7.24	0.72	2.449E-01	0.17

H	134	25.91	-4.66	0.95	1.731E-01	0.02
H	135	29.06	7.51	0.60	1.762E-01	0.03
H	136	27.77	5.24	0.79	1.815E-01	0.02
H	137	23.60	5.12	0.46	1.817E-01	0.07
H	138	23.38	3.25	0.66	1.865E-01	0.06
H	139	25.44	-4.85	0.69	1.914E-01	0.04
H	140	23.94	-3.78	0.93	1.916E-01	0.04
H	141	24.06	3.76	0.88	1.895E-01	0.07
H	142	24.11	-6.88	0.44	2.443E-01	0.18
H	143	25.47	-3.88	0.38	1.773E-01	0.03
H	144	27.38	5.99	0.53	1.794E-01	0.02
H	145	26.45	8.47	0.59	1.811E-01	0.04
H	146	23.28	4.72	0.60	1.919E-01	0.07
H	147	23.84	3.01	0.71	1.902E-01	0.06
H	148	25.04	6.61	0.40	1.905E-01	0.06
H	149	23.67	-3.80	1.00	1.912E-01	0.06
H	150	22.75	3.81	0.94	1.898E-01	0.07
H	151	27.98	17.10	0.32	2.781E-01	0.12
H	152	23.81	32.45	0.08	2.151E-01	0.15
H	153	26.38	20.07	0.12	2.731E-01	0.07
H	154	20.40	33.22	0.04	1.766E-01	0.14
H	155	23.89	28.81	0.04	2.407E-01	0.11
H	156	23.52	22.03	0.16	2.358E-01	0.13
C	1	119.35	-28.10	0.84	2.617E+00	0.25
C	2	131.56	30.11	0.98	1.144E+00	0.71
C	3	49.67	172.77	0.66	1.732E+00	0.70
C	4	36.53	177.01	0.76	2.750E+00	0.20
C	5	53.91	146.22	0.74	2.007E+00	0.35
C	6	9.66	149.40	0.65	-3.001E+00	0.42
C	7	57.71	137.33	0.79	1.770E+00	0.32
C	8	38.27	168.08	0.81	2.649E+00	0.21
C	9	3.09	-115.78	0.99	2.763E+00	0.36
C	10	107.79	37.60	0.67	2.528E+00	0.33
C	11	143.27	-36.90	0.47	1.193E+00	0.62
C	12	151.38	-31.68	0.10	8.948E-01	0.78
C	13	124.14	47.79	0.71	2.941E+00	0.21
C	14	2.75	-120.22	0.83	3.118E+00	0.42
C	15	113.27	44.17	0.14	2.160E+00	0.79
C	16	129.66	29.52	0.29	9.025E-01	0.61
C	17	34.23	195.61	0.54	2.536E+00	0.46
C	18	39.10	172.48	0.84	2.733E+00	0.21
C	19	39.14	195.61	0.65	3.047E+00	0.07
C	20	43.08	194.07	0.66	2.883E+00	0.12
C	21	40.37	193.48	0.69	2.898E+00	0.14
C	22	42.29	176.82	0.75	2.642E+00	0.20
C	23	-4.01	128.56	0.61	3.304E+00	0.35
C	24	114.51	36.24	0.94	2.184E+00	0.56
C	25	128.61	26.98	0.64	9.132E-01	0.70
C	26	32.64	199.64	0.49	2.552E+00	0.42
C	27	38.50	169.63	0.88	2.632E+00	0.22
C	28	41.69	186.34	0.72	2.749E+00	0.20
C	29	43.14	187.38	0.68	2.757E+00	0.16
C	30	41.11	189.95	0.70	2.929E+00	0.09

C	31	39.95	182.52	0.74	2.626E+00	0.24
C	32	-10.61	111.09	0.67	3.584E+00	0.18
C	33	116.19	23.56	0.80	3.134E+00	0.23
C	34	133.80	25.55	0.70	1.185E+00	0.74
C	35	47.90	174.78	0.65	1.822E+00	0.69
C	36	37.80	177.96	0.73	2.741E+00	0.16
C	37	55.59	146.33	0.70	1.949E+00	0.28
C	38	9.27	147.94	0.67	-3.105E+00	0.26
C	39	56.12	146.57	0.70	1.979E+00	0.31
C	40	34.43	173.90	0.73	2.740E+00	0.15
C	41	5.23	-122.31	0.76	2.659E+00	0.41
C	42	108.48	37.07	0.86	2.536E+00	0.35
C	43	142.16	-35.65	0.46	1.180E+00	0.57
C	44	150.75	-30.73	0.23	8.761E-01	0.75
C	45	124.41	48.11	0.75	3.106E+00	0.25
C	46	2.63	-122.80	0.96	3.188E+00	0.48
C	47	116.14	48.72	0.27	2.257E+00	0.71
C	48	138.34	27.15	0.05	6.214E-01	0.75
C	49	35.27	194.34	0.55	2.417E+00	0.59
C	50	40.85	177.51	0.76	2.771E+00	0.13
C	51	38.74	194.87	0.66	3.027E+00	0.08
C	52	41.98	196.50	0.66	2.976E+00	0.10
C	53	39.76	196.14	0.65	3.001E+00	0.08
C	54	41.07	179.54	0.70	2.674E+00	0.18
C	55	1.50	-120.85	0.94	3.143E+00	0.36
C	56	112.78	37.16	0.52	2.401E+00	0.51
C	57	135.86	22.74	0.35	-8.397E-01	0.85
C	58	29.84	198.89	0.48	2.587E+00	0.41
C	59	39.87	173.50	0.81	2.610E+00	0.24
C	60	41.93	187.96	0.73	2.828E+00	0.15
C	61	44.80	192.28	0.70	2.867E+00	0.12
C	62	41.69	185.36	0.77	2.782E+00	0.21
C	63	40.15	175.50	0.75	2.769E+00	0.13
C	64	-11.07	107.28	0.78	3.525E+00	0.09
C	65	119.35	-28.10	0.84	2.617E+00	0.25
C	66	131.56	30.11	0.98	1.144E+00	0.71
C	67	49.67	172.77	0.66	1.732E+00	0.70
C	68	36.53	177.01	0.76	2.750E+00	0.20
C	69	53.91	146.22	0.74	2.007E+00	0.35
C	70	9.66	149.40	0.65	-3.001E+00	0.42
C	71	57.71	137.33	0.79	1.770E+00	0.32
C	72	38.27	168.08	0.81	2.649E+00	0.21
C	73	3.09	-115.78	0.99	2.763E+00	0.36
C	74	107.79	37.60	0.67	2.528E+00	0.33
C	75	143.27	-36.90	0.47	1.193E+00	0.62
C	76	151.38	-31.68	0.10	8.948E-01	0.78
C	77	124.14	47.79	0.71	2.941E+00	0.21
C	78	2.75	-120.22	0.83	3.118E+00	0.42
C	79	113.27	44.17	0.14	2.160E+00	0.79
C	80	129.66	29.52	0.29	9.025E-01	0.61
C	81	34.23	195.61	0.54	2.536E+00	0.46
C	82	39.10	172.48	0.84	2.733E+00	0.21
C	83	39.14	195.61	0.65	3.047E+00	0.07

C	84	43.08	194.07	0.66	2.883E+00	0.12
C	85	40.37	193.48	0.69	2.898E+00	0.14
C	86	42.29	176.82	0.75	2.642E+00	0.20
C	87	-4.01	128.56	0.61	3.304E+00	0.35
C	88	114.51	36.24	0.94	2.184E+00	0.56
C	89	128.61	26.98	0.64	9.132E-01	0.70
C	90	32.64	199.64	0.49	2.552E+00	0.42
C	91	38.50	169.63	0.88	2.632E+00	0.22
C	92	41.69	186.34	0.72	2.749E+00	0.20
C	93	43.14	187.38	0.68	2.757E+00	0.16
C	94	41.11	189.95	0.70	2.929E+00	0.09
C	95	39.95	182.52	0.74	2.626E+00	0.24
C	96	-10.61	111.09	0.67	3.584E+00	0.18
C	97	116.19	23.56	0.80	3.134E+00	0.23
C	98	133.80	25.55	0.70	1.185E+00	0.74
C	99	47.90	174.78	0.65	1.822E+00	0.69
C	100	37.80	177.96	0.73	2.741E+00	0.16
C	101	55.59	146.33	0.70	1.949E+00	0.28
C	102	9.27	147.94	0.67	-3.105E+00	0.26
C	103	56.12	146.57	0.70	1.979E+00	0.31
C	104	34.43	173.90	0.73	2.740E+00	0.15
C	105	5.23	-122.31	0.76	2.659E+00	0.41
C	106	108.48	37.07	0.86	2.536E+00	0.35
C	107	142.16	-35.65	0.46	1.180E+00	0.57
C	108	150.75	-30.73	0.23	8.761E-01	0.75
C	109	124.41	48.11	0.75	3.106E+00	0.25
C	110	2.63	-122.80	0.96	3.188E+00	0.48
C	111	116.14	48.72	0.27	2.257E+00	0.71
C	112	138.34	27.15	0.05	6.214E-01	0.75
C	113	35.27	194.34	0.55	2.417E+00	0.59
C	114	40.85	177.51	0.76	2.771E+00	0.13
C	115	38.74	194.87	0.66	3.027E+00	0.08
C	116	41.98	196.50	0.66	2.976E+00	0.10
C	117	39.76	196.14	0.65	3.001E+00	0.08
C	118	41.07	179.54	0.70	2.674E+00	0.18
C	119	1.50	-120.85	0.94	3.143E+00	0.36
C	120	112.78	37.16	0.52	2.401E+00	0.51
C	121	135.86	22.74	0.35	-8.397E-01	0.85
C	122	29.84	198.89	0.48	2.587E+00	0.41
C	123	39.87	173.50	0.81	2.610E+00	0.24
C	124	41.93	187.96	0.73	2.828E+00	0.15
C	125	44.80	192.28	0.70	2.867E+00	0.12
C	126	41.69	185.36	0.77	2.782E+00	0.21
C	127	40.15	175.50	0.75	2.769E+00	0.13
C	128	-11.07	107.28	0.78	3.525E+00	0.09
N	1	182.39	29.45	0.12	1.609E+00	0.89
N	2	77.45	-161.47	0.59	-3.764E+00	0.13
N	3	101.54	-174.76	0.03	-3.387E+00	0.45
N	4	95.64	-163.40	0.11	-3.214E+00	0.44
N	5	190.61	24.85	0.28	-1.346E+00	0.86
N	6	79.06	-158.91	0.65	-3.789E+00	0.13
N	7	104.55	-166.05	0.19	-3.894E+00	0.22
N	8	92.78	-165.69	0.18	-3.507E+00	0.17

	N	9	182.39	29.45	0.12	1.609E+00	0.89
	N	10	77.45	-161.47	0.59	-3.764E+00	0.13
	N	11	101.54	-174.76	0.03	-3.387E+00	0.45
	N	12	95.64	-163.40	0.11	-3.214E+00	0.44
	N	13	190.61	24.85	0.28	-1.346E+00	0.86
	N	14	79.06	-158.91	0.65	-3.789E+00	0.13
	N	15	104.55	-166.05	0.19	-3.894E+00	0.22
	N	16	92.78	-165.69	0.18	-3.507E+00	0.17
	O	1	149.47	116.50	0.67	-9.058E+00	0.49
	O	2	-63.08	585.88	0.46	8.913E+00	0.24
	O	3	-52.63	578.77	0.41	8.527E+00	0.24
	O	4	-28.15	497.03	0.39	9.156E+00	0.32
	O	5	-45.83	374.13	0.43	7.408E+00	0.48
	O	6	-4.05	334.70	0.64	8.114E+00	0.52
	O	7	164.75	100.32	0.88	-8.673E+00	0.52
	O	8	-72.51	597.49	0.46	8.885E+00	0.21
	O	9	-60.12	604.60	0.41	8.557E+00	0.21
	O	10	-50.88	557.91	0.34	8.781E+00	0.24
	O	11	-64.36	366.56	0.47	8.374E+00	0.32
	O	12	-12.02	352.69	0.55	8.322E+00	0.42
	O	13	266.27	36.21	0.85	8.559E+00	0.80
	O	14	249.18	15.54	0.82	7.329E+00	0.91
	O	15	261.60	-42.35	0.97	8.032E+00	0.80
	O	16	149.47	116.50	0.67	-9.058E+00	0.49
	O	17	-63.08	585.88	0.46	8.913E+00	0.24
	O	18	-52.63	578.77	0.41	8.527E+00	0.24
	O	19	-28.15	497.03	0.39	9.156E+00	0.32
	O	20	-45.83	374.13	0.43	7.408E+00	0.48
	O	21	-4.05	334.70	0.64	8.114E+00	0.52
	O	22	164.75	100.32	0.88	-8.673E+00	0.52
	O	23	-72.51	597.49	0.46	8.885E+00	0.21
	O	24	-60.12	604.60	0.41	8.557E+00	0.21
	O	25	-50.88	557.91	0.34	8.781E+00	0.24
	O	26	-64.36	366.56	0.47	8.374E+00	0.32
	O	27	-12.02	352.69	0.55	8.322E+00	0.42
	O	28	266.27	36.21	0.85	8.559E+00	0.80
	O	29	249.18	15.54	0.82	7.329E+00	0.91
	O	30	261.60	-42.35	0.97	8.032E+00	0.80

=====

GIPAW coordinates and calculated NMR parameters for 2 (structure 3)

xx

x	Element	Atom	Fractional coordinates of atoms x			
x		Number	u	v	w	x
x-----x						
x H		1	0.958471	-0.201023	0.167803	x
x H		2	0.931030	-0.022294	0.206344	x
x H		3	1.005048	0.020531	0.181101	x
x H		4	0.874061	0.150163	0.133910	x
x H		5	0.967469	0.272214	0.097999	x
x H		6	1.002768	0.023997	0.095465	x
x H		7	0.945415	-0.228760	0.025084	x
x H		8	0.915497	-0.252645	-0.072272	x
x H		9	0.876441	0.397353	-0.082213	x
x H		10	0.906737	0.421574	0.015344	x
x H		11	0.872434	0.175203	-0.157363	x
x H		12	0.805996	0.169746	0.048316	x
x H		13	0.692235	0.083630	-0.024369	x
x H		14	0.773616	-0.019277	-0.031985	x
x H		15	0.702774	-0.332545	-0.034720	x
x H		16	0.661480	-0.238419	0.015516	x
x H		17	0.749526	-0.428357	0.071738	x
x H		18	0.807267	-0.413469	0.027209	x
x H		19	0.733857	-0.083456	0.137143	x
x H		20	0.629396	0.251957	0.131071	x
x H		21	0.639914	-0.150158	0.194869	x
x H		22	0.582520	0.053947	0.199806	x
x H		23	0.614662	-0.397842	0.125549	x
x H		24	0.531275	-0.543406	0.049667	x
x H		25	0.426677	-0.340784	0.008281	x
x H		26	0.406869	0.003306	0.043115	x
x H		27	0.490349	0.149543	0.118731	x
x H		28	0.753883	-0.028894	0.222411	x
x H		29	0.793397	0.356468	0.283097	x
x H		30	0.776482	-0.062713	0.333609	x
x H		31	0.804143	0.169772	0.366898	x
x H		32	0.656792	-0.139832	0.305247	x
x H		33	0.533400	-0.045110	0.297052	x
x H		34	0.501328	0.312563	0.319195	x
x H		35	0.593449	0.568811	0.349468	x
x H		36	0.717266	0.475054	0.355966	x
x H		37	0.047150	-0.187114	0.319132	x
x H		38	0.089553	0.036597	0.311130	x
x H		39	0.132892	-0.191356	0.314094	x
x H		40	0.160145	0.035558	0.393872	x
x H		41	0.042072	0.143703	0.396222	x
x H		42	0.014768	-0.115165	0.399536	x
x H		43	0.053824	-0.322368	0.481812	x
x H		44	0.075018	-0.308372	0.579101	x
x H		45	0.121162	0.336604	0.574632	x
x H		46	0.097312	0.323285	0.476277	x
x H		47	0.101013	-0.109840	0.652890	x

x H	48	0.215049	-0.004328	0.475837	x
x H	49	0.335914	-0.134103	0.534861	x
x H	50	0.255769	-0.225299	0.547631	x
x H	51	0.315170	-0.549340	0.534730	x
x H	52	0.348467	-0.443212	0.481779	x
x H	53	0.246867	-0.600102	0.430578	x
x H	54	0.200121	-0.576300	0.482468	x
x H	55	0.257507	-0.197558	0.368854	x
x H	56	0.361478	0.131637	0.371624	x
x H	57	0.341461	-0.251041	0.300257	x
x H	58	0.402952	-0.051175	0.299536	x
x H	59	0.361128	-0.522480	0.361822	x
x H	60	0.437768	-0.701454	0.435878	x
x H	61	0.545052	-0.527922	0.484119	x
x H	62	0.572787	-0.175855	0.458859	x
x H	63	0.495044	0.005892	0.386219	x
x H	64	0.288414	-0.044854	0.248180	x
x H	65	0.197338	0.323486	0.227658	x
x H	66	0.257368	0.042230	0.152721	x
x H	67	0.202511	0.256413	0.133402	x
x H	68	0.380911	0.103877	0.203603	x
x H	69	0.482182	0.335723	0.213955	x
x H	70	0.467260	0.698880	0.183549	x
x H	71	0.349713	0.829674	0.145160	x
x H	72	0.247071	0.601765	0.138568	x
x H	73	0.817599	-0.252023	0.217501	x
x H	74	0.749040	-0.391955	0.202971	x
x H	75	0.957473	-0.372154	0.324280	x
x H	76	0.940772	-0.195310	0.283093	x
x H	77	0.207979	-0.476424	0.302545	x
x H	78	0.191524	-0.294369	0.259494	x
x H	79	-0.958471	0.298977	-0.167803	x
x H	80	-0.931030	0.477706	-0.206344	x
x H	81	-1.005048	0.520531	-0.181101	x
x H	82	-0.874061	0.650163	-0.133910	x
x H	83	-0.967469	0.772214	-0.097999	x
x H	84	-1.002768	0.523997	-0.095465	x
x H	85	-0.945415	0.271240	-0.025084	x
x H	86	-0.915497	0.247355	0.072272	x
x H	87	-0.876441	0.897353	0.082213	x
x H	88	-0.906737	0.921574	-0.015344	x
x H	89	-0.872434	0.675203	0.157363	x
x H	90	-0.805996	0.669746	-0.048316	x
x H	91	-0.692235	0.583630	0.024369	x
x H	92	-0.773616	0.480723	0.031985	x
x H	93	-0.702774	0.167455	0.034720	x
x H	94	-0.661480	0.261581	-0.015516	x
x H	95	-0.749526	0.071643	-0.071738	x
x H	96	-0.807267	0.086531	-0.027209	x
x H	97	-0.733857	0.416544	-0.137143	x
x H	98	-0.629396	0.751957	-0.131071	x
x H	99	-0.639914	0.349842	-0.194869	x
x H	100	-0.582520	0.553947	-0.199806	x

x H	101	-0.614662	0.102158	-0.125549	x
x H	102	-0.531275	-0.043406	-0.049667	x
x H	103	-0.426677	0.159216	-0.008281	x
x H	104	-0.406869	0.503306	-0.043115	x
x H	105	-0.490349	0.649543	-0.118731	x
x H	106	-0.753883	0.471106	-0.222411	x
x H	107	-0.793397	0.856468	-0.283097	x
x H	108	-0.776482	0.437287	-0.333609	x
x H	109	-0.804143	0.669772	-0.366898	x
x H	110	-0.656792	0.360168	-0.305247	x
x H	111	-0.533400	0.454890	-0.297052	x
x H	112	-0.501328	0.812563	-0.319195	x
x H	113	-0.593449	1.068811	-0.349468	x
x H	114	-0.717266	0.975054	-0.355966	x
x H	115	-0.047150	0.312886	-0.319132	x
x H	116	-0.089553	0.536597	-0.311130	x
x H	117	-0.132892	0.308644	-0.314094	x
x H	118	-0.160145	0.535558	-0.393872	x
x H	119	-0.042072	0.643703	-0.396222	x
x H	120	-0.014768	0.384835	-0.399536	x
x H	121	-0.053824	0.177632	-0.481812	x
x H	122	-0.075018	0.191628	-0.579101	x
x H	123	-0.121162	0.836604	-0.574632	x
x H	124	-0.097312	0.823285	-0.476277	x
x H	125	-0.101013	0.390160	-0.652890	x
x H	126	-0.215049	0.495672	-0.475837	x
x H	127	-0.335914	0.365897	-0.534861	x
x H	128	-0.255769	0.274701	-0.547631	x
x H	129	-0.315170	-0.049340	-0.534730	x
x H	130	-0.348467	0.056788	-0.481779	x
x H	131	-0.246867	-0.100102	-0.430578	x
x H	132	-0.200121	-0.076300	-0.482468	x
x H	133	-0.257507	0.302442	-0.368854	x
x H	134	-0.361478	0.631637	-0.371624	x
x H	135	-0.341461	0.248959	-0.300257	x
x H	136	-0.402952	0.448825	-0.299536	x
x H	137	-0.361128	-0.022480	-0.361822	x
x H	138	-0.437768	-0.201454	-0.435878	x
x H	139	-0.545052	-0.027922	-0.484119	x
x H	140	-0.572787	0.324145	-0.458859	x
x H	141	-0.495044	0.505892	-0.386219	x
x H	142	-0.288414	0.455146	-0.248180	x
x H	143	-0.197338	0.823486	-0.227658	x
x H	144	-0.257368	0.542230	-0.152721	x
x H	145	-0.202511	0.756413	-0.133402	x
x H	146	-0.380911	0.603877	-0.203603	x
x H	147	-0.482182	0.835723	-0.213955	x
x H	148	-0.467260	1.198880	-0.183549	x
x H	149	-0.349713	1.329674	-0.145160	x
x H	150	-0.247071	1.101765	-0.138568	x
x H	151	-0.817599	0.247977	-0.217501	x
x H	152	-0.749040	0.108045	-0.202971	x
x H	153	-0.957473	0.127846	-0.324280	x

x H	154	-0.940772	0.304690	-0.283093	x
x H	155	-0.207979	0.023576	-0.302545	x
x H	156	-0.191524	0.205631	-0.259494	x
x C	1	0.907852	0.028731	0.123795	x
x C	2	0.954182	0.112576	0.086398	x
x C	3	0.927790	0.098486	0.027658	x
x C	4	0.929077	-0.090909	0.001927	x
x C	5	0.912882	-0.105777	-0.052588	x
x C	6	0.896032	0.070364	-0.083909	x
x C	7	0.891376	0.259700	-0.058611	x
x C	8	0.907683	0.272007	-0.003645	x
x C	9	0.866156	-0.164456	0.102135	x
x C	10	0.768342	0.045953	0.049002	x
x C	11	0.734348	-0.020441	-0.007142	x
x C	12	0.710598	-0.239917	0.001361	x
x C	13	0.768690	-0.327293	0.043931	x
x C	14	0.713182	0.134144	0.077608	x
x C	15	0.659435	0.131956	0.155131	x
x C	16	0.609787	-0.025818	0.172380	x
x C	17	0.558536	-0.114291	0.126945	x
x C	18	0.569211	-0.309342	0.107128	x
x C	19	0.522024	-0.391767	0.064793	x
x C	20	0.463553	-0.279314	0.041740	x
x C	21	0.452418	-0.084706	0.061279	x
x C	22	0.499576	-0.002542	0.103571	x
x C	23	0.702488	0.241229	0.203412	x
x C	24	0.794568	0.187672	0.282185	x
x C	25	0.769856	0.105389	0.331949	x
x C	26	0.695445	0.160834	0.331067	x
x C	27	0.642974	0.016209	0.314829	x
x C	28	0.573400	0.070092	0.310048	x
x C	29	0.555478	0.269169	0.322242	x
x C	30	0.607452	0.414151	0.339165	x
x C	31	0.676837	0.360463	0.343232	x
x C	32	0.869533	0.116056	0.284123	x
x C	33	0.119036	-0.080792	0.387693	x
x C	34	0.058265	-0.008781	0.412439	x
x C	35	0.075150	-0.000735	0.471896	x
x C	36	0.069791	-0.177468	0.501789	x
x C	37	0.081848	-0.170829	0.556610	x
x C	38	0.099807	0.015226	0.583221	x
x C	39	0.107151	0.192136	0.553889	x
x C	40	0.094294	0.183353	0.498990	x
x C	41	0.146149	-0.293240	0.408450	x
x C	42	0.249508	-0.127196	0.467200	x
x C	43	0.289447	-0.223080	0.518447	x
x C	44	0.303979	-0.441539	0.501590	x
x C	45	0.237803	-0.500220	0.462700	x
x C	46	0.298430	-0.025776	0.435183	x
x C	47	0.328060	0.017016	0.347796	x
x C	48	0.374031	-0.136539	0.324974	x
x C	49	0.423298	-0.247713	0.368120	x
x C	50	0.408268	-0.447408	0.382664	x

x C	51	0.451594	-0.548472	0.424168	x
x C	52	0.511107	-0.451227	0.451428	x
x C	53	0.526595	-0.252243	0.437287	x
x C	54	0.482783	-0.150799	0.396233	x
x C	55	0.275034	0.142097	0.308106	x
x C	56	0.213225	0.173750	0.214876	x
x C	57	0.243893	0.197157	0.164615	x
x C	58	0.306231	0.336891	0.170993	x
x C	59	0.373166	0.264880	0.192063	x
x C	60	0.430583	0.394663	0.197490	x
x C	61	0.422305	0.598949	0.181113	x
x C	62	0.356115	0.672106	0.159700	x
x C	63	0.298622	0.543104	0.155190	x
x C	64	0.149100	0.029072	0.203565	x
x C	65	-0.907852	0.528731	-0.123795	x
x C	66	-0.954182	0.612576	-0.086398	x
x C	67	-0.927790	0.598486	-0.027658	x
x C	68	-0.929077	0.409091	-0.001927	x
x C	69	-0.912882	0.394223	0.052588	x
x C	70	-0.896032	0.570364	0.083909	x
x C	71	-0.891376	0.759700	0.058611	x
x C	72	-0.907683	0.772007	0.003645	x
x C	73	-0.866156	0.335544	-0.102135	x
x C	74	-0.768342	0.545953	-0.049002	x
x C	75	-0.734348	0.479559	0.007142	x
x C	76	-0.710598	0.260083	-0.001361	x
x C	77	-0.768690	0.172707	-0.043931	x
x C	78	-0.713182	0.634144	-0.077608	x
x C	79	-0.659435	0.631956	-0.155131	x
x C	80	-0.609787	0.474182	-0.172380	x
x C	81	-0.558536	0.385709	-0.126945	x
x C	82	-0.569211	0.190658	-0.107128	x
x C	83	-0.522024	0.108233	-0.064793	x
x C	84	-0.463553	0.220686	-0.041740	x
x C	85	-0.452418	0.415294	-0.061279	x
x C	86	-0.499576	0.497458	-0.103571	x
x C	87	-0.702488	0.741229	-0.203412	x
x C	88	-0.794568	0.687672	-0.282185	x
x C	89	-0.769856	0.605389	-0.331949	x
x C	90	-0.695445	0.660834	-0.331067	x
x C	91	-0.642974	0.516209	-0.314829	x
x C	92	-0.573400	0.570092	-0.310048	x
x C	93	-0.555478	0.769169	-0.322242	x
x C	94	-0.607452	0.914151	-0.339165	x
x C	95	-0.676837	0.860463	-0.343232	x
x C	96	-0.869533	0.616056	-0.284123	x
x C	97	-0.119036	0.419208	-0.387693	x
x C	98	-0.058265	0.491219	-0.412439	x
x C	99	-0.075150	0.499265	-0.471896	x
x C	100	-0.069791	0.322532	-0.501789	x
x C	101	-0.081848	0.329171	-0.556610	x
x C	102	-0.099807	0.515226	-0.583221	x
x C	103	-0.107151	0.692136	-0.553889	x

x C	104	-0.094294	0.683353	-0.498990	x
x C	105	-0.146149	0.206760	-0.408450	x
x C	106	-0.249508	0.372804	-0.467200	x
x C	107	-0.289447	0.276920	-0.518447	x
x C	108	-0.303979	0.058461	-0.501590	x
x C	109	-0.237803	-0.000220	-0.462700	x
x C	110	-0.298430	0.474224	-0.435183	x
x C	111	-0.328060	0.517016	-0.347796	x
x C	112	-0.374031	0.363461	-0.324974	x
x C	113	-0.423298	0.252287	-0.368120	x
x C	114	-0.408268	0.052592	-0.382664	x
x C	115	-0.451594	-0.048472	-0.424168	x
x C	116	-0.511107	0.048773	-0.451428	x
x C	117	-0.526595	0.247757	-0.437287	x
x C	118	-0.482783	0.349201	-0.396233	x
x C	119	-0.275034	0.642097	-0.308106	x
x C	120	-0.213225	0.673750	-0.214876	x
x C	121	-0.243893	0.697157	-0.164615	x
x C	122	-0.306231	0.836891	-0.170993	x
x C	123	-0.373166	0.764880	-0.192063	x
x C	124	-0.430583	0.894663	-0.197490	x
x C	125	-0.422305	1.098949	-0.181113	x
x C	126	-0.356115	1.172106	-0.159700	x
x C	127	-0.298622	1.043104	-0.155190	x
x C	128	-0.149100	0.529072	-0.203565	x
x N	1	0.954406	-0.042835	0.173587	x
x N	2	0.803113	-0.143611	0.071101	x
x N	3	0.704518	0.041967	0.122727	x
x N	4	0.749102	0.120930	0.234253	x
x N	5	0.095727	-0.104501	0.329239	x
x N	6	0.208934	-0.301109	0.441151	x
x N	7	0.290650	-0.082235	0.383936	x
x N	8	0.265329	0.086746	0.257163	x
x N	9	-0.954406	0.457165	-0.173587	x
x N	10	-0.803113	0.356389	-0.071101	x
x N	11	-0.704518	0.541967	-0.122727	x
x N	12	-0.749102	0.620930	-0.234253	x
x N	13	-0.095727	0.395499	-0.329239	x
x N	14	-0.208934	0.198891	-0.441151	x
x N	15	-0.290650	0.417765	-0.383936	x
x N	16	-0.265329	0.586746	-0.257163	x
x O	1	0.886266	0.045262	-0.136487	x
x O	2	0.893619	-0.335399	0.113622	x
x O	3	0.680023	0.286347	0.058233	x
x O	4	0.693138	0.426458	0.212173	x
x O	5	0.916853	0.197932	0.317400	x
x O	6	0.879183	-0.029862	0.253114	x
x O	7	0.109400	0.029785	0.636646	x
x O	8	0.111131	-0.448528	0.393983	x
x O	9	0.339821	0.105957	0.456335	x
x O	10	0.243456	0.285612	0.324878	x
x O	11	0.089840	0.105288	0.199759	x
x O	12	0.164009	-0.160628	0.198886	x

x O	13	0.774291	-0.272097	0.192049	x
x O	14	0.976458	-0.300863	0.296809	x
x O	15	0.199691	-0.326468	0.297677	x
x O	16	-0.886266	0.545262	0.136487	x
x O	17	-0.893619	0.164601	-0.113622	x
x O	18	-0.680023	0.786347	-0.058233	x
x O	19	-0.693138	0.926458	-0.212173	x
x O	20	-0.916853	0.697932	-0.317400	x
x O	21	-0.879183	0.470138	-0.253114	x
x O	22	-0.109400	0.529785	-0.636646	x
x O	23	-0.111131	0.051472	-0.393983	x
x O	24	-0.339821	0.605957	-0.456335	x
x O	25	-0.243456	0.785612	-0.324878	x
x O	26	-0.089840	0.605288	-0.199759	x
x O	27	-0.164009	0.339372	-0.198886	x
x O	28	-0.774291	0.227903	-0.192049	x
x O	29	-0.976458	0.199137	-0.296809	x
x O	30	-0.199691	0.173532	-0.297677	x

xx

---

### Chemical Shielding and Electric Field Gradient Tensors

---

Nucleus	Shielding tensor			EFG Tensor		
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
H	1	23.18	11.94	0.32	1.841E-01	0.02
H	2	20.93	29.28	0.19	1.603E-01	0.04
H	3	19.23	26.04	0.20	1.397E-01	0.06
H	4	26.08	4.47	0.49	1.765E-01	0.06
H	5	26.63	7.44	0.38	1.776E-01	0.04
H	6	27.43	-6.53	0.73	1.762E-01	0.06
H	7	24.45	7.02	0.18	1.883E-01	0.07
H	8	23.50	-2.90	0.90	1.951E-01	0.06
H	9	23.34	-3.74	0.61	1.929E-01	0.08
H	10	23.42	-2.24	0.69	1.891E-01	0.06
H	11	17.56	29.36	0.19	1.755E-01	0.14
H	12	26.52	-6.52	0.98	1.783E-01	0.06
H	13	29.55	9.17	0.44	1.837E-01	0.00
H	14	30.81	11.37	0.73	1.806E-01	0.02
H	15	29.83	8.34	0.36	1.868E-01	0.01
H	16	30.10	11.03	0.20	1.790E-01	0.00
H	17	26.85	12.21	0.22	1.787E-01	0.03
H	18	27.27	8.95	0.52	1.806E-01	0.06
H	19	21.32	-13.28	0.85	2.095E-01	0.18
H	20	25.98	3.90	0.80	1.748E-01	0.02
H	21	27.76	4.28	0.74	1.785E-01	0.03
H	22	28.11	8.51	0.97	1.795E-01	0.03
H	23	23.30	3.67	0.84	1.874E-01	0.07
H	24	24.26	3.72	0.70	1.900E-01	0.05
H	25	25.18	-4.12	0.65	1.900E-01	0.04
H	26	24.16	-2.92	0.95	1.930E-01	0.05
H	27	24.27	3.09	0.76	1.883E-01	0.07

H	28	20.00	16.13	0.69	1.940E-01	0.22
H	29	25.29	-6.33	0.29	1.755E-01	0.04
H	30	27.77	5.30	0.58	1.782E-01	0.03
H	31	26.72	8.46	0.49	1.810E-01	0.02
H	32	23.57	3.77	0.51	1.890E-01	0.07
H	33	23.55	4.09	0.17	1.915E-01	0.06
H	34	24.38	4.04	0.74	1.907E-01	0.06
H	35	24.70	6.34	0.41	1.904E-01	0.06
H	36	23.60	3.92	0.31	1.893E-01	0.07
H	37	16.51	33.95	0.11	1.015E-01	0.08
H	38	27.04	11.91	0.15	2.264E-01	0.04
H	39	19.83	28.33	0.19	1.412E-01	0.08
H	40	26.36	5.60	0.13	1.748E-01	0.06
H	41	26.94	6.81	0.46	1.768E-01	0.05
H	42	27.42	5.87	0.89	1.779E-01	0.04
H	43	24.81	6.22	0.27	1.883E-01	0.06
H	44	23.29	3.83	0.81	1.910E-01	0.07
H	45	23.68	-2.27	0.52	1.935E-01	0.07
H	46	23.09	-2.59	0.52	1.854E-01	0.06
H	47	15.85	28.03	0.14	1.394E-01	0.17
H	48	27.49	9.45	0.54	1.748E-01	0.04
H	49	29.85	9.01	0.52	1.835E-01	0.00
H	50	30.55	10.65	0.79	1.824E-01	0.02
H	51	30.20	7.24	0.56	1.861E-01	0.02
H	52	30.38	12.80	0.18	1.792E-01	0.01
H	53	27.25	10.42	0.31	1.779E-01	0.05
H	54	27.34	10.73	0.51	1.801E-01	0.05
H	55	22.77	-10.48	0.62	2.313E-01	0.15
H	56	25.63	4.92	0.63	1.728E-01	0.01
H	57	28.51	6.52	0.53	1.767E-01	0.05
H	58	27.51	5.32	0.96	1.802E-01	0.02
H	59	23.95	4.41	0.47	1.868E-01	0.08
H	60	22.93	3.36	0.51	1.856E-01	0.06
H	61	24.85	-4.27	0.43	1.897E-01	0.04
H	62	24.00	-3.37	0.91	1.923E-01	0.05
H	63	23.78	3.36	0.70	1.895E-01	0.07
H	64	23.91	-6.38	0.38	2.432E-01	0.17
H	65	25.77	-4.93	0.47	1.824E-01	0.04
H	66	27.22	6.19	0.58	1.792E-01	0.01
H	67	26.58	8.49	0.63	1.808E-01	0.04
H	68	23.30	4.28	0.67	1.913E-01	0.07
H	69	23.77	2.86	0.76	1.903E-01	0.06
H	70	25.06	7.22	0.41	1.907E-01	0.06
H	71	23.61	-4.02	0.94	1.919E-01	0.06
H	72	22.92	3.21	0.82	1.903E-01	0.07
H	73	26.48	19.52	0.15	2.709E-01	0.09
H	74	23.52	32.64	0.07	2.164E-01	0.12
H	75	25.47	24.38	0.07	2.587E-01	0.08
H	76	22.67	30.51	0.07	2.119E-01	0.14
H	77	23.40	28.84	0.31	2.214E-01	0.13
H	78	24.40	27.10	0.24	2.281E-01	0.13
H	79	23.18	11.94	0.32	1.841E-01	0.02
H	80	20.93	29.28	0.19	1.603E-01	0.04

H	81	19.23	26.04	0.20	1.397E-01	0.06
H	82	26.08	4.47	0.49	1.765E-01	0.06
H	83	26.63	7.44	0.38	1.776E-01	0.04
H	84	27.43	-6.53	0.73	1.762E-01	0.06
H	85	24.45	7.02	0.18	1.883E-01	0.07
H	86	23.50	-2.90	0.90	1.951E-01	0.06
H	87	23.34	-3.74	0.61	1.929E-01	0.08
H	88	23.42	-2.24	0.69	1.891E-01	0.06
H	89	17.56	29.36	0.19	1.755E-01	0.14
H	90	26.52	-6.52	0.98	1.783E-01	0.06
H	91	29.55	9.17	0.44	1.837E-01	0.00
H	92	30.81	11.37	0.73	1.806E-01	0.02
H	93	29.83	8.34	0.36	1.868E-01	0.01
H	94	30.10	11.03	0.20	1.790E-01	0.00
H	95	26.85	12.21	0.22	1.787E-01	0.03
H	96	27.27	8.95	0.52	1.806E-01	0.06
H	97	21.32	-13.28	0.85	2.095E-01	0.18
H	98	25.98	3.90	0.80	1.748E-01	0.02
H	99	27.76	4.28	0.74	1.785E-01	0.03
H	100	28.11	8.51	0.97	1.795E-01	0.03
H	101	23.30	3.67	0.84	1.874E-01	0.07
H	102	24.26	3.72	0.70	1.900E-01	0.05
H	103	25.18	-4.12	0.65	1.900E-01	0.04
H	104	24.16	-2.92	0.95	1.930E-01	0.05
H	105	24.27	3.09	0.76	1.883E-01	0.07
H	106	20.00	16.13	0.69	1.940E-01	0.22
H	107	25.29	-6.33	0.29	1.755E-01	0.04
H	108	27.77	5.30	0.58	1.782E-01	0.03
H	109	26.72	8.46	0.49	1.810E-01	0.02
H	110	23.57	3.77	0.51	1.890E-01	0.07
H	111	23.55	4.09	0.17	1.915E-01	0.06
H	112	24.38	4.04	0.74	1.907E-01	0.06
H	113	24.70	6.34	0.41	1.904E-01	0.06
H	114	23.60	3.92	0.31	1.893E-01	0.07
H	115	16.51	33.95	0.11	1.015E-01	0.08
H	116	27.04	11.91	0.15	2.264E-01	0.04
H	117	19.83	28.33	0.19	1.412E-01	0.08
H	118	26.36	5.60	0.13	1.748E-01	0.06
H	119	26.94	6.81	0.46	1.768E-01	0.05
H	120	27.42	5.87	0.89	1.779E-01	0.04
H	121	24.81	6.22	0.27	1.883E-01	0.06
H	122	23.29	3.83	0.81	1.910E-01	0.07
H	123	23.68	-2.27	0.52	1.935E-01	0.07
H	124	23.09	-2.59	0.52	1.854E-01	0.06
H	125	15.85	28.03	0.14	1.394E-01	0.17
H	126	27.49	9.45	0.54	1.748E-01	0.04
H	127	29.85	9.01	0.52	1.835E-01	0.00
H	128	30.55	10.65	0.79	1.824E-01	0.02
H	129	30.20	7.24	0.56	1.861E-01	0.02
H	130	30.38	12.80	0.18	1.792E-01	0.01
H	131	27.25	10.42	0.31	1.779E-01	0.05
H	132	27.34	10.73	0.51	1.801E-01	0.05
H	133	22.77	-10.48	0.62	2.313E-01	0.15

H	134	25.63	4.92	0.63	1.728E-01	0.01
H	135	28.51	6.52	0.53	1.767E-01	0.05
H	136	27.51	5.32	0.96	1.802E-01	0.02
H	137	23.95	4.41	0.47	1.868E-01	0.08
H	138	22.93	3.36	0.51	1.856E-01	0.06
H	139	24.85	-4.27	0.43	1.897E-01	0.04
H	140	24.00	-3.37	0.91	1.923E-01	0.05
H	141	23.78	3.36	0.70	1.895E-01	0.07
H	142	23.91	-6.38	0.38	2.432E-01	0.17
H	143	25.77	-4.93	0.47	1.824E-01	0.04
H	144	27.22	6.19	0.58	1.792E-01	0.01
H	145	26.58	8.49	0.63	1.808E-01	0.04
H	146	23.30	4.28	0.67	1.913E-01	0.07
H	147	23.77	2.86	0.76	1.903E-01	0.06
H	148	25.06	7.22	0.41	1.907E-01	0.06
H	149	23.61	-4.02	0.94	1.919E-01	0.06
H	150	22.92	3.21	0.82	1.903E-01	0.07
H	151	26.48	19.52	0.15	2.709E-01	0.09
H	152	23.52	32.64	0.07	2.164E-01	0.12
H	153	25.47	24.38	0.07	2.587E-01	0.08
H	154	22.67	30.51	0.07	2.119E-01	0.14
H	155	23.40	28.84	0.31	2.214E-01	0.13
H	156	24.40	27.10	0.24	2.281E-01	0.13
C	1	119.29	-31.25	0.83	2.787E+00	0.30
C	2	133.31	-31.75	0.82	1.221E+00	0.64
C	3	49.29	173.58	0.63	1.719E+00	0.73
C	4	35.38	182.63	0.70	2.824E+00	0.16
C	5	54.45	146.50	0.73	2.023E+00	0.35
C	6	9.84	150.00	0.63	-3.012E+00	0.42
C	7	58.90	138.49	0.77	1.746E+00	0.35
C	8	36.38	172.33	0.77	2.711E+00	0.17
C	9	4.32	-116.50	0.97	2.744E+00	0.29
C	10	107.42	-34.82	0.98	2.566E+00	0.32
C	11	142.67	-36.16	0.53	1.183E+00	0.70
C	12	152.26	-29.91	0.09	7.913E-01	0.77
C	13	123.83	49.66	0.83	3.031E+00	0.24
C	14	3.22	-119.77	0.86	3.139E+00	0.40
C	15	112.76	42.71	0.19	2.237E+00	0.74
C	16	131.42	29.86	0.14	8.547E-01	0.65
C	17	33.45	196.66	0.52	2.532E+00	0.46
C	18	39.63	174.41	0.81	2.774E+00	0.16
C	19	39.41	194.61	0.66	3.015E+00	0.09
C	20	43.05	195.02	0.65	2.901E+00	0.10
C	21	40.17	194.30	0.70	2.900E+00	0.14
C	22	42.53	175.97	0.77	2.611E+00	0.23
C	23	-2.55	126.16	0.64	3.314E+00	0.36
C	24	115.32	37.71	0.89	2.035E+00	0.57
C	25	129.51	27.59	0.51	9.056E-01	0.71
C	26	32.96	199.46	0.49	2.524E+00	0.44
C	27	38.49	169.12	0.88	2.619E+00	0.24
C	28	41.88	186.02	0.71	2.746E+00	0.21
C	29	42.57	188.57	0.67	2.778E+00	0.15
C	30	41.26	188.92	0.71	2.890E+00	0.11

C	31	40.38	180.89	0.75	2.604E+00	0.25
C	32	-10.47	110.10	0.70	3.555E+00	0.23
C	33	117.63	20.40	0.72	2.847E+00	0.28
C	34	135.69	26.46	0.54	1.011E+00	0.85
C	35	47.06	177.76	0.62	1.931E+00	0.60
C	36	36.58	179.75	0.70	2.839E+00	0.12
C	37	56.11	147.14	0.71	1.989E+00	0.29
C	38	10.67	145.90	0.72	-3.134E+00	0.21
C	39	57.14	144.92	0.73	1.972E+00	0.34
C	40	35.00	179.04	0.70	2.821E+00	0.09
C	41	4.21	-123.25	0.80	2.744E+00	0.42
C	42	108.82	-36.59	0.97	2.471E+00	0.36
C	43	141.96	-35.28	0.49	1.151E+00	0.61
C	44	150.84	-30.17	0.14	8.501E-01	0.77
C	45	124.99	44.83	0.80	2.923E+00	0.19
C	46	2.78	-121.41	0.95	3.204E+00	0.45
C	47	117.13	48.64	0.41	2.063E+00	0.84
C	48	137.05	28.81	0.09	6.364E-01	0.83
C	49	35.39	193.76	0.56	2.416E+00	0.57
C	50	40.60	170.70	0.85	2.637E+00	0.24
C	51	39.06	197.16	0.64	3.023E+00	0.07
C	52	41.50	197.65	0.64	2.988E+00	0.08
C	53	40.46	194.94	0.66	2.976E+00	0.10
C	54	39.78	182.43	0.68	2.679E+00	0.18
C	55	0.94	120.10	0.82	3.174E+00	0.36
C	56	111.69	34.48	0.45	2.448E+00	0.44
C	57	134.44	25.97	0.35	8.813E-01	0.98
C	58	31.76	196.95	0.50	2.541E+00	0.42
C	59	39.88	170.96	0.84	2.570E+00	0.28
C	60	41.79	188.51	0.73	2.842E+00	0.15
C	61	44.33	194.39	0.69	2.917E+00	0.10
C	62	41.48	186.01	0.77	2.798E+00	0.20
C	63	40.10	176.41	0.75	2.763E+00	0.14
C	64	-8.10	103.18	0.94	3.455E+00	0.18
C	65	119.29	-31.25	0.83	2.787E+00	0.30
C	66	133.31	-31.75	0.82	1.221E+00	0.64
C	67	49.29	173.58	0.63	1.719E+00	0.73
C	68	35.38	182.63	0.70	2.824E+00	0.16
C	69	54.45	146.50	0.73	2.023E+00	0.35
C	70	9.84	150.00	0.63	-3.012E+00	0.42
C	71	58.90	138.49	0.77	1.746E+00	0.35
C	72	36.38	172.33	0.77	2.711E+00	0.17
C	73	4.32	-116.50	0.97	2.744E+00	0.29
C	74	107.42	-34.82	0.98	2.566E+00	0.32
C	75	142.67	-36.16	0.53	1.183E+00	0.70
C	76	152.26	-29.91	0.09	7.913E-01	0.77
C	77	123.83	49.66	0.83	3.031E+00	0.24
C	78	3.22	-119.77	0.86	3.139E+00	0.40
C	79	112.76	42.71	0.19	2.237E+00	0.74
C	80	131.42	29.86	0.14	8.547E-01	0.65
C	81	33.45	196.66	0.52	2.532E+00	0.46
C	82	39.63	174.41	0.81	2.774E+00	0.16
C	83	39.41	194.61	0.66	3.015E+00	0.09

C	84	43.05	195.02	0.65	2.901E+00	0.10
C	85	40.17	194.30	0.70	2.900E+00	0.14
C	86	42.53	175.97	0.77	2.611E+00	0.23
C	87	-2.55	126.16	0.64	3.314E+00	0.36
C	88	115.32	37.71	0.89	2.035E+00	0.57
C	89	129.51	27.59	0.51	9.056E-01	0.71
C	90	32.96	199.46	0.49	2.524E+00	0.44
C	91	38.49	169.12	0.88	2.619E+00	0.24
C	92	41.88	186.02	0.71	2.746E+00	0.21
C	93	42.57	188.57	0.67	2.778E+00	0.15
C	94	41.26	188.92	0.71	2.890E+00	0.11
C	95	40.38	180.89	0.75	2.604E+00	0.25
C	96	-10.47	110.10	0.70	3.555E+00	0.23
C	97	117.63	20.40	0.72	2.847E+00	0.28
C	98	135.69	26.46	0.54	1.011E+00	0.85
C	99	47.06	177.76	0.62	1.931E+00	0.60
C	100	36.58	179.75	0.70	2.839E+00	0.12
C	101	56.11	147.14	0.71	1.989E+00	0.29
C	102	10.67	145.90	0.72	-3.134E+00	0.21
C	103	57.14	144.92	0.73	1.972E+00	0.34
C	104	35.00	179.04	0.70	2.821E+00	0.09
C	105	4.21	-123.25	0.80	2.744E+00	0.42
C	106	108.82	-36.59	0.97	2.471E+00	0.36
C	107	141.96	-35.28	0.49	1.151E+00	0.61
C	108	150.84	-30.17	0.14	8.501E-01	0.77
C	109	124.99	44.83	0.80	2.923E+00	0.19
C	110	2.78	-121.41	0.95	3.204E+00	0.45
C	111	117.13	48.64	0.41	2.063E+00	0.84
C	112	137.05	28.81	0.09	6.364E-01	0.83
C	113	35.39	193.76	0.56	2.416E+00	0.57
C	114	40.60	170.70	0.85	2.637E+00	0.24
C	115	39.06	197.16	0.64	3.023E+00	0.07
C	116	41.50	197.65	0.64	2.988E+00	0.08
C	117	40.46	194.94	0.66	2.976E+00	0.10
C	118	39.78	182.43	0.68	2.679E+00	0.18
C	119	0.94	120.10	0.82	3.174E+00	0.36
C	120	111.69	34.48	0.45	2.448E+00	0.44
C	121	134.44	25.97	0.35	8.813E-01	0.98
C	122	31.76	196.95	0.50	2.541E+00	0.42
C	123	39.88	170.96	0.84	2.570E+00	0.28
C	124	41.79	188.51	0.73	2.842E+00	0.15
C	125	44.33	194.39	0.69	2.917E+00	0.10
C	126	41.48	186.01	0.77	2.798E+00	0.20
C	127	40.10	176.41	0.75	2.763E+00	0.14
C	128	-8.10	103.18	0.94	3.455E+00	0.18
N	1	184.83	27.13	0.60	1.466E+00	0.33
N	2	80.94	-155.79	0.52	-3.745E+00	0.12
N	3	100.44	-178.11	0.09	-3.445E+00	0.43
N	4	98.25	-157.59	0.12	-3.239E+00	0.48
N	5	187.81	16.74	0.36	-1.637E+00	1.00
N	6	80.04	-159.85	0.71	-3.869E+00	0.16
N	7	103.18	-170.31	0.09	-3.723E+00	0.36
N	8	92.42	-166.23	0.07	-3.443E+00	0.20

	N	9	184.83	27.13	0.60	1.466E+00	0.33
	N	10	80.94	-155.79	0.52	-3.745E+00	0.12
	N	11	100.44	-178.11	0.09	-3.445E+00	0.43
	N	12	98.25	-157.59	0.12	-3.239E+00	0.48
	N	13	187.81	16.74	0.36	-1.637E+00	1.00
	N	14	80.04	-159.85	0.71	-3.869E+00	0.16
	N	15	103.18	-170.31	0.09	-3.723E+00	0.36
	N	16	92.42	-166.23	0.07	-3.443E+00	0.20
	O	1	153.19	121.36	0.47	-8.829E+00	0.46
	O	2	-56.02	584.28	0.46	8.136E+00	0.33
	O	3	-50.35	577.77	0.39	8.567E+00	0.25
	O	4	-20.11	486.70	0.36	8.886E+00	0.34
	O	5	-47.90	381.06	0.43	7.378E+00	0.45
	O	6	4.68	295.77	0.71	7.570E+00	0.66
	O	7	164.88	97.90	0.82	-8.570E+00	0.50
	O	8	-76.39	606.41	0.44	8.859E+00	0.21
	O	9	-48.77	586.18	0.39	8.499E+00	0.23
	O	10	-21.18	499.97	0.29	8.316E+00	0.43
	O	11	-69.86	377.35	0.44	8.538E+00	0.29
	O	12	-0.76	322.11	0.66	7.826E+00	0.59
	O	13	259.54	45.75	0.43	8.039E+00	0.86
	O	14	254.17	-37.41	0.60	7.687E+00	0.83
	O	15	261.20	-37.26	0.80	7.899E+00	0.79
	O	16	153.19	121.36	0.47	-8.829E+00	0.46
	O	17	-56.02	584.28	0.46	8.136E+00	0.33
	O	18	-50.35	577.77	0.39	8.567E+00	0.25
	O	19	-20.11	486.70	0.36	8.886E+00	0.34
	O	20	-47.90	381.06	0.43	7.378E+00	0.45
	O	21	4.68	295.77	0.71	7.570E+00	0.66
	O	22	164.88	97.90	0.82	-8.570E+00	0.50
	O	23	-76.39	606.41	0.44	8.859E+00	0.21
	O	24	-48.77	586.18	0.39	8.499E+00	0.23
	O	25	-21.18	499.97	0.29	8.316E+00	0.43
	O	26	-69.86	377.35	0.44	8.538E+00	0.29
	O	27	-0.76	322.11	0.66	7.826E+00	0.59
	O	28	259.54	45.75	0.43	8.039E+00	0.86
	O	29	254.17	-37.41	0.60	7.687E+00	0.83
	O	30	261.20	-37.26	0.80	7.899E+00	0.79

=====

GIPAW coordinates and calculated NMR parameters for 2 (structure 4)

xx

x	Element	Atom	Fractional coordinates of atoms x			
x		Number	u	v	w	x
x-----x						
x H		1	0.975575	-0.040800	0.174562	x
x H		2	0.909889	0.072166	0.197714	x
x H		3	0.968433	0.218274	0.175348	x
x H		4	0.861524	0.220079	0.110370	x
x H		5	0.973162	0.283737	0.086328	x
x H		6	0.992478	0.017604	0.087392	x
x H		7	0.941915	-0.207632	0.013451	x
x H		8	0.904227	-0.226573	-0.084235	x
x H		9	0.862434	0.421995	-0.089534	x
x H		10	0.900137	0.441346	0.007642	x
x H		11	0.840551	0.204379	-0.164271	x
x H		12	0.795505	0.181408	0.033304	x
x H		13	0.677021	0.054750	-0.028818	x
x H		14	0.758357	-0.037112	-0.039207	x
x H		15	0.699394	-0.362230	-0.028828	x
x H		16	0.658340	-0.256690	0.020045	x
x H		17	0.752325	-0.401186	0.079675	x
x H		18	0.806740	-0.406924	0.032572	x
x H		19	0.734649	-0.054621	0.132851	x
x H		20	0.637712	0.296885	0.131739	x
x H		21	0.641984	-0.104119	0.195072	x
x H		22	0.584157	0.102924	0.195123	x
x H		23	0.625902	-0.356280	0.127398	x
x H		24	0.546742	-0.525049	0.053213	x
x H		25	0.438669	-0.345179	0.008738	x
x H		26	0.412358	0.001933	0.038265	x
x H		27	0.492635	0.173756	0.111950	x
x H		28	0.764715	-0.005239	0.220374	x
x H		29	0.792386	0.366777	0.288435	x
x H		30	0.783194	-0.075871	0.328256	x
x H		31	0.805932	0.146392	0.367429	x
x H		32	0.665430	-0.174495	0.301748	x
x H		33	0.540791	-0.107651	0.298058	x
x H		34	0.502215	0.235419	0.325548	x
x H		35	0.589022	0.505856	0.356716	x
x H		36	0.714034	0.439626	0.359400	x
x H		37	0.032026	-0.218501	0.310877	x
x H		38	0.070206	0.012037	0.301665	x
x H		39	0.112414	-0.203594	0.296044	x
x H		40	0.153167	0.005891	0.379081	x
x H		41	0.033806	0.100224	0.386398	x
x H		42	0.012685	-0.160715	0.393777	x
x H		43	0.055297	-0.347664	0.477483	x
x H		44	0.079553	-0.314294	0.574499	x
x H		45	0.120070	0.331064	0.560624	x
x H		46	0.092415	0.297922	0.462670	x
x H		47	0.103589	-0.103289	0.644559	x

x H	48	0.204344	-0.036897	0.464124	x
x H	49	0.318179	-0.167154	0.531476	x
x H	50	0.235446	-0.267086	0.536052	x
x H	51	0.300169	-0.584411	0.526313	x
x H	52	0.343011	-0.466527	0.480095	x
x H	53	0.251247	-0.617876	0.417377	x
x H	54	0.194414	-0.621554	0.462792	x
x H	55	0.270412	-0.247140	0.368221	x
x H	56	0.380041	0.069617	0.379330	x
x H	57	0.354024	-0.305177	0.305452	x
x H	58	0.419163	-0.117951	0.304726	x
x H	59	0.369126	-0.572232	0.370320	x
x H	60	0.444408	-0.753144	0.444515	x
x H	61	0.554774	-0.591592	0.490598	x
x H	62	0.587181	-0.246419	0.463401	x
x H	63	0.511101	-0.061994	0.390391	x
x H	64	0.320971	-0.046086	0.249298	x
x H	65	0.236176	0.334876	0.235173	x
x H	66	0.298451	0.088584	0.154450	x
x H	67	0.243075	0.303924	0.139797	x
x H	68	0.419792	0.150158	0.215630	x
x H	69	0.519786	0.387610	0.231703	x
x H	70	0.504979	0.751728	0.202703	x
x H	71	0.389192	0.876543	0.157574	x
x H	72	0.287702	0.642901	0.144552	x
x H	73	0.818560	-0.301131	0.182631	x
x H	74	0.746900	-0.370268	0.196935	x
x H	75	0.938276	-0.354642	0.324827	x
x H	76	0.931343	-0.193178	0.278619	x
x H	77	0.079331	-0.070110	0.199031	x
x H	78	0.054499	-0.297251	0.181808	x
x H	79	-0.975575	0.459200	-0.174562	x
x H	80	-0.909889	0.572166	-0.197714	x
x H	81	-0.968433	0.718274	-0.175348	x
x H	82	-0.861524	0.720079	-0.110370	x
x H	83	-0.973162	0.783737	-0.086328	x
x H	84	-0.992478	0.517604	-0.087392	x
x H	85	-0.941915	0.292368	-0.013451	x
x H	86	-0.904227	0.273427	0.084235	x
x H	87	-0.862434	0.921995	0.089534	x
x H	88	-0.900137	0.941346	-0.007642	x
x H	89	-0.840551	0.704379	0.164271	x
x H	90	-0.795505	0.681408	-0.033304	x
x H	91	-0.677021	0.554750	0.028818	x
x H	92	-0.758357	0.462888	0.039207	x
x H	93	-0.699394	0.137770	0.028828	x
x H	94	-0.658340	0.243310	-0.020045	x
x H	95	-0.752325	0.098814	-0.079675	x
x H	96	-0.806740	0.093076	-0.032572	x
x H	97	-0.734649	0.445379	-0.132851	x
x H	98	-0.637712	0.796885	-0.131739	x
x H	99	-0.641984	0.395881	-0.195072	x
x H	100	-0.584157	0.602924	-0.195123	x

x H	101	-0.625902	0.143720	-0.127398	x
x H	102	-0.546742	-0.025049	-0.053213	x
x H	103	-0.438669	0.154821	-0.008738	x
x H	104	-0.412358	0.501933	-0.038265	x
x H	105	-0.492635	0.673756	-0.111950	x
x H	106	-0.764715	0.494761	-0.220374	x
x H	107	-0.792386	0.866777	-0.288435	x
x H	108	-0.783194	0.424129	-0.328256	x
x H	109	-0.805932	0.646392	-0.367429	x
x H	110	-0.665430	0.325505	-0.301748	x
x H	111	-0.540791	0.392349	-0.298058	x
x H	112	-0.502215	0.735419	-0.325548	x
x H	113	-0.589022	1.005856	-0.356716	x
x H	114	-0.714034	0.939626	-0.359400	x
x H	115	-0.032026	0.281499	-0.310877	x
x H	116	-0.070206	0.512037	-0.301665	x
x H	117	-0.112414	0.296406	-0.296044	x
x H	118	-0.153167	0.505891	-0.379081	x
x H	119	-0.033806	0.600224	-0.386398	x
x H	120	-0.012685	0.339285	-0.393777	x
x H	121	-0.055297	0.152336	-0.477483	x
x H	122	-0.079553	0.185706	-0.574499	x
x H	123	-0.120070	0.831064	-0.560624	x
x H	124	-0.092415	0.797922	-0.462670	x
x H	125	-0.103589	0.396711	-0.644559	x
x H	126	-0.204344	0.463103	-0.464124	x
x H	127	-0.318179	0.332846	-0.531476	x
x H	128	-0.235446	0.232914	-0.536052	x
x H	129	-0.300169	-0.084411	-0.526313	x
x H	130	-0.343011	0.033473	-0.480095	x
x H	131	-0.251247	-0.117876	-0.417377	x
x H	132	-0.194414	-0.121554	-0.462792	x
x H	133	-0.270412	0.252860	-0.368221	x
x H	134	-0.380041	0.569617	-0.379330	x
x H	135	-0.354024	0.194823	-0.305452	x
x H	136	-0.419163	0.382049	-0.304726	x
x H	137	-0.369126	-0.072232	-0.370320	x
x H	138	-0.444408	-0.253144	-0.444515	x
x H	139	-0.554774	-0.091592	-0.490598	x
x H	140	-0.587181	0.253581	-0.463401	x
x H	141	-0.511101	0.438006	-0.390391	x
x H	142	-0.320971	0.453914	-0.249298	x
x H	143	-0.236176	0.834876	-0.235173	x
x H	144	-0.298451	0.588584	-0.154450	x
x H	145	-0.243075	0.803924	-0.139797	x
x H	146	-0.419792	0.650158	-0.215630	x
x H	147	-0.519786	0.887610	-0.231703	x
x H	148	-0.504979	1.251728	-0.202703	x
x H	149	-0.389192	1.376543	-0.157574	x
x H	150	-0.287702	1.142901	-0.144552	x
x H	151	-0.818560	0.198869	-0.182631	x
x H	152	-0.746900	0.129732	-0.196935	x
x H	153	-0.938276	0.145358	-0.324827	x

x H	154	-0.931343	0.306822	-0.278619	x
x H	155	-0.079331	0.429890	-0.199031	x
x H	156	-0.054499	0.202749	-0.181808	x
x C	1	0.898411	0.092166	0.112959	x
x C	2	0.950463	0.130701	0.076354	x
x C	3	0.923331	0.118132	0.017824	x
x C	4	0.923752	-0.069189	-0.008917	x
x C	5	0.903476	-0.081115	-0.063459	x
x C	6	0.882699	0.096270	-0.093412	x
x C	7	0.879702	0.283890	-0.066841	x
x C	8	0.900311	0.293064	-0.012160	x
x C	9	0.861284	-0.115104	0.101542	x
x C	10	0.760783	0.057996	0.040873	x
x C	11	0.722786	-0.035575	-0.011379	x
x C	12	0.706219	-0.254267	0.004308	x
x C	13	0.767980	-0.314860	0.047594	x
x C	14	0.710145	0.157202	0.071975	x
x C	15	0.665897	0.169729	0.154147	x
x C	16	0.613518	0.017040	0.170152	x
x C	17	0.565097	-0.079749	0.124386	x
x C	18	0.579415	-0.276323	0.107277	x
x C	19	0.534384	-0.372388	0.066006	x
x C	20	0.474068	-0.272193	0.041269	x
x C	21	0.459410	-0.075803	0.057863	x
x C	22	0.504702	0.020513	0.098997	x
x C	23	0.709742	0.264920	0.204264	x
x C	24	0.797902	0.199957	0.284205	x
x C	25	0.773319	0.090108	0.330705	x
x C	26	0.698090	0.127942	0.330784	x
x C	27	0.648725	-0.024656	0.313685	x
x C	28	0.578471	0.013420	0.311485	x
x C	29	0.556930	0.204258	0.326826	x
x C	30	0.605841	0.357402	0.344269	x
x C	31	0.675867	0.319321	0.346044	x
x C	32	0.874365	0.143509	0.287680	x
x C	33	0.112931	-0.113164	0.375315	x
x C	34	0.054491	-0.046753	0.403774	x
x C	35	0.074120	-0.027813	0.462906	x
x C	36	0.071047	-0.198704	0.495307	x
x C	37	0.084658	-0.181153	0.549976	x
x C	38	0.102155	0.010340	0.573983	x
x C	39	0.106782	0.181988	0.542091	x
x C	40	0.091996	0.162151	0.487382	x
x C	41	0.143205	-0.325559	0.393199	x
x C	42	0.240694	-0.158506	0.458174	x
x C	43	0.274232	-0.257875	0.510859	x
x C	44	0.293909	-0.472038	0.494171	x
x C	45	0.234376	-0.531123	0.448963	x
x C	46	0.295454	-0.056084	0.431880	x
x C	47	0.344946	-0.029680	0.351717	x
x C	48	0.388179	-0.194003	0.330235	x
x C	49	0.435429	-0.306687	0.374270	x
x C	50	0.417532	-0.501456	0.390226	x

x C	51	0.460087	-0.603702	0.431886	x
x C	52	0.521456	-0.512881	0.457957	x
x C	53	0.539532	-0.317957	0.442664	x
x C	54	0.496578	-0.215121	0.401449	x
x C	55	0.301368	0.119597	0.311849	x
x C	56	0.252815	0.192863	0.218644	x
x C	57	0.284560	0.237280	0.169864	x
x C	58	0.346099	0.379789	0.179443	x
x C	59	0.412222	0.310750	0.203771	x
x C	60	0.468859	0.443904	0.212620	x
x C	61	0.460527	0.648692	0.196790	x
x C	62	0.395328	0.718664	0.171826	x
x C	63	0.338583	0.585828	0.163582	x
x C	64	0.190443	0.046867	0.202892	x
x C	65	-0.898411	0.592166	-0.112959	x
x C	66	-0.950463	0.630701	-0.076354	x
x C	67	-0.923331	0.618132	-0.017824	x
x C	68	-0.923752	0.430811	0.008917	x
x C	69	-0.903476	0.418885	0.063459	x
x C	70	-0.882699	0.596270	0.093412	x
x C	71	-0.879702	0.783890	0.066841	x
x C	72	-0.900311	0.793064	0.012160	x
x C	73	-0.861284	0.384896	-0.101542	x
x C	74	-0.760783	0.557996	-0.040873	x
x C	75	-0.722786	0.464425	0.011379	x
x C	76	-0.706219	0.245733	-0.004308	x
x C	77	-0.767980	0.185140	-0.047594	x
x C	78	-0.710145	0.657202	-0.071975	x
x C	79	-0.665897	0.669729	-0.154147	x
x C	80	-0.613518	0.517040	-0.170152	x
x C	81	-0.565097	0.420251	-0.124386	x
x C	82	-0.579415	0.223677	-0.107277	x
x C	83	-0.534384	0.127612	-0.066006	x
x C	84	-0.474068	0.227807	-0.041269	x
x C	85	-0.459410	0.424197	-0.057863	x
x C	86	-0.504702	0.520513	-0.098997	x
x C	87	-0.709742	0.764920	-0.204264	x
x C	88	-0.797902	0.699957	-0.284205	x
x C	89	-0.773319	0.590108	-0.330705	x
x C	90	-0.698090	0.627942	-0.330784	x
x C	91	-0.648725	0.475344	-0.313685	x
x C	92	-0.578471	0.513420	-0.311485	x
x C	93	-0.556930	0.704258	-0.326826	x
x C	94	-0.605841	0.857402	-0.344269	x
x C	95	-0.675867	0.819321	-0.346044	x
x C	96	-0.874365	0.643509	-0.287680	x
x C	97	-0.112931	0.386836	-0.375315	x
x C	98	-0.054491	0.453247	-0.403774	x
x C	99	-0.074120	0.472187	-0.462906	x
x C	100	-0.071047	0.301296	-0.495307	x
x C	101	-0.084658	0.318847	-0.549976	x
x C	102	-0.102155	0.510340	-0.573983	x
x C	103	-0.106782	0.681988	-0.542091	x

x C	104	-0.091996	0.662151	-0.487382	x
x C	105	-0.143205	0.174441	-0.393199	x
x C	106	-0.240694	0.341494	-0.458174	x
x C	107	-0.274232	0.242125	-0.510859	x
x C	108	-0.293909	0.027962	-0.494171	x
x C	109	-0.234376	-0.031123	-0.448963	x
x C	110	-0.295454	0.443916	-0.431880	x
x C	111	-0.344946	0.470320	-0.351717	x
x C	112	-0.388179	0.305997	-0.330235	x
x C	113	-0.435429	0.193313	-0.374270	x
x C	114	-0.417532	-0.001456	-0.390226	x
x C	115	-0.460087	-0.103702	-0.431886	x
x C	116	-0.521456	-0.012881	-0.457957	x
x C	117	-0.539532	0.182043	-0.442664	x
x C	118	-0.496578	0.284879	-0.401449	x
x C	119	-0.301368	0.619597	-0.311849	x
x C	120	-0.252815	0.692863	-0.218644	x
x C	121	-0.284560	0.737280	-0.169864	x
x C	122	-0.346099	0.879789	-0.179443	x
x C	123	-0.412222	0.810750	-0.203771	x
x C	124	-0.468859	0.943904	-0.212620	x
x C	125	-0.460527	1.148692	-0.196790	x
x C	126	-0.395328	1.218664	-0.171826	x
x C	127	-0.338583	1.085828	-0.163582	x
x C	128	-0.190443	0.546867	-0.202892	x
x N	1	0.939392	0.086550	0.167809	x
x N	2	0.800185	-0.117281	0.067109	x
x N	3	0.708562	0.078622	0.120232	x
x N	4	0.756368	0.140374	0.233748	x
x N	5	0.081062	-0.131429	0.317759	x
x N	6	0.203946	-0.331547	0.428560	x
x N	7	0.299111	-0.122568	0.382818	x
x N	8	0.302041	0.089539	0.260168	x
x N	9	-0.939392	0.586550	-0.167809	x
x N	10	-0.800185	0.382719	-0.067109	x
x N	11	-0.708562	0.578622	-0.120232	x
x N	12	-0.756368	0.640374	-0.233748	x
x N	13	-0.081062	0.368571	-0.317759	x
x N	14	-0.203946	0.168453	-0.428560	x
x N	15	-0.299111	0.377432	-0.382818	x
x N	16	-0.302041	0.589539	-0.260168	x
x O	1	0.868189	0.078787	-0.146370	x
x O	2	0.889205	-0.274240	0.122534	x
x O	3	0.675450	0.305952	0.052267	x
x O	4	0.699626	0.446599	0.216525	x
x O	5	0.918154	0.212999	0.325723	x
x O	6	0.888165	0.017536	0.253425	x
x O	7	0.113773	0.033332	0.627243	x
x O	8	0.111909	-0.482250	0.374514	x
x O	9	0.332064	0.081585	0.455344	x
x O	10	0.268594	0.259331	0.328255	x
x O	11	0.130143	0.112834	0.202799	x
x O	12	0.206734	-0.134710	0.191767	x

x O	13	0.772158	-0.253349	0.184346	x
x O	14	0.959323	-0.312861	0.295026	x
x O	15	0.041534	-0.177551	0.200597	x
x O	16	-0.868189	0.578787	0.146370	x
x O	17	-0.889205	0.225760	-0.122534	x
x O	18	-0.675450	0.805952	-0.052267	x
x O	19	-0.699626	0.946599	-0.216525	x
x O	20	-0.918154	0.712999	-0.325723	x
x O	21	-0.888165	0.517536	-0.253425	x
x O	22	-0.113773	0.533332	-0.627243	x
x O	23	-0.111909	0.017750	-0.374514	x
x O	24	-0.332064	0.581585	-0.455344	x
x O	25	-0.268594	0.759331	-0.328255	x
x O	26	-0.130143	0.612834	-0.202799	x
x O	27	-0.206734	0.365290	-0.191767	x
x O	28	-0.772158	0.246651	-0.184346	x
x O	29	-0.959323	0.187139	-0.295026	x
x O	30	-0.041534	0.322449	-0.200597	x

xx

=====

### Chemical Shielding and Electric Field Gradient Tensors |

Nucleus		Shielding tensor		EFG Tensor		Species	
		Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
H	1	16.60	31.31	0.05	1.037E-01	0.04	
H	2	19.86	31.18	0.11	1.445E-01	0.05	
H	3	27.41	10.51	0.39	2.267E-01	0.05	
H	4	26.24	5.30	0.50	1.757E-01	0.06	
H	5	27.28	8.23	0.50	1.765E-01	0.04	
H	6	27.54	-6.61	0.79	1.749E-01	0.04	
H	7	24.32	5.87	0.33	1.893E-01	0.07	
H	8	23.23	-2.61	0.56	1.927E-01	0.06	
H	9	23.06	-4.43	0.90	1.919E-01	0.08	
H	10	23.45	2.48	0.87	1.898E-01	0.06	
H	11	15.04	31.01	0.05	1.233E-01	0.16	
H	12	26.80	7.39	0.74	1.783E-01	0.05	
H	13	29.48	9.52	0.30	1.827E-01	0.00	
H	14	30.23	10.71	0.69	1.808E-01	0.02	
H	15	29.35	7.83	0.38	1.864E-01	0.01	
H	16	29.66	12.05	0.17	1.791E-01	0.01	
H	17	27.00	9.44	0.56	1.808E-01	0.03	
H	18	27.31	9.76	0.54	1.809E-01	0.06	
H	19	21.09	-12.90	0.95	2.062E-01	0.18	
H	20	25.86	4.65	0.89	1.749E-01	0.02	
H	21	27.92	4.14	0.52	1.794E-01	0.04	
H	22	28.25	6.97	0.94	1.796E-01	0.04	
H	23	23.44	3.76	0.38	1.887E-01	0.08	
H	24	24.03	3.78	0.64	1.896E-01	0.05	
H	25	25.54	-4.57	0.17	1.910E-01	0.04	
H	26	24.03	3.52	0.60	1.928E-01	0.05	

H	27	24.70	-2.75	0.50	1.878E-01	0.07
H	28	19.92	14.21	0.71	1.932E-01	0.21
H	29	24.94	-6.04	0.34	1.749E-01	0.04
H	30	27.57	5.17	0.67	1.775E-01	0.03
H	31	26.62	8.17	0.57	1.814E-01	0.02
H	32	23.40	3.21	0.56	1.880E-01	0.07
H	33	23.46	2.97	0.47	1.911E-01	0.06
H	34	24.36	4.13	0.47	1.912E-01	0.06
H	35	25.05	7.86	0.23	1.892E-01	0.06
H	36	23.54	4.37	0.44	1.892E-01	0.07
H	37	14.74	34.00	0.14	7.772E-02	0.08
H	38	26.43	11.08	0.35	2.251E-01	0.04
H	39	26.29	13.02	0.45	2.271E-01	0.04
H	40	26.07	6.26	0.41	1.725E-01	0.07
H	41	26.41	7.27	0.83	1.741E-01	0.06
H	42	27.28	-6.57	0.93	1.782E-01	0.04
H	43	24.64	5.78	0.31	1.892E-01	0.07
H	44	23.20	4.15	0.73	1.906E-01	0.07
H	45	23.74	-1.92	0.42	1.932E-01	0.07
H	46	23.14	-2.76	0.47	1.870E-01	0.06
H	47	15.45	28.47	0.19	1.311E-01	0.20
H	48	27.30	10.56	0.47	1.758E-01	0.05
H	49	29.72	9.08	0.41	1.833E-01	0.00
H	50	30.38	9.99	0.90	1.818E-01	0.02
H	51	29.99	6.82	0.56	1.863E-01	0.01
H	52	30.29	12.47	0.21	1.794E-01	0.01
H	53	26.63	11.20	0.25	1.732E-01	0.05
H	54	27.06	11.19	0.54	1.811E-01	0.06
H	55	24.87	-7.99	0.68	2.457E-01	0.17
H	56	25.82	-4.18	0.97	1.722E-01	0.02
H	57	29.21	7.52	0.57	1.759E-01	0.02
H	58	27.81	5.73	0.61	1.809E-01	0.03
H	59	23.70	4.78	0.26	1.826E-01	0.07
H	60	23.35	3.28	0.67	1.880E-01	0.06
H	61	25.46	-4.79	0.42	1.916E-01	0.04
H	62	23.95	3.48	0.88	1.912E-01	0.04
H	63	23.95	-3.27	0.94	1.894E-01	0.07
H	64	24.15	-7.95	0.55	2.412E-01	0.17
H	65	25.59	-4.26	0.29	1.783E-01	0.03
H	66	27.19	5.52	0.72	1.797E-01	0.01
H	67	27.35	7.51	0.72	1.800E-01	0.04
H	68	23.40	4.56	0.64	1.922E-01	0.07
H	69	24.21	4.92	0.36	1.901E-01	0.06
H	70	24.52	5.08	0.35	1.936E-01	0.06
H	71	23.80	4.16	0.69	1.925E-01	0.06
H	72	23.12	-3.25	0.90	1.902E-01	0.08
H	73	28.23	15.47	0.28	2.847E-01	0.12
H	74	23.41	33.05	0.06	2.102E-01	0.16
H	75	25.53	24.32	0.06	2.541E-01	0.08
H	76	22.61	30.30	0.03	2.077E-01	0.13
H	77	18.41	33.40	0.08	1.437E-01	0.17
H	78	26.35	19.91	0.21	2.727E-01	0.08
H	79	16.60	31.31	0.05	1.037E-01	0.04

H	80	19.86	31.18	0.11	1.445E-01	0.05
H	81	27.41	10.51	0.39	2.267E-01	0.05
H	82	26.24	5.30	0.50	1.757E-01	0.06
H	83	27.28	8.23	0.50	1.765E-01	0.04
H	84	27.54	-6.61	0.79	1.749E-01	0.04
H	85	24.32	5.87	0.33	1.893E-01	0.07
H	86	23.23	-2.61	0.56	1.927E-01	0.06
H	87	23.06	-4.43	0.90	1.919E-01	0.08
H	88	23.45	2.48	0.87	1.898E-01	0.06
H	89	15.04	31.01	0.05	1.233E-01	0.16
H	90	26.80	7.39	0.74	1.783E-01	0.05
H	91	29.48	9.52	0.30	1.827E-01	0.00
H	92	30.23	10.71	0.69	1.808E-01	0.02
H	93	29.35	7.83	0.38	1.864E-01	0.01
H	94	29.66	12.05	0.17	1.791E-01	0.01
H	95	27.00	9.44	0.56	1.808E-01	0.03
H	96	27.31	9.76	0.54	1.809E-01	0.06
H	97	21.09	-12.90	0.95	2.062E-01	0.18
H	98	25.86	4.65	0.89	1.749E-01	0.02
H	99	27.92	4.14	0.52	1.794E-01	0.04
H	100	28.25	6.97	0.94	1.796E-01	0.04
H	101	23.44	3.76	0.38	1.887E-01	0.08
H	102	24.03	3.78	0.64	1.896E-01	0.05
H	103	25.54	-4.57	0.17	1.910E-01	0.04
H	104	24.03	3.52	0.60	1.928E-01	0.05
H	105	24.70	-2.75	0.50	1.878E-01	0.07
H	106	19.92	14.21	0.71	1.932E-01	0.21
H	107	24.94	-6.04	0.34	1.749E-01	0.04
H	108	27.57	5.17	0.67	1.775E-01	0.03
H	109	26.62	8.17	0.57	1.814E-01	0.02
H	110	23.40	3.21	0.56	1.880E-01	0.07
H	111	23.46	2.97	0.47	1.911E-01	0.06
H	112	24.36	4.13	0.47	1.912E-01	0.06
H	113	25.05	7.86	0.23	1.892E-01	0.06
H	114	23.54	4.37	0.44	1.892E-01	0.07
H	115	14.74	34.00	0.14	7.772E-02	0.08
H	116	26.43	11.08	0.35	2.251E-01	0.04
H	117	26.29	13.02	0.45	2.271E-01	0.04
H	118	26.07	6.26	0.41	1.725E-01	0.07
H	119	26.41	7.27	0.83	1.741E-01	0.06
H	120	27.28	-6.57	0.93	1.782E-01	0.04
H	121	24.64	5.78	0.31	1.892E-01	0.07
H	122	23.20	4.15	0.73	1.906E-01	0.07
H	123	23.74	-1.92	0.42	1.932E-01	0.07
H	124	23.14	-2.76	0.47	1.870E-01	0.06
H	125	15.45	28.47	0.19	1.311E-01	0.20
H	126	27.30	10.56	0.47	1.758E-01	0.05
H	127	29.72	9.08	0.41	1.833E-01	0.00
H	128	30.38	9.99	0.90	1.818E-01	0.02
H	129	29.99	6.82	0.56	1.863E-01	0.01
H	130	30.29	12.47	0.21	1.794E-01	0.01
H	131	26.63	11.20	0.25	1.732E-01	0.05
H	132	27.06	11.19	0.54	1.811E-01	0.06

H	133	24.87	-7.99	0.68	2.457E-01	0.17
H	134	25.82	-4.18	0.97	1.722E-01	0.02
H	135	29.21	7.52	0.57	1.759E-01	0.02
H	136	27.81	5.73	0.61	1.809E-01	0.03
H	137	23.70	4.78	0.26	1.826E-01	0.07
H	138	23.35	3.28	0.67	1.880E-01	0.06
H	139	25.46	-4.79	0.42	1.916E-01	0.04
H	140	23.95	3.48	0.88	1.912E-01	0.04
H	141	23.95	-3.27	0.94	1.894E-01	0.07
H	142	24.15	-7.95	0.55	2.412E-01	0.17
H	143	25.59	-4.26	0.29	1.783E-01	0.03
H	144	27.19	5.52	0.72	1.797E-01	0.01
H	145	27.35	7.51	0.72	1.800E-01	0.04
H	146	23.40	4.56	0.64	1.922E-01	0.07
H	147	24.21	4.92	0.36	1.901E-01	0.06
H	148	24.52	5.08	0.35	1.936E-01	0.06
H	149	23.80	4.16	0.69	1.925E-01	0.06
H	150	23.12	-3.25	0.90	1.902E-01	0.08
H	151	28.23	15.47	0.28	2.847E-01	0.12
H	152	23.41	33.05	0.06	2.102E-01	0.16
H	153	25.53	24.32	0.06	2.541E-01	0.08
H	154	22.61	30.30	0.03	2.077E-01	0.13
H	155	18.41	33.40	0.08	1.437E-01	0.17
H	156	26.35	19.91	0.21	2.727E-01	0.08
C	1	118.46	25.46	0.89	2.677E+00	0.23
C	2	130.45	30.06	0.87	1.067E+00	0.62
C	3	49.84	173.55	0.67	1.743E+00	0.72
C	4	37.09	173.87	0.78	2.747E+00	0.20
C	5	53.03	147.84	0.72	2.093E+00	0.28
C	6	8.25	152.09	0.62	-2.975E+00	0.47
C	7	55.50	147.13	0.72	1.988E+00	0.23
C	8	38.52	169.58	0.82	2.633E+00	0.24
C	9	4.52	-115.74	0.94	2.704E+00	0.35
C	10	106.84	37.76	0.71	2.566E+00	0.33
C	11	143.54	-37.02	0.49	1.186E+00	0.64
C	12	151.09	-33.18	0.13	9.369E-01	0.76
C	13	124.01	49.03	0.72	2.939E+00	0.20
C	14	3.13	-120.56	0.81	3.111E+00	0.42
C	15	113.69	43.17	0.19	2.192E+00	0.76
C	16	130.01	29.46	0.33	8.889E-01	0.60
C	17	34.54	196.12	0.54	2.493E+00	0.48
C	18	39.10	173.78	0.83	2.704E+00	0.22
C	19	39.26	195.89	0.64	3.033E+00	0.08
C	20	43.46	194.40	0.65	2.897E+00	0.12
C	21	39.35	196.02	0.67	2.925E+00	0.12
C	22	42.52	177.65	0.75	2.624E+00	0.21
C	23	-3.86	127.99	0.58	3.298E+00	0.34
C	24	114.79	-37.03	0.99	2.168E+00	0.56
C	25	128.57	28.92	0.55	9.248E-01	0.66
C	26	32.86	199.40	0.48	2.558E+00	0.42
C	27	39.33	168.01	0.89	2.627E+00	0.23
C	28	41.85	186.15	0.70	2.770E+00	0.19
C	29	41.49	188.85	0.66	2.761E+00	0.15

C	30	40.83	191.25	0.67	2.959E+00	0.07
C	31	40.58	181.06	0.75	2.625E+00	0.25
C	32	-10.31	110.75	0.64	3.594E+00	0.19
C	33	115.77	26.40	0.58	3.018E+00	0.23
C	34	134.38	28.07	0.62	1.169E+00	0.72
C	35	47.17	177.25	0.63	1.881E+00	0.64
C	36	37.50	176.52	0.75	2.777E+00	0.17
C	37	55.40	148.51	0.69	2.011E+00	0.27
C	38	9.97	146.73	0.70	-3.115E+00	0.24
C	39	56.54	147.06	0.70	1.992E+00	0.31
C	40	35.21	176.81	0.72	2.759E+00	0.13
C	41	4.93	-122.16	0.75	2.673E+00	0.42
C	42	108.31	35.60	0.92	2.525E+00	0.36
C	43	142.34	-35.60	0.55	1.169E+00	0.62
C	44	151.53	-32.37	0.21	8.843E-01	0.76
C	45	124.79	49.21	0.76	3.082E+00	0.23
C	46	2.67	-122.57	0.95	3.197E+00	0.47
C	47	116.01	48.47	0.40	2.256E+00	0.69
C	48	138.63	25.61	0.12	6.200E-01	0.79
C	49	34.74	195.51	0.54	2.449E+00	0.57
C	50	40.91	176.49	0.78	2.763E+00	0.15
C	51	38.01	196.25	0.64	3.035E+00	0.07
C	52	42.24	196.43	0.65	2.950E+00	0.11
C	53	39.52	196.77	0.65	2.993E+00	0.08
C	54	40.87	182.31	0.66	2.681E+00	0.17
C	55	0.40	-123.85	0.88	3.144E+00	0.38
C	56	113.88	34.53	0.35	2.419E+00	0.53
C	57	134.74	29.99	0.27	7.325E-01	1.00
C	58	31.75	197.92	0.48	2.586E+00	0.40
C	59	40.58	175.95	0.79	2.601E+00	0.25
C	60	42.32	189.96	0.69	2.883E+00	0.12
C	61	44.95	192.51	0.70	2.824E+00	0.15
C	62	42.52	186.61	0.74	2.799E+00	0.19
C	63	39.54	171.59	0.77	2.756E+00	0.15
C	64	-11.20	112.47	0.71	3.519E+00	0.19
C	65	118.46	25.46	0.89	2.677E+00	0.23
C	66	130.45	30.06	0.87	1.067E+00	0.62
C	67	49.84	173.55	0.67	1.743E+00	0.72
C	68	37.09	173.87	0.78	2.747E+00	0.20
C	69	53.03	147.84	0.72	2.093E+00	0.28
C	70	8.25	152.09	0.62	-2.975E+00	0.47
C	71	55.50	147.13	0.72	1.988E+00	0.23
C	72	38.52	169.58	0.82	2.633E+00	0.24
C	73	4.52	-115.74	0.94	2.704E+00	0.35
C	74	106.84	37.76	0.71	2.566E+00	0.33
C	75	143.54	-37.02	0.49	1.186E+00	0.64
C	76	151.09	-33.18	0.13	9.369E-01	0.76
C	77	124.01	49.03	0.72	2.939E+00	0.20
C	78	3.13	-120.56	0.81	3.111E+00	0.42
C	79	113.69	43.17	0.19	2.192E+00	0.76
C	80	130.01	29.46	0.33	8.889E-01	0.60
C	81	34.54	196.12	0.54	2.493E+00	0.48
C	82	39.10	173.78	0.83	2.704E+00	0.22

C	83	39.26	195.89	0.64	3.033E+00	0.08
C	84	43.46	194.40	0.65	2.897E+00	0.12
C	85	39.35	196.02	0.67	2.925E+00	0.12
C	86	42.52	177.65	0.75	2.624E+00	0.21
C	87	-3.86	127.99	0.58	3.298E+00	0.34
C	88	114.79	-37.03	0.99	2.168E+00	0.56
C	89	128.57	28.92	0.55	9.248E-01	0.66
C	90	32.86	199.40	0.48	2.558E+00	0.42
C	91	39.33	168.01	0.89	2.627E+00	0.23
C	92	41.85	186.15	0.70	2.770E+00	0.19
C	93	41.49	188.85	0.66	2.761E+00	0.15
C	94	40.83	191.25	0.67	2.959E+00	0.07
C	95	40.58	181.06	0.75	2.625E+00	0.25
C	96	-10.31	110.75	0.64	3.594E+00	0.19
C	97	115.77	26.40	0.58	3.018E+00	0.23
C	98	134.38	28.07	0.62	1.169E+00	0.72
C	99	47.17	177.25	0.63	1.881E+00	0.64
C	100	37.50	176.52	0.75	2.777E+00	0.17
C	101	55.40	148.51	0.69	2.011E+00	0.27
C	102	9.97	146.73	0.70	-3.115E+00	0.24
C	103	56.54	147.06	0.70	1.992E+00	0.31
C	104	35.21	176.81	0.72	2.759E+00	0.13
C	105	4.93	-122.16	0.75	2.673E+00	0.42
C	106	108.31	35.60	0.92	2.525E+00	0.36
C	107	142.34	-35.60	0.55	1.169E+00	0.62
C	108	151.53	-32.37	0.21	8.843E-01	0.76
C	109	124.79	49.21	0.76	3.082E+00	0.23
C	110	2.67	-122.57	0.95	3.197E+00	0.47
C	111	116.01	48.47	0.40	2.256E+00	0.69
C	112	138.63	25.61	0.12	6.200E-01	0.79
C	113	34.74	195.51	0.54	2.449E+00	0.57
C	114	40.91	176.49	0.78	2.763E+00	0.15
C	115	38.01	196.25	0.64	3.035E+00	0.07
C	116	42.24	196.43	0.65	2.950E+00	0.11
C	117	39.52	196.77	0.65	2.993E+00	0.08
C	118	40.87	182.31	0.66	2.681E+00	0.17
C	119	0.40	-123.85	0.88	3.144E+00	0.38
C	120	113.88	34.53	0.35	2.419E+00	0.53
C	121	134.74	29.99	0.27	7.325E-01	1.00
C	122	31.75	197.92	0.48	2.586E+00	0.40
C	123	40.58	175.95	0.79	2.601E+00	0.25
C	124	42.32	189.96	0.69	2.883E+00	0.12
C	125	44.95	192.51	0.70	2.824E+00	0.15
C	126	42.52	186.61	0.74	2.799E+00	0.19
C	127	39.54	171.59	0.77	2.756E+00	0.15
C	128	-11.20	112.47	0.71	3.519E+00	0.19
N	1	183.00	22.52	0.74	-1.683E+00	0.99
N	2	76.82	-162.25	0.57	-3.728E+00	0.12
N	3	101.63	-175.31	0.03	-3.398E+00	0.45
N	4	93.93	-163.66	0.14	-3.142E+00	0.47
N	5	183.33	27.50	0.91	-1.773E+00	0.48
N	6	79.81	-158.87	0.65	-3.800E+00	0.13
N	7	104.55	-166.69	0.20	-3.914E+00	0.22

	N	8	95.39	-161.96	0.23	-3.536E+00	0.21
	N	9	183.00	22.52	0.74	-1.683E+00	0.99
	N	10	76.82	-162.25	0.57	-3.728E+00	0.12
	N	11	101.63	-175.31	0.03	-3.398E+00	0.45
	N	12	93.93	-163.66	0.14	-3.142E+00	0.47
	N	13	183.33	27.50	0.91	-1.773E+00	0.48
	N	14	79.81	-158.87	0.65	-3.800E+00	0.13
	N	15	104.55	-166.69	0.20	-3.914E+00	0.22
	N	16	95.39	-161.96	0.23	-3.536E+00	0.21
	O	1	143.24	149.21	0.15	-8.569E+00	0.47
	O	2	-60.50	581.02	0.48	8.994E+00	0.25
	O	3	-52.99	578.61	0.41	8.490E+00	0.24
	O	4	-21.66	489.48	0.38	9.108E+00	0.34
	O	5	-47.37	379.40	0.42	7.256E+00	0.48
	O	6	-3.15	331.75	0.67	8.372E+00	0.49
	O	7	163.47	102.92	0.79	-8.537E+00	0.51
	O	8	-75.83	604.37	0.47	8.973E+00	0.19
	O	9	-54.91	595.26	0.40	8.523E+00	0.22
	O	10	-56.60	582.73	0.35	8.806E+00	0.22
	O	11	-35.05	335.09	0.48	7.504E+00	0.48
	O	12	-5.95	324.81	0.52	7.080E+00	0.68
	O	13	265.48	34.00	0.78	8.557E+00	0.81
	O	14	250.83	-35.97	0.59	7.506E+00	0.85
	O	15	245.66	-43.42	0.47	-7.080E+00	0.95
	O	16	143.24	149.21	0.15	-8.569E+00	0.47
	O	17	-60.50	581.02	0.48	8.994E+00	0.25
	O	18	-52.99	578.61	0.41	8.490E+00	0.24
	O	19	-21.66	489.48	0.38	9.108E+00	0.34
	O	20	-47.37	379.40	0.42	7.256E+00	0.48
	O	21	-3.15	331.75	0.67	8.372E+00	0.49
	O	22	163.47	102.92	0.79	-8.537E+00	0.51
	O	23	-75.83	604.37	0.47	8.973E+00	0.19
	O	24	-54.91	595.26	0.40	8.523E+00	0.22
	O	25	-56.60	582.73	0.35	8.806E+00	0.22
	O	26	-35.05	335.09	0.48	7.504E+00	0.48
	O	27	-5.95	324.81	0.52	7.080E+00	0.68
	O	28	265.48	34.00	0.78	8.557E+00	0.81
	O	29	250.83	-35.97	0.59	7.506E+00	0.85
	O	30	245.66	-43.42	0.47	-7.080E+00	0.95

=====

GIPAW coordinates and calculated NMR parameters for 2 (structure 6)

xx

x	Element	Atom	Fractional coordinates of atoms x			
x		Number	u	v	w	x
x-----x						
x H		1	0.989980	-0.024351	0.169889	x
x H		2	0.923538	0.019422	0.199576	x
x H		3	0.971617	0.215281	0.186429	x
x H		4	0.865079	0.208472	0.119661	x
x H		5	0.965184	0.331797	0.089095	x
x H		6	1.001735	0.082457	0.091110	x
x H		7	0.944934	-0.186174	0.023811	x
x H		8	0.906915	-0.235370	-0.072708	x
x H		9	0.868339	0.412717	-0.091984	x
x H		10	0.905705	0.461504	0.004595	x
x H		11	0.854327	0.176582	-0.161863	x
x H		12	0.801322	0.171238	0.036239	x
x H		13	0.680306	0.038340	-0.021498	x
x H		14	0.760448	-0.048737	-0.035575	x
x H		15	0.703623	-0.376886	-0.022346	x
x H		16	0.669256	-0.273591	0.030231	x
x H		17	0.770451	-0.423950	0.082218	x
x H		18	0.818186	-0.404201	0.030937	x
x H		19	0.752961	-0.053027	0.139711	x
x H		20	0.653094	0.289611	0.140952	x
x H		21	0.660412	-0.116515	0.202691	x
x H		22	0.605100	0.092721	0.208282	x
x H		23	0.633736	-0.359483	0.132564	x
x H		24	0.551051	-0.497089	0.055564	x
x H		25	0.447313	-0.289927	0.014425	x
x H		26	0.428962	0.055120	0.050621	x
x H		27	0.512344	0.193391	0.127037	x
x H		28	0.780477	-0.013956	0.226337	x
x H		29	0.816306	0.358871	0.293468	x
x H		30	0.806091	-0.085285	0.331779	x
x H		31	0.831054	0.133123	0.371906	x
x H		32	0.686982	-0.178848	0.311371	x
x H		33	0.563352	-0.100418	0.309356	x
x H		34	0.528337	0.252525	0.332716	x
x H		35	0.617869	0.520325	0.358982	x
x H		36	0.741705	0.441866	0.360367	x
x H		37	0.042211	-0.376662	0.327593	x
x H		38	0.024199	-0.135510	0.304236	x
x H		39	0.101698	-0.261690	0.300324	x
x H		40	0.133231	-0.036747	0.371694	x
x H		41	0.019618	0.046362	0.388201	x
x H		42	0.002071	-0.213423	0.401473	x
x H		43	0.041653	-0.367322	0.487060	x
x H		44	0.065586	-0.301628	0.582696	x
x H		45	0.126731	0.317439	0.555663	x
x H		46	0.096974	0.255704	0.458815	x
x H		47	0.088597	-0.054333	0.647954	x

x H	48	0.193592	-0.032097	0.459647	x
x H	49	0.305708	-0.121994	0.533163	x
x H	50	0.225120	-0.241292	0.536520	x
x H	51	0.302094	-0.540934	0.535843	x
x H	52	0.342974	-0.422706	0.488310	x
x H	53	0.258304	-0.610352	0.427108	x
x H	54	0.200138	-0.620100	0.471446	x
x H	55	0.250336	-0.190655	0.359938	x
x H	56	0.363900	0.116172	0.378821	x
x H	57	0.346481	-0.253737	0.303035	x
x H	58	0.409418	-0.056595	0.305215	x
x H	59	0.357924	-0.518594	0.369881	x
x H	60	0.434467	-0.705085	0.442468	x
x H	61	0.548084	-0.552443	0.485625	x
x H	62	0.581843	-0.209961	0.457427	x
x H	63	0.503846	-0.018800	0.386851	x
x H	64	0.299121	-0.038065	0.250937	x
x H	65	0.211723	0.335800	0.227664	x
x H	66	0.275979	0.056733	0.154668	x
x H	67	0.222582	0.273454	0.134587	x
x H	68	0.396810	0.117008	0.213317	x
x H	69	0.498784	0.346387	0.229256	x
x H	70	0.488181	0.707790	0.196732	x
x H	71	0.373817	0.838005	0.149983	x
x H	72	0.269995	0.613108	0.138116	x
x H	73	0.847451	-0.240274	0.226690	x
x H	74	0.777231	-0.369468	0.212261	x
x H	75	0.006001	0.323363	0.268115	x
x H	76	0.061849	0.308343	0.231605	x
x H	77	0.207381	-0.466602	0.300149	x
x H	78	0.190896	-0.281205	0.258533	x
x H	79	-0.989980	0.475649	-0.169889	x
x H	80	-0.923538	0.519422	-0.199576	x
x H	81	-0.971617	0.715281	-0.186429	x
x H	82	-0.865079	0.708472	-0.119661	x
x H	83	-0.965184	0.831797	-0.089095	x
x H	84	-1.001735	0.582457	-0.091110	x
x H	85	-0.944934	0.313826	-0.023811	x
x H	86	-0.906915	0.264630	0.072708	x
x H	87	-0.868339	0.912717	0.091984	x
x H	88	-0.905705	0.961504	-0.004595	x
x H	89	-0.854327	0.676582	0.161863	x
x H	90	-0.801322	0.671238	-0.036239	x
x H	91	-0.680306	0.538340	0.021498	x
x H	92	-0.760448	0.451263	0.035575	x
x H	93	-0.703623	0.123114	0.022346	x
x H	94	-0.669256	0.226409	-0.030231	x
x H	95	-0.770451	0.076050	-0.082218	x
x H	96	-0.818186	0.095799	-0.030937	x
x H	97	-0.752961	0.446973	-0.139711	x
x H	98	-0.653094	0.789611	-0.140952	x
x H	99	-0.660412	0.383485	-0.202691	x
x H	100	-0.605100	0.592721	-0.208282	x

x H	101	-0.633736	0.140517	-0.132564	x
x H	102	-0.551051	0.002911	-0.055564	x
x H	103	-0.447313	0.210073	-0.014425	x
x H	104	-0.428962	0.555120	-0.050621	x
x H	105	-0.512344	0.693391	-0.127037	x
x H	106	-0.780477	0.486044	-0.226337	x
x H	107	-0.816306	0.858871	-0.293468	x
x H	108	-0.806091	0.414715	-0.331779	x
x H	109	-0.831054	0.633123	-0.371906	x
x H	110	-0.686982	0.321152	-0.311371	x
x H	111	-0.563352	0.399582	-0.309356	x
x H	112	-0.528337	0.752525	-0.332716	x
x H	113	-0.617869	1.020325	-0.358982	x
x H	114	-0.741705	0.941866	-0.360367	x
x H	115	-0.042211	0.123338	-0.327593	x
x H	116	-0.024199	0.364490	-0.304236	x
x H	117	-0.101698	0.238310	-0.300324	x
x H	118	-0.133231	0.463253	-0.371694	x
x H	119	-0.019618	0.546362	-0.388201	x
x H	120	-0.002071	0.286577	-0.401473	x
x H	121	-0.041653	0.132678	-0.487060	x
x H	122	-0.065586	0.198372	-0.582696	x
x H	123	-0.126731	0.817439	-0.555663	x
x H	124	-0.096974	0.755704	-0.458815	x
x H	125	-0.088597	0.445667	-0.647954	x
x H	126	-0.193592	0.467903	-0.459647	x
x H	127	-0.305708	0.378006	-0.533163	x
x H	128	-0.225120	0.258708	-0.536520	x
x H	129	-0.302094	-0.040934	-0.535843	x
x H	130	-0.342974	0.077294	-0.488310	x
x H	131	-0.258304	-0.110352	-0.427108	x
x H	132	-0.200138	-0.120100	-0.471446	x
x H	133	-0.250336	0.309345	-0.359938	x
x H	134	-0.363900	0.616172	-0.378821	x
x H	135	-0.346481	0.246263	-0.303035	x
x H	136	-0.409418	0.443405	-0.305215	x
x H	137	-0.357924	-0.018594	-0.369881	x
x H	138	-0.434467	-0.205085	-0.442468	x
x H	139	-0.548084	-0.052443	-0.485625	x
x H	140	-0.581843	0.290039	-0.457427	x
x H	141	-0.503846	0.481200	-0.386851	x
x H	142	-0.299121	0.461935	-0.250937	x
x H	143	-0.211723	0.835800	-0.227664	x
x H	144	-0.275979	0.556733	-0.154668	x
x H	145	-0.222582	0.773454	-0.134587	x
x H	146	-0.396810	0.617008	-0.213317	x
x H	147	-0.498784	0.846387	-0.229256	x
x H	148	-0.488181	1.207790	-0.196732	x
x H	149	-0.373817	1.338005	-0.149983	x
x H	150	-0.269995	1.113108	-0.138116	x
x H	151	-0.847451	0.259726	-0.226690	x
x H	152	-0.777231	0.130532	-0.212261	x
x H	153	-0.006001	0.823363	-0.268115	x

x H	154	-0.061849	0.808343	-0.231605	x
x H	155	-0.207381	0.033398	-0.300149	x
x H	156	-0.190896	0.218795	-0.258533	x
x C	1	0.905198	0.094128	0.116938	x
x C	2	0.952967	0.169386	0.079930	x
x C	3	0.926632	0.141116	0.021594	x
x C	4	0.926783	-0.054513	-0.001233	x
x C	5	0.906186	-0.083306	-0.055197	x
x C	6	0.886127	0.084735	-0.088816	x
x C	7	0.884643	0.281205	-0.066404	x
x C	8	0.904986	0.307188	-0.012033	x
x C	9	0.873967	-0.118929	0.101241	x
x C	10	0.767860	0.046685	0.045276	x
x C	11	0.727422	-0.049324	-0.005945	x
x C	12	0.714023	-0.268912	0.010793	x
x C	13	0.780218	-0.325838	0.050023	x
x C	14	0.718782	0.144671	0.077708	x
x C	15	0.682407	0.163459	0.162997	x
x C	16	0.631258	0.010484	0.180576	x
x C	17	0.579129	-0.073714	0.134954	x
x C	18	0.588892	-0.268018	0.114288	x
x C	19	0.541971	-0.346020	0.071158	x
x C	20	0.484208	-0.230199	0.048163	x
x C	21	0.473870	-0.036357	0.068565	x
x C	22	0.520976	0.041477	0.111545	x
x C	23	0.729956	0.262514	0.210879	x
x C	24	0.821756	0.192532	0.288641	x
x C	25	0.797684	0.081059	0.335025	x
x C	26	0.722870	0.125835	0.336088	x
x C	27	0.671958	-0.025165	0.321945	x
x C	28	0.602223	0.019511	0.320492	x
x C	29	0.582617	0.216038	0.333485	x
x C	30	0.633045	0.367509	0.348099	x
x C	31	0.702515	0.322556	0.349222	x
x C	32	0.898973	0.143329	0.290298	x
x C	33	0.098540	-0.164141	0.376679	x
x C	34	0.042890	-0.095174	0.407261	x
x C	35	0.067252	-0.060317	0.465698	x
x C	36	0.060779	-0.216539	0.501587	x
x C	37	0.074781	-0.181012	0.555715	x
x C	38	0.097313	0.013066	0.575726	x
x C	39	0.108570	0.166848	0.540273	x
x C	40	0.092342	0.130907	0.486135	x
x C	41	0.138302	-0.357175	0.400458	x
x C	42	0.233140	-0.149405	0.457913	x
x C	43	0.265777	-0.227355	0.513100	x
x C	44	0.293466	-0.438730	0.501481	x
x C	45	0.237617	-0.522615	0.456704	x
x C	46	0.288063	-0.046577	0.431687	x
x C	47	0.331332	0.013652	0.350504	x
x C	48	0.378340	-0.141508	0.329165	x
x C	49	0.425809	-0.256863	0.372638	x
x C	50	0.407232	-0.450674	0.388938	x

x C	51	0.450626	-0.556457	0.429525	x
x C	52	0.513823	-0.470928	0.453988	x
x C	53	0.532737	-0.277684	0.438138	x
x C	54	0.488765	-0.170997	0.398183	x
x C	55	0.286107	0.155323	0.309743	x
x C	56	0.228935	0.186818	0.215427	x
x C	57	0.262394	0.211526	0.166553	x
x C	58	0.325396	0.349363	0.175381	x
x C	59	0.390712	0.277101	0.200682	x
x C	60	0.448616	0.405640	0.209229	x
x C	61	0.442666	0.608705	0.191545	x
x C	62	0.378296	0.681677	0.165518	x
x C	63	0.320186	0.554004	0.158059	x
x C	64	0.166884	0.034822	0.204388	x
x C	65	-0.905198	0.594128	-0.116938	x
x C	66	-0.952967	0.669386	-0.079930	x
x C	67	-0.926632	0.641116	-0.021594	x
x C	68	-0.926783	0.445487	0.001233	x
x C	69	-0.906186	0.416694	0.055197	x
x C	70	-0.886127	0.584735	0.088816	x
x C	71	-0.884643	0.781205	0.066404	x
x C	72	-0.904986	0.807188	0.012033	x
x C	73	-0.873967	0.381071	-0.101241	x
x C	74	-0.767860	0.546685	-0.045276	x
x C	75	-0.727422	0.450676	0.005945	x
x C	76	-0.714023	0.231088	-0.010793	x
x C	77	-0.780218	0.174162	-0.050023	x
x C	78	-0.718782	0.644671	-0.077708	x
x C	79	-0.682407	0.663459	-0.162997	x
x C	80	-0.631258	0.510484	-0.180576	x
x C	81	-0.579129	0.426286	-0.134954	x
x C	82	-0.588892	0.231982	-0.114288	x
x C	83	-0.541971	0.153980	-0.071158	x
x C	84	-0.484208	0.269801	-0.048163	x
x C	85	-0.473870	0.463643	-0.068565	x
x C	86	-0.520976	0.541477	-0.111545	x
x C	87	-0.729956	0.762514	-0.210879	x
x C	88	-0.821756	0.692532	-0.288641	x
x C	89	-0.797684	0.581059	-0.335025	x
x C	90	-0.722870	0.625835	-0.336088	x
x C	91	-0.671958	0.474835	-0.321945	x
x C	92	-0.602223	0.519511	-0.320492	x
x C	93	-0.582617	0.716038	-0.333485	x
x C	94	-0.633045	0.867509	-0.348099	x
x C	95	-0.702515	0.822556	-0.349222	x
x C	96	-0.898973	0.643329	-0.290298	x
x C	97	-0.098540	0.335859	-0.376679	x
x C	98	-0.042890	0.404826	-0.407261	x
x C	99	-0.067252	0.439683	-0.465698	x
x C	100	-0.060779	0.283461	-0.501587	x
x C	101	-0.074781	0.318988	-0.555715	x
x C	102	-0.097313	0.513066	-0.575726	x
x C	103	-0.108570	0.666848	-0.540273	x

x C	104	-0.092342	0.630907	-0.486135	x
x C	105	-0.138302	0.142825	-0.400458	x
x C	106	-0.233140	0.350595	-0.457913	x
x C	107	-0.265777	0.272645	-0.513100	x
x C	108	-0.293466	0.061270	-0.501481	x
x C	109	-0.237617	-0.022615	-0.456704	x
x C	110	-0.288063	0.453423	-0.431687	x
x C	111	-0.331332	0.513652	-0.350504	x
x C	112	-0.378340	0.358492	-0.329165	x
x C	113	-0.425809	0.243137	-0.372638	x
x C	114	-0.407232	0.049326	-0.388938	x
x C	115	-0.450626	-0.056457	-0.429525	x
x C	116	-0.513823	0.029072	-0.453988	x
x C	117	-0.532737	0.222316	-0.438138	x
x C	118	-0.488765	0.329003	-0.398183	x
x C	119	-0.286107	0.655323	-0.309743	x
x C	120	-0.228935	0.686818	-0.215427	x
x C	121	-0.262394	0.711526	-0.166553	x
x C	122	-0.325396	0.849363	-0.175381	x
x C	123	-0.390712	0.777101	-0.200682	x
x C	124	-0.448616	0.905640	-0.209229	x
x C	125	-0.442666	1.108705	-0.191545	x
x C	126	-0.378296	1.181677	-0.165518	x
x C	127	-0.320186	1.054004	-0.158059	x
x C	128	-0.166884	0.534822	-0.204388	x
x N	1	0.949287	0.074959	0.170753	x
x N	2	0.809536	-0.126402	0.070833	x
x N	3	0.722471	0.071708	0.127338	x
x N	4	0.777973	0.137012	0.238691	x
x N	5	0.063102	-0.233459	0.322584	x
x N	6	0.201063	-0.336871	0.432069	x
x N	7	0.285492	-0.088525	0.380066	x
x N	8	0.278971	0.099649	0.258975	x
x N	9	-0.949287	0.574959	-0.170753	x
x N	10	-0.809536	0.373598	-0.070833	x
x N	11	-0.722471	0.571708	-0.127338	x
x N	12	-0.777973	0.637012	-0.238691	x
x N	13	-0.063102	0.266541	-0.322584	x
x N	14	-0.201063	0.163129	-0.432069	x
x N	15	-0.285492	0.411475	-0.380066	x
x N	16	-0.278971	0.599649	-0.258975	x
x O	1	0.870018	0.047712	-0.140929	x
x O	2	0.908798	-0.274386	0.115905	x
x O	3	0.680650	0.286833	0.058244	x
x O	4	0.722053	0.446349	0.222082	x
x O	5	0.942850	0.266357	0.316557	x
x O	6	0.915104	-0.016434	0.267098	x
x O	7	0.106947	0.059416	0.627864	x
x O	8	0.110491	-0.526935	0.388423	x
x O	9	0.329666	0.074545	0.457568	x
x O	10	0.257706	0.308716	0.325019	x
x O	11	0.106273	0.095805	0.202878	x
x O	12	0.185504	-0.151586	0.198798	x

x O	13	0.803351	-0.250810	0.201613	x
x O	14	0.019416	0.381252	0.236395	x
x O	15	0.187646	-0.326112	0.294707	x
x O	16	-0.870018	0.547712	0.140929	x
x O	17	-0.908798	0.225614	-0.115905	x
x O	18	-0.680650	0.786833	-0.058244	x
x O	19	-0.722053	0.946349	-0.222082	x
x O	20	-0.942850	0.766357	-0.316557	x
x O	21	-0.915104	0.483566	-0.267098	x
x O	22	-0.106947	0.559416	-0.627864	x
x O	23	-0.110491	-0.026935	-0.388423	x
x O	24	-0.329666	0.574545	-0.457568	x
x O	25	-0.257706	0.808716	-0.325019	x
x O	26	-0.106273	0.595805	-0.202878	x
x O	27	-0.185504	0.348414	-0.198798	x
x O	28	-0.803351	0.249190	-0.201613	x
x O	29	-0.019416	0.881252	-0.236395	x
x O	30	-0.187646	0.173888	-0.294707	x

xx

=====

| Chemical Shielding and Electric Field Gradient Tensors |

Nucleus	Shielding tensor			EFG Tensor		
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
H	1	24.94	10.31	0.40	2.104E-01	0.08
H	2	22.36	25.95	0.24	1.754E-01	0.03
H	3	19.78	27.59	0.16	1.480E-01	0.02
H	4	26.36	4.29	0.33	1.764E-01	0.07
H	5	27.08	6.74	0.56	1.759E-01	0.04
H	6	27.60	-5.48	0.72	1.754E-01	0.06
H	7	24.31	6.61	0.19	1.878E-01	0.07
H	8	23.51	-2.68	0.68	1.944E-01	0.06
H	9	23.26	-5.11	0.81	1.930E-01	0.08
H	10	23.51	-2.20	0.68	1.908E-01	0.06
H	11	17.28	29.42	0.27	1.703E-01	0.17
H	12	27.05	8.04	0.64	1.763E-01	0.05
H	13	29.73	8.84	0.40	1.835E-01	0.00
H	14	30.18	10.83	0.71	1.812E-01	0.02
H	15	29.60	7.68	0.35	1.868E-01	0.02
H	16	29.71	12.85	0.12	1.797E-01	0.02
H	17	27.39	10.02	0.33	1.821E-01	0.04
H	18	27.15	10.12	0.44	1.806E-01	0.06
H	19	22.60	-11.45	0.52	2.236E-01	0.17
H	20	25.95	4.17	0.71	1.743E-01	0.02
H	21	28.02	4.86	0.57	1.783E-01	0.03
H	22	28.43	8.00	0.99	1.797E-01	0.03
H	23	23.48	3.67	0.56	1.883E-01	0.07
H	24	23.86	3.41	0.51	1.893E-01	0.05
H	25	24.88	-3.96	0.36	1.887E-01	0.05
H	26	24.35	3.60	0.79	1.920E-01	0.06

H	27	24.39	3.42	0.72	1.884E-01	0.07
H	28	18.82	18.84	0.56	1.791E-01	0.23
H	29	24.75	-5.33	0.61	1.747E-01	0.03
H	30	27.22	6.45	0.37	1.768E-01	0.03
H	31	26.36	8.80	0.25	1.803E-01	0.02
H	32	23.22	3.10	0.92	1.880E-01	0.07
H	33	23.52	4.51	0.26	1.909E-01	0.06
H	34	24.25	-3.23	0.63	1.908E-01	0.06
H	35	24.17	5.55	0.59	1.899E-01	0.06
H	36	23.20	4.12	0.27	1.886E-01	0.07
H	37	24.19	12.49	0.30	2.028E-01	0.03
H	38	23.86	18.15	0.13	1.972E-01	0.03
H	39	19.94	24.86	0.22	1.538E-01	0.02
H	40	25.98	5.03	0.10	1.743E-01	0.06
H	41	26.36	8.84	0.72	1.729E-01	0.05
H	42	27.51	7.60	0.67	1.737E-01	0.05
H	43	25.51	7.36	0.46	1.883E-01	0.06
H	44	23.37	4.16	0.87	1.929E-01	0.07
H	45	23.94	-1.79	0.54	1.925E-01	0.07
H	46	22.57	3.46	0.89	1.803E-01	0.07
H	47	18.00	24.18	0.07	1.738E-01	0.14
H	48	26.59	11.18	0.45	1.757E-01	0.06
H	49	29.45	7.90	0.61	1.848E-01	0.01
H	50	31.05	-10.47	0.98	1.818E-01	0.02
H	51	30.44	7.89	0.59	1.858E-01	0.01
H	52	30.54	11.95	0.26	1.794E-01	0.01
H	53	27.13	11.38	0.33	1.775E-01	0.04
H	54	27.32	9.67	0.57	1.820E-01	0.06
H	55	22.12	-11.78	0.84	2.190E-01	0.18
H	56	25.64	4.85	0.73	1.727E-01	0.01
H	57	28.88	6.53	0.54	1.766E-01	0.04
H	58	27.78	-5.45	0.92	1.801E-01	0.02
H	59	23.62	4.52	0.85	1.831E-01	0.07
H	60	23.22	3.49	0.63	1.862E-01	0.06
H	61	24.97	-4.71	0.37	1.897E-01	0.05
H	62	23.89	-3.29	0.50	1.914E-01	0.05
H	63	23.65	4.61	0.31	1.909E-01	0.07
H	64	23.96	-6.60	0.36	2.419E-01	0.17
H	65	25.90	-4.69	0.58	1.827E-01	0.03
H	66	27.29	6.15	0.55	1.793E-01	0.01
H	67	26.81	8.00	0.49	1.812E-01	0.04
H	68	23.45	4.80	0.55	1.918E-01	0.07
H	69	23.83	2.90	0.83	1.902E-01	0.06
H	70	24.89	5.80	0.51	1.912E-01	0.06
H	71	23.88	4.34	0.70	1.915E-01	0.06
H	72	23.15	3.26	0.54	1.904E-01	0.07
H	73	26.76	17.25	0.25	2.709E-01	0.10
H	74	23.36	32.09	0.06	2.151E-01	0.12
H	75	26.13	23.01	0.16	2.501E-01	0.08
H	76	24.45	22.63	0.16	2.361E-01	0.10
H	77	23.97	25.71	0.32	2.249E-01	0.12
H	78	24.10	29.75	0.14	2.196E-01	0.13
H	79	24.94	10.31	0.40	2.104E-01	0.08

H	80	22.36	25.95	0.24	1.754E-01	0.03
H	81	19.78	27.59	0.16	1.480E-01	0.02
H	82	26.36	4.29	0.33	1.764E-01	0.07
H	83	27.08	6.74	0.56	1.759E-01	0.04
H	84	27.60	-5.48	0.72	1.754E-01	0.06
H	85	24.31	6.61	0.19	1.878E-01	0.07
H	86	23.51	-2.68	0.68	1.944E-01	0.06
H	87	23.26	-5.11	0.81	1.930E-01	0.08
H	88	23.51	-2.20	0.68	1.908E-01	0.06
H	89	17.28	29.42	0.27	1.703E-01	0.17
H	90	27.05	8.04	0.64	1.763E-01	0.05
H	91	29.73	8.84	0.40	1.835E-01	0.00
H	92	30.18	10.83	0.71	1.812E-01	0.02
H	93	29.60	7.68	0.35	1.868E-01	0.02
H	94	29.71	12.85	0.12	1.797E-01	0.02
H	95	27.39	10.02	0.33	1.821E-01	0.04
H	96	27.15	10.12	0.44	1.806E-01	0.06
H	97	22.60	-11.45	0.52	2.236E-01	0.17
H	98	25.95	4.17	0.71	1.743E-01	0.02
H	99	28.02	4.86	0.57	1.783E-01	0.03
H	100	28.43	8.00	0.99	1.797E-01	0.03
H	101	23.48	3.67	0.56	1.883E-01	0.07
H	102	23.86	3.41	0.51	1.893E-01	0.05
H	103	24.88	-3.96	0.36	1.887E-01	0.05
H	104	24.35	3.60	0.79	1.920E-01	0.06
H	105	24.39	3.42	0.72	1.884E-01	0.07
H	106	18.82	18.84	0.56	1.791E-01	0.23
H	107	24.75	-5.33	0.61	1.747E-01	0.03
H	108	27.22	6.45	0.37	1.768E-01	0.03
H	109	26.36	8.80	0.25	1.803E-01	0.02
H	110	23.22	3.10	0.92	1.880E-01	0.07
H	111	23.52	4.51	0.26	1.909E-01	0.06
H	112	24.25	-3.23	0.63	1.908E-01	0.06
H	113	24.17	5.55	0.59	1.899E-01	0.06
H	114	23.20	4.12	0.27	1.886E-01	0.07
H	115	24.19	12.49	0.30	2.028E-01	0.03
H	116	23.86	18.15	0.13	1.972E-01	0.03
H	117	19.94	24.86	0.22	1.538E-01	0.02
H	118	25.98	5.03	0.10	1.743E-01	0.06
H	119	26.36	8.84	0.72	1.729E-01	0.05
H	120	27.51	7.60	0.67	1.737E-01	0.05
H	121	25.51	7.36	0.46	1.883E-01	0.06
H	122	23.37	4.16	0.87	1.929E-01	0.07
H	123	23.94	-1.79	0.54	1.925E-01	0.07
H	124	22.57	3.46	0.89	1.803E-01	0.07
H	125	18.00	24.18	0.07	1.738E-01	0.14
H	126	26.59	11.18	0.45	1.757E-01	0.06
H	127	29.45	7.90	0.61	1.848E-01	0.01
H	128	31.05	-10.47	0.98	1.818E-01	0.02
H	129	30.44	7.89	0.59	1.858E-01	0.01
H	130	30.54	11.95	0.26	1.794E-01	0.01
H	131	27.13	11.38	0.33	1.775E-01	0.04
H	132	27.32	9.67	0.57	1.820E-01	0.06

H	133	22.12	-11.78	0.84	2.190E-01	0.18
H	134	25.64	4.85	0.73	1.727E-01	0.01
H	135	28.88	6.53	0.54	1.766E-01	0.04
H	136	27.78	-5.45	0.92	1.801E-01	0.02
H	137	23.62	4.52	0.85	1.831E-01	0.07
H	138	23.22	3.49	0.63	1.862E-01	0.06
H	139	24.97	-4.71	0.37	1.897E-01	0.05
H	140	23.89	-3.29	0.50	1.914E-01	0.05
H	141	23.65	4.61	0.31	1.909E-01	0.07
H	142	23.96	-6.60	0.36	2.419E-01	0.17
H	143	25.90	-4.69	0.58	1.827E-01	0.03
H	144	27.29	6.15	0.55	1.793E-01	0.01
H	145	26.81	8.00	0.49	1.812E-01	0.04
H	146	23.45	4.80	0.55	1.918E-01	0.07
H	147	23.83	2.90	0.83	1.902E-01	0.06
H	148	24.89	5.80	0.51	1.912E-01	0.06
H	149	23.88	4.34	0.70	1.915E-01	0.06
H	150	23.15	3.26	0.54	1.904E-01	0.07
H	151	26.76	17.25	0.25	2.709E-01	0.10
H	152	23.36	32.09	0.06	2.151E-01	0.12
H	153	26.13	23.01	0.16	2.501E-01	0.08
H	154	24.45	22.63	0.16	2.361E-01	0.10
H	155	23.97	25.71	0.32	2.249E-01	0.12
H	156	24.10	29.75	0.14	2.196E-01	0.13
C	1	118.87	-26.87	0.83	2.918E+00	0.20
C	2	132.66	-27.74	0.91	1.171E+00	0.64
C	3	50.81	171.05	0.66	1.702E+00	0.74
C	4	36.48	182.32	0.69	2.816E+00	0.14
C	5	54.77	146.91	0.73	2.006E+00	0.36
C	6	8.97	150.00	0.61	-3.008E+00	0.44
C	7	58.71	139.80	0.76	1.813E+00	0.31
C	8	37.95	168.65	0.81	2.687E+00	0.21
C	9	5.27	-123.67	0.79	2.691E+00	0.41
C	10	107.81	36.89	0.85	2.529E+00	0.34
C	11	142.88	-36.95	0.48	1.186E+00	0.61
C	12	151.60	-31.62	0.16	8.998E-01	0.79
C	13	124.47	46.42	0.82	2.870E+00	0.16
C	14	3.59	-122.96	0.85	3.162E+00	0.46
C	15	112.85	44.43	0.08	2.238E+00	0.75
C	16	130.15	28.20	0.30	8.765E-01	0.64
C	17	33.75	196.57	0.53	2.519E+00	0.46
C	18	39.23	172.39	0.86	2.705E+00	0.21
C	19	40.07	194.01	0.68	2.976E+00	0.09
C	20	43.18	194.59	0.67	2.892E+00	0.11
C	21	41.13	190.87	0.73	2.858E+00	0.16
C	22	41.49	178.04	0.75	2.656E+00	0.20
C	23	-2.84	125.99	0.67	3.287E+00	0.35
C	24	112.89	35.85	0.55	2.111E+00	0.59
C	25	131.05	23.85	0.62	9.190E-01	0.74
C	26	32.34	198.22	0.50	2.554E+00	0.43
C	27	38.33	169.06	0.89	2.637E+00	0.22
C	28	41.61	186.39	0.72	2.779E+00	0.18
C	29	43.23	187.19	0.69	2.746E+00	0.18

C	30	41.07	188.94	0.72	2.883E+00	0.13
C	31	39.38	185.19	0.71	2.654E+00	0.21
C	32	-13.72	114.85	0.60	3.582E+00	0.15
C	33	117.01	25.36	0.87	3.085E+00	0.25
C	34	136.00	30.67	0.69	1.145E+00	0.77
C	35	48.02	174.92	0.66	1.811E+00	0.73
C	36	35.66	176.10	0.71	2.880E+00	0.12
C	37	55.38	145.44	0.69	1.944E+00	0.29
C	38	9.61	148.66	0.66	-3.108E+00	0.27
C	39	56.09	148.98	0.70	1.984E+00	0.32
C	40	33.20	188.66	0.62	2.878E+00	0.03
C	41	4.85	-118.22	0.88	2.700E+00	0.30
C	42	108.14	-37.34	0.58	2.627E+00	0.37
C	43	142.23	-32.61	0.75	1.141E+00	0.72
C	44	152.84	-30.86	0.17	8.452E-01	0.78
C	45	124.39	50.20	0.86	3.093E+00	0.21
C	46	3.85	-121.64	0.90	3.178E+00	0.43
C	47	117.06	46.30	0.39	2.101E+00	0.88
C	48	136.45	27.51	0.14	5.868E-01	0.85
C	49	35.46	192.92	0.57	2.406E+00	0.59
C	50	40.77	176.56	0.78	2.757E+00	0.15
C	51	39.96	193.43	0.67	2.982E+00	0.08
C	52	41.60	197.58	0.65	2.993E+00	0.07
C	53	40.24	193.59	0.68	2.938E+00	0.11
C	54	39.97	177.42	0.73	2.655E+00	0.20
C	55	1.58	119.93	0.84	3.152E+00	0.36
C	56	112.06	35.74	0.26	2.396E+00	0.45
C	57	135.10	26.23	0.30	8.776E-01	0.99
C	58	31.87	197.04	0.50	2.547E+00	0.42
C	59	39.35	173.15	0.83	2.586E+00	0.26
C	60	42.79	186.65	0.75	2.808E+00	0.16
C	61	44.70	191.74	0.71	2.855E+00	0.13
C	62	41.77	185.84	0.77	2.807E+00	0.18
C	63	39.69	174.03	0.77	2.744E+00	0.16
C	64	-8.84	105.40	0.85	3.494E+00	0.19
C	65	118.87	-26.87	0.83	2.918E+00	0.20
C	66	132.66	-27.74	0.91	1.171E+00	0.64
C	67	50.81	171.05	0.66	1.702E+00	0.74
C	68	36.48	182.32	0.69	2.816E+00	0.14
C	69	54.77	146.91	0.73	2.006E+00	0.36
C	70	8.97	150.00	0.61	-3.008E+00	0.44
C	71	58.71	139.80	0.76	1.813E+00	0.31
C	72	37.95	168.65	0.81	2.687E+00	0.21
C	73	5.27	-123.67	0.79	2.691E+00	0.41
C	74	107.81	36.89	0.85	2.529E+00	0.34
C	75	142.88	-36.95	0.48	1.186E+00	0.61
C	76	151.60	-31.62	0.16	8.998E-01	0.79
C	77	124.47	46.42	0.82	2.870E+00	0.16
C	78	3.59	-122.96	0.85	3.162E+00	0.46
C	79	112.85	44.43	0.08	2.238E+00	0.75
C	80	130.15	28.20	0.30	8.765E-01	0.64
C	81	33.75	196.57	0.53	2.519E+00	0.46
C	82	39.23	172.39	0.86	2.705E+00	0.21

C	83	40.07	194.01	0.68	2.976E+00	0.09
C	84	43.18	194.59	0.67	2.892E+00	0.11
C	85	41.13	190.87	0.73	2.858E+00	0.16
C	86	41.49	178.04	0.75	2.656E+00	0.20
C	87	-2.84	125.99	0.67	3.287E+00	0.35
C	88	112.89	35.85	0.55	2.111E+00	0.59
C	89	131.05	23.85	0.62	9.190E-01	0.74
C	90	32.34	198.22	0.50	2.554E+00	0.43
C	91	38.33	169.06	0.89	2.637E+00	0.22
C	92	41.61	186.39	0.72	2.779E+00	0.18
C	93	43.23	187.19	0.69	2.746E+00	0.18
C	94	41.07	188.94	0.72	2.883E+00	0.13
C	95	39.38	185.19	0.71	2.654E+00	0.21
C	96	-13.72	114.85	0.60	3.582E+00	0.15
C	97	117.01	25.36	0.87	3.085E+00	0.25
C	98	136.00	30.67	0.69	1.145E+00	0.77
C	99	48.02	174.92	0.66	1.811E+00	0.73
C	100	35.66	176.10	0.71	2.880E+00	0.12
C	101	55.38	145.44	0.69	1.944E+00	0.29
C	102	9.61	148.66	0.66	-3.108E+00	0.27
C	103	56.09	148.98	0.70	1.984E+00	0.32
C	104	33.20	188.66	0.62	2.878E+00	0.03
C	105	4.85	-118.22	0.88	2.700E+00	0.30
C	106	108.14	-37.34	0.58	2.627E+00	0.37
C	107	142.23	-32.61	0.75	1.141E+00	0.72
C	108	152.84	-30.86	0.17	8.452E-01	0.78
C	109	124.39	50.20	0.86	3.093E+00	0.21
C	110	3.85	-121.64	0.90	3.178E+00	0.43
C	111	117.06	46.30	0.39	2.101E+00	0.88
C	112	136.45	27.51	0.14	5.868E-01	0.85
C	113	35.46	192.92	0.57	2.406E+00	0.59
C	114	40.77	176.56	0.78	2.757E+00	0.15
C	115	39.96	193.43	0.67	2.982E+00	0.08
C	116	41.60	197.58	0.65	2.993E+00	0.07
C	117	40.24	193.59	0.68	2.938E+00	0.11
C	118	39.97	177.42	0.73	2.655E+00	0.20
C	119	1.58	119.93	0.84	3.152E+00	0.36
C	120	112.06	35.74	0.26	2.396E+00	0.45
C	121	135.10	26.23	0.30	8.776E-01	0.99
C	122	31.87	197.04	0.50	2.547E+00	0.42
C	123	39.35	173.15	0.83	2.586E+00	0.26
C	124	42.79	186.65	0.75	2.808E+00	0.16
C	125	44.70	191.74	0.71	2.855E+00	0.13
C	126	41.77	185.84	0.77	2.807E+00	0.18
C	127	39.69	174.03	0.77	2.744E+00	0.16
C	128	-8.84	105.40	0.85	3.494E+00	0.19
N	1	181.66	32.16	0.06	1.244E+00	0.52
N	2	81.13	-158.50	0.65	-3.916E+00	0.13
N	3	103.96	-178.46	0.09	-3.608E+00	0.32
N	4	95.92	-160.04	0.16	-3.098E+00	0.56
N	5	182.51	31.78	0.40	1.134E+00	0.74
N	6	78.84	-153.64	0.54	-3.720E+00	0.12
N	7	103.61	-168.01	0.04	-3.702E+00	0.36

	N	8	91.36	-160.42	0.20	-3.417E+00	0.22
	N	9	181.66	32.16	0.06	1.244E+00	0.52
	N	10	81.13	-158.50	0.65	-3.916E+00	0.13
	N	11	103.96	-178.46	0.09	-3.608E+00	0.32
	N	12	95.92	-160.04	0.16	-3.098E+00	0.56
	N	13	182.51	31.78	0.40	1.134E+00	0.74
	N	14	78.84	-153.64	0.54	-3.720E+00	0.12
	N	15	103.61	-168.01	0.04	-3.702E+00	0.36
	N	16	91.36	-160.42	0.20	-3.417E+00	0.22
	O	1	152.92	127.21	0.46	-8.701E+00	0.49
	O	2	-76.40	618.04	0.46	8.732E+00	0.21
	O	3	-49.12	592.07	0.38	8.579E+00	0.23
	O	4	-23.57	490.46	0.39	8.915E+00	0.35
	O	5	-45.31	329.79	0.53	7.328E+00	0.52
	O	6	-22.42	359.08	0.47	7.787E+00	0.51
	O	7	164.05	104.10	0.72	-8.844E+00	0.59
	O	8	-56.50	582.13	0.42	8.338E+00	0.32
	O	9	-49.59	581.31	0.40	8.595E+00	0.23
	O	10	-23.97	496.26	0.29	8.195E+00	0.45
	O	11	-65.47	379.12	0.40	8.422E+00	0.27
	O	12	1.15	312.43	0.70	7.723E+00	0.62
	O	13	261.20	46.82	0.35	8.183E+00	0.84
	O	14	269.05	-32.31	1.00	7.732E+00	0.93
	O	15	266.02	-30.78	0.72	7.648E+00	0.83
	O	16	152.92	127.21	0.46	-8.701E+00	0.49
	O	17	-76.40	618.04	0.46	8.732E+00	0.21
	O	18	-49.12	592.07	0.38	8.579E+00	0.23
	O	19	-23.57	490.46	0.39	8.915E+00	0.35
	O	20	-45.31	329.79	0.53	7.328E+00	0.52
	O	21	-22.42	359.08	0.47	7.787E+00	0.51
	O	22	164.05	104.10	0.72	-8.844E+00	0.59
	O	23	-56.50	582.13	0.42	8.338E+00	0.32
	O	24	-49.59	581.31	0.40	8.595E+00	0.23
	O	25	-23.97	496.26	0.29	8.195E+00	0.45
	O	26	-65.47	379.12	0.40	8.422E+00	0.27
	O	27	1.15	312.43	0.70	7.723E+00	0.62
	O	28	261.20	46.82	0.35	8.183E+00	0.84
	O	29	269.05	-32.31	1.00	7.732E+00	0.93
	O	30	266.02	-30.78	0.72	7.648E+00	0.83

=====

GIPAW coordinates and calculated NMR parameters for 2 (structure 10)

xx

x	Element	Atom	Fractional coordinates of atoms x			
x		Number	u	v	w	x
x-----x						
x H		1	0.973970	-0.076179	0.174725	x
x H		2	0.914494	0.049785	0.201762	x
x H		3	0.974901	0.181123	0.178326	x
x H		4	0.860740	0.196390	0.116405	x
x H		5	0.966490	0.300708	0.090246	x
x H		6	0.996773	0.043452	0.090995	x
x H		7	0.945520	-0.201093	0.019191	x
x H		8	0.907432	-0.230456	-0.078357	x
x H		9	0.862068	0.416179	-0.087760	x
x H		10	0.900133	0.445060	0.009278	x
x H		11	0.840202	0.186702	-0.161266	x
x H		12	0.796773	0.159685	0.035578	x
x H		13	0.677210	0.031904	-0.024923	x
x H		14	0.758051	-0.061693	-0.036220	x
x H		15	0.697674	-0.385198	-0.024146	x
x H		16	0.661288	-0.276467	0.026862	x
x H		17	0.759579	-0.429501	0.081896	x
x H		18	0.809894	-0.419560	0.032050	x
x H		19	0.747186	-0.042270	0.139991	x
x H		20	0.645397	0.299174	0.135804	x
x H		21	0.652468	-0.098629	0.200783	x
x H		22	0.595128	0.108408	0.202960	x
x H		23	0.630771	-0.352182	0.133934	x
x H		24	0.551557	-0.508685	0.057547	x
x H		25	0.446512	-0.315317	0.012304	x
x H		26	0.423820	0.033695	0.043296	x
x H		27	0.504010	0.191648	0.118933	x
x H		28	0.769927	0.006765	0.225660	x
x H		29	0.803050	0.382715	0.291991	x
x H		30	0.796784	-0.061868	0.331085	x
x H		31	0.818899	0.159359	0.370674	x
x H		32	0.678666	-0.166448	0.308067	x
x H		33	0.554046	-0.101456	0.305138	x
x H		34	0.514819	0.244651	0.330077	x
x H		35	0.601151	0.519068	0.358515	x
x H		36	0.726065	0.454553	0.360532	x
x H		37	0.046066	-0.392578	0.327353	x
x H		38	0.028789	-0.153052	0.302202	x
x H		39	0.105274	-0.276972	0.299293	x
x H		40	0.134110	-0.044231	0.370235	x
x H		41	0.017974	0.026758	0.384921	x
x H		42	0.004912	-0.233632	0.400534	x
x H		43	0.042721	-0.369851	0.487600	x
x H		44	0.070616	-0.293784	0.582821	x
x H		45	0.129206	0.321993	0.549565	x
x H		46	0.096799	0.248917	0.453398	x
x H		47	0.098523	-0.044801	0.645975	x

x H	48	0.194802	-0.028744	0.456971	x
x H	49	0.306626	-0.105647	0.532003	x
x H	50	0.226335	-0.225411	0.535952	x
x H	51	0.304568	-0.523916	0.538911	x
x H	52	0.345919	-0.412248	0.490723	x
x H	53	0.263028	-0.610376	0.430890	x
x H	54	0.203829	-0.614695	0.474423	x
x H	55	0.253541	-0.197381	0.358811	x
x H	56	0.367634	0.107326	0.378002	x
x H	57	0.351723	-0.264869	0.303027	x
x H	58	0.415605	-0.069899	0.306659	x
x H	59	0.360664	-0.530446	0.369364	x
x H	60	0.435484	-0.720205	0.442235	x
x H	61	0.548420	-0.569514	0.487389	x
x H	62	0.582975	-0.224902	0.461302	x
x H	63	0.506723	-0.030681	0.390353	x
x H	64	0.315301	-0.033728	0.249313	x
x H	65	0.224494	0.332062	0.224230	x
x H	66	0.296452	0.071411	0.152110	x
x H	67	0.240957	0.283621	0.132376	x
x H	68	0.414012	0.141346	0.216412	x
x H	69	0.513066	0.381205	0.235157	x
x H	70	0.499922	0.741354	0.202289	x
x H	71	0.386218	0.860352	0.151940	x
x H	72	0.284975	0.624735	0.136680	x
x H	73	0.837872	-0.212547	0.227324	x
x H	74	0.769320	-0.351097	0.211250	x
x H	75	0.212055	-0.480150	0.298659	x
x H	76	0.200315	-0.290326	0.258802	x
x H	77	0.077023	-0.108762	0.196430	x
x H	78	0.055592	-0.335371	0.181925	x
x H	79	-0.973970	0.423821	-0.174725	x
x H	80	-0.914494	0.549785	-0.201762	x
x H	81	-0.974901	0.681123	-0.178326	x
x H	82	-0.860740	0.696390	-0.116405	x
x H	83	-0.966490	0.800708	-0.090246	x
x H	84	-0.996773	0.543452	-0.090995	x
x H	85	-0.945520	0.298907	-0.019191	x
x H	86	-0.907432	0.269544	0.078357	x
x H	87	-0.862068	0.916179	0.087760	x
x H	88	-0.900133	0.945060	-0.009278	x
x H	89	-0.840202	0.686702	0.161266	x
x H	90	-0.796773	0.659685	-0.035578	x
x H	91	-0.677210	0.531904	0.024923	x
x H	92	-0.758051	0.438307	0.036220	x
x H	93	-0.697674	0.114802	0.024146	x
x H	94	-0.661288	0.223533	-0.026862	x
x H	95	-0.759579	0.070499	-0.081896	x
x H	96	-0.809894	0.080440	-0.032050	x
x H	97	-0.747186	0.457730	-0.139991	x
x H	98	-0.645397	0.799174	-0.135804	x
x H	99	-0.652468	0.401371	-0.200783	x
x H	100	-0.595128	0.608408	-0.202960	x

x H	101	-0.630771	0.147818	-0.133934	x
x H	102	-0.551557	-0.008685	-0.057547	x
x H	103	-0.446512	0.184683	-0.012304	x
x H	104	-0.423820	0.533695	-0.043296	x
x H	105	-0.504010	0.691648	-0.118933	x
x H	106	-0.769927	0.506765	-0.225660	x
x H	107	-0.803050	0.882715	-0.291991	x
x H	108	-0.796784	0.438132	-0.331085	x
x H	109	-0.818899	0.659359	-0.370674	x
x H	110	-0.678666	0.333552	-0.308067	x
x H	111	-0.554046	0.398544	-0.305138	x
x H	112	-0.514819	0.744651	-0.330077	x
x H	113	-0.601151	1.019068	-0.358515	x
x H	114	-0.726065	0.954553	-0.360532	x
x H	115	-0.046066	0.107422	-0.327353	x
x H	116	-0.028789	0.346948	-0.302202	x
x H	117	-0.105274	0.223028	-0.299293	x
x H	118	-0.134110	0.455769	-0.370235	x
x H	119	-0.017974	0.526758	-0.384921	x
x H	120	-0.004912	0.266368	-0.400534	x
x H	121	-0.042721	0.130149	-0.487600	x
x H	122	-0.070616	0.206216	-0.582821	x
x H	123	-0.129206	0.821993	-0.549565	x
x H	124	-0.096799	0.748917	-0.453398	x
x H	125	-0.098523	0.455199	-0.645975	x
x H	126	-0.194802	0.471256	-0.456971	x
x H	127	-0.306626	0.394353	-0.532003	x
x H	128	-0.226335	0.274589	-0.535952	x
x H	129	-0.304568	-0.023916	-0.538911	x
x H	130	-0.345919	0.087752	-0.490723	x
x H	131	-0.263028	-0.110376	-0.430890	x
x H	132	-0.203829	-0.114695	-0.474423	x
x H	133	-0.253541	0.302619	-0.358811	x
x H	134	-0.367634	0.607326	-0.378002	x
x H	135	-0.351723	0.235131	-0.303027	x
x H	136	-0.415605	0.430101	-0.306659	x
x H	137	-0.360664	-0.030446	-0.369364	x
x H	138	-0.435484	-0.220205	-0.442235	x
x H	139	-0.548420	-0.069514	-0.487389	x
x H	140	-0.582975	0.275098	-0.461302	x
x H	141	-0.506723	0.469319	-0.390353	x
x H	142	-0.315301	0.466272	-0.249313	x
x H	143	-0.224494	0.832062	-0.224230	x
x H	144	-0.296452	0.571411	-0.152110	x
x H	145	-0.240957	0.783621	-0.132376	x
x H	146	-0.414012	0.641346	-0.216412	x
x H	147	-0.513066	0.881205	-0.235157	x
x H	148	-0.499922	1.241354	-0.202289	x
x H	149	-0.386218	1.360352	-0.151940	x
x H	150	-0.284975	1.124735	-0.136680	x
x H	151	-0.837872	0.287453	-0.227324	x
x H	152	-0.769320	0.148903	-0.211250	x
x H	153	-0.212055	0.019850	-0.298659	x

x H	154	-0.200315	0.209674	-0.258802	x
x H	155	-0.077023	0.391238	-0.196430	x
x H	156	-0.055592	0.164629	-0.181925	x
x C	1	0.899858	0.076707	0.115847	x
x C	2	0.950510	0.141338	0.079984	x
x C	3	0.924325	0.123781	0.021387	x
x C	4	0.926171	-0.065877	-0.004085	x
x C	5	0.905411	-0.083668	-0.058435	x
x C	6	0.882735	0.089718	-0.089315	x
x C	7	0.879449	0.280037	-0.064254	x
x C	8	0.900522	0.295222	-0.009652	x
x C	9	0.866910	-0.134289	0.100155	x
x C	10	0.762122	0.037083	0.043863	x
x C	11	0.723165	-0.058379	-0.007884	x
x C	12	0.707285	-0.276146	0.008779	x
x C	13	0.771616	-0.335728	0.049656	x
x C	14	0.712045	0.139639	0.074780	x
x C	15	0.674531	0.176267	0.159338	x
x C	16	0.623190	0.023859	0.176867	x
x C	17	0.573357	-0.069551	0.131264	x
x C	18	0.585644	-0.266791	0.113471	x
x C	19	0.540517	-0.355581	0.070942	x
x C	20	0.482050	-0.247799	0.045667	x
x C	21	0.469285	-0.051023	0.063169	x
x C	22	0.514597	0.037795	0.105554	x
x C	23	0.719871	0.280845	0.207464	x
x C	24	0.809474	0.216667	0.287364	x
x C	25	0.786289	0.103525	0.333879	x
x C	26	0.710917	0.139623	0.334415	x
x C	27	0.661787	-0.015394	0.319034	x
x C	28	0.591497	0.021537	0.317184	x
x C	29	0.569550	0.214099	0.331109	x
x C	30	0.618171	0.369515	0.346907	x
x C	31	0.688203	0.332463	0.348332	x
x C	32	0.886953	0.169285	0.289524	x
x C	33	0.100774	-0.174650	0.375543	x
x C	34	0.043680	-0.109571	0.405253	x
x C	35	0.067747	-0.066150	0.463329	x
x C	36	0.062336	-0.217812	0.500688	x
x C	37	0.078514	-0.176512	0.554526	x
x C	38	0.101994	0.019439	0.572713	x
x C	39	0.110918	0.169615	0.535616	x
x C	40	0.092850	0.127615	0.481845	x
x C	41	0.142169	-0.363304	0.400323	x
x C	42	0.234978	-0.145495	0.456677	x
x C	43	0.267332	-0.214578	0.512771	x
x C	44	0.296116	-0.427190	0.503520	x
x C	45	0.241237	-0.518532	0.459176	x
x C	46	0.290000	-0.046242	0.429904	x
x C	47	0.335484	0.004188	0.349537	x
x C	48	0.383031	-0.153309	0.329727	x
x C	49	0.428923	-0.269030	0.373963	x
x C	50	0.409708	-0.463484	0.389326	x

x C	51	0.452107	-0.570962	0.430103	x
x C	52	0.514863	-0.486257	0.455720	x
x C	53	0.534217	-0.291831	0.441043	x
x C	54	0.491224	-0.183455	0.400894	x
x C	55	0.292433	0.145980	0.307612	x
x C	56	0.245099	0.187426	0.212193	x
x C	57	0.280540	0.222593	0.164730	x
x C	58	0.341760	0.366568	0.175762	x
x C	59	0.406789	0.300654	0.203288	x
x C	60	0.463026	0.435160	0.213566	x
x C	61	0.455573	0.637744	0.195715	x
x C	62	0.391490	0.704520	0.167698	x
x C	63	0.335017	0.570679	0.158278	x
x C	64	0.185552	0.030693	0.197506	x
x C	65	-0.899858	0.576707	-0.115847	x
x C	66	-0.950510	0.641338	-0.079984	x
x C	67	-0.924325	0.623781	-0.021387	x
x C	68	-0.926171	0.434123	0.004085	x
x C	69	-0.905411	0.416332	0.058435	x
x C	70	-0.882735	0.589718	0.089315	x
x C	71	-0.879449	0.780037	0.064254	x
x C	72	-0.900522	0.795222	0.009652	x
x C	73	-0.866910	0.365711	-0.100155	x
x C	74	-0.762122	0.537083	-0.043863	x
x C	75	-0.723165	0.441621	0.007884	x
x C	76	-0.707285	0.223854	-0.008779	x
x C	77	-0.7711616	0.164272	-0.049656	x
x C	78	-0.712045	0.639639	-0.074780	x
x C	79	-0.674531	0.676267	-0.159338	x
x C	80	-0.623190	0.523859	-0.176867	x
x C	81	-0.573357	0.430449	-0.131264	x
x C	82	-0.585644	0.233209	-0.113471	x
x C	83	-0.540517	0.144419	-0.070942	x
x C	84	-0.482050	0.252201	-0.045667	x
x C	85	-0.469285	0.448977	-0.063169	x
x C	86	-0.514597	0.537795	-0.105554	x
x C	87	-0.719871	0.780845	-0.207464	x
x C	88	-0.809474	0.716667	-0.287364	x
x C	89	-0.786289	0.603525	-0.333879	x
x C	90	-0.710917	0.639623	-0.334415	x
x C	91	-0.661787	0.484606	-0.319034	x
x C	92	-0.591497	0.521537	-0.317184	x
x C	93	-0.569550	0.714099	-0.331109	x
x C	94	-0.618171	0.869515	-0.346907	x
x C	95	-0.688203	0.832463	-0.348332	x
x C	96	-0.886953	0.669285	-0.289524	x
x C	97	-0.100774	0.325350	-0.375543	x
x C	98	-0.043680	0.390429	-0.405253	x
x C	99	-0.067747	0.433850	-0.463329	x
x C	100	-0.062336	0.282188	-0.500688	x
x C	101	-0.078514	0.323488	-0.554526	x
x C	102	-0.101994	0.519439	-0.572713	x
x C	103	-0.110918	0.669615	-0.535616	x

x C	104	-0.092850	0.627615	-0.481845	x
x C	105	-0.142169	0.136696	-0.400323	x
x C	106	-0.234978	0.354505	-0.456677	x
x C	107	-0.267332	0.285422	-0.512771	x
x C	108	-0.296116	0.072810	-0.503520	x
x C	109	-0.241237	-0.018532	-0.459176	x
x C	110	-0.290000	0.453758	-0.429904	x
x C	111	-0.335484	0.504188	-0.349537	x
x C	112	-0.383031	0.346691	-0.329727	x
x C	113	-0.428923	0.230970	-0.373963	x
x C	114	-0.409708	0.036516	-0.389326	x
x C	115	-0.452107	-0.070962	-0.430103	x
x C	116	-0.514863	0.013743	-0.455720	x
x C	117	-0.534217	0.208169	-0.441043	x
x C	118	-0.491224	0.316545	-0.400894	x
x C	119	-0.292433	0.645980	-0.307612	x
x C	120	-0.245099	0.687426	-0.212193	x
x C	121	-0.280540	0.722593	-0.164730	x
x C	122	-0.341760	0.866568	-0.175762	x
x C	123	-0.406789	0.800654	-0.203288	x
x C	124	-0.463026	0.935160	-0.213566	x
x C	125	-0.455573	1.137744	-0.195715	x
x C	126	-0.391490	1.204520	-0.167698	x
x C	127	-0.335017	1.070679	-0.158278	x
x C	128	-0.185552	0.530693	-0.197506	x
x N	1	0.941843	0.057878	0.170348	x
x N	2	0.802257	-0.137429	0.070163	x
x N	3	0.716621	0.080325	0.125603	x
x N	4	0.766304	0.157614	0.237483	x
x N	5	0.066886	-0.249690	0.321660	x
x N	6	0.204152	-0.337112	0.432542	x
x N	7	0.288421	-0.093930	0.378712	x
x N	8	0.293605	0.102214	0.256909	x
x N	9	-0.941843	0.557878	-0.170348	x
x N	10	-0.802257	0.362571	-0.070163	x
x N	11	-0.716621	0.580325	-0.125603	x
x N	12	-0.766304	0.657614	-0.237483	x
x N	13	-0.066886	0.250310	-0.321660	x
x N	14	-0.204152	0.162888	-0.432542	x
x N	15	-0.288421	0.406070	-0.378712	x
x N	16	-0.293605	0.602214	-0.256909	x
x O	1	0.866711	0.064404	-0.142242	x
x O	2	0.900610	-0.292373	0.114198	x
x O	3	0.672852	0.275496	0.052928	x
x O	4	0.711331	0.466221	0.216879	x
x O	5	0.930411	0.279759	0.319570	x
x O	6	0.902339	0.017425	0.262792	x
x O	7	0.114816	0.069908	0.624565	x
x O	8	0.116200	-0.535547	0.388543	x
x O	9	0.331257	0.077586	0.455104	x
x O	10	0.259106	0.290826	0.321803	x
x O	11	0.123886	0.091013	0.187136	x
x O	12	0.205517	-0.157279	0.197562	x

x O	13	0.795347	-0.231827	0.200829	x
x O	14	0.193070	-0.338513	0.293565	x
x O	15	0.043467	-0.219696	0.202548	x
x O	16	-0.866711	0.564404	0.142242	x
x O	17	-0.900610	0.207627	-0.114198	x
x O	18	-0.672852	0.775496	-0.052928	x
x O	19	-0.711331	0.966221	-0.216879	x
x O	20	-0.930411	0.779759	-0.319570	x
x O	21	-0.902339	0.517425	-0.262792	x
x O	22	-0.114816	0.569908	-0.624565	x
x O	23	-0.116200	-0.035547	-0.388543	x
x O	24	-0.331257	0.577586	-0.455104	x
x O	25	-0.259106	0.790826	-0.321803	x
x O	26	-0.123886	0.591013	-0.187136	x
x O	27	-0.205517	0.342721	-0.197562	x
x O	28	-0.795347	0.268173	-0.200829	x
x O	29	-0.193070	0.161487	-0.293565	x
x O	30	-0.043467	0.280304	-0.202548	x

xx

=====

| Chemical Shielding and Electric Field Gradient Tensors |

Nucleus	Shielding tensor			EFG Tensor		
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
H	1	18.13	27.81	0.08	1.267E-01	0.01
H	2	20.11	31.35	0.15	1.443E-01	0.03
H	3	27.27	9.96	0.41	2.256E-01	0.05
H	4	26.23	5.28	0.14	1.758E-01	0.07
H	5	27.29	7.29	0.33	1.761E-01	0.05
H	6	27.51	-5.73	0.91	1.753E-01	0.05
H	7	24.37	6.09	0.33	1.882E-01	0.07
H	8	23.25	-2.88	0.59	1.922E-01	0.05
H	9	23.32	-4.54	0.88	1.919E-01	0.08
H	10	23.35	-2.14	0.84	1.895E-01	0.06
H	11	16.83	29.81	0.13	1.507E-01	0.15
H	12	27.00	8.41	0.63	1.770E-01	0.05
H	13	29.48	9.03	0.40	1.828E-01	0.00
H	14	30.31	10.66	0.72	1.813E-01	0.02
H	15	29.50	7.71	0.36	1.867E-01	0.02
H	16	29.72	12.85	0.11	1.789E-01	0.01
H	17	27.48	10.14	0.31	1.818E-01	0.04
H	18	27.16	9.88	0.53	1.808E-01	0.06
H	19	22.18	-11.90	0.63	2.190E-01	0.17
H	20	25.95	4.45	0.75	1.749E-01	0.02
H	21	27.94	4.78	0.54	1.783E-01	0.03
H	22	28.37	7.36	0.96	1.801E-01	0.03
H	23	23.35	3.70	0.63	1.864E-01	0.07
H	24	23.86	3.09	0.62	1.885E-01	0.05
H	25	25.04	-4.34	0.30	1.887E-01	0.05
H	26	24.19	3.64	0.65	1.926E-01	0.05

H	27	24.67	-2.79	0.77	1.881E-01	0.07
H	28	19.23	17.73	0.58	1.852E-01	0.23
H	29	24.99	-5.81	0.43	1.762E-01	0.04
H	30	27.31	5.86	0.35	1.770E-01	0.03
H	31	26.47	8.93	0.37	1.801E-01	0.02
H	32	23.23	3.00	0.75	1.881E-01	0.07
H	33	23.48	3.65	0.10	1.911E-01	0.06
H	34	24.23	2.90	0.95	1.910E-01	0.06
H	35	24.50	6.38	0.36	1.899E-01	0.06
H	36	23.26	4.13	0.37	1.886E-01	0.07
H	37	24.14	11.68	0.38	1.998E-01	0.04
H	38	24.93	15.22	0.42	2.127E-01	0.02
H	39	20.14	24.30	0.46	1.570E-01	0.04
H	40	25.94	4.97	0.30	1.741E-01	0.07
H	41	26.41	8.60	0.64	1.720E-01	0.05
H	42	27.58	8.08	0.61	1.744E-01	0.05
H	43	25.38	7.20	0.38	1.880E-01	0.07
H	44	23.34	4.60	0.71	1.915E-01	0.07
H	45	23.98	-1.27	0.58	1.919E-01	0.07
H	46	22.42	4.13	0.71	1.789E-01	0.07
H	47	17.04	25.13	0.10	1.580E-01	0.16
H	48	26.47	11.39	0.43	1.750E-01	0.06
H	49	29.32	7.86	0.56	1.849E-01	0.01
H	50	30.86	10.56	0.99	1.815E-01	0.02
H	51	30.45	8.47	0.52	1.856E-01	0.01
H	52	30.70	11.65	0.31	1.795E-01	0.01
H	53	27.25	11.82	0.24	1.784E-01	0.04
H	54	27.31	9.73	0.54	1.811E-01	0.06
H	55	22.12	-12.05	0.85	2.184E-01	0.18
H	56	25.47	4.91	0.58	1.717E-01	0.01
H	57	28.94	6.71	0.49	1.767E-01	0.04
H	58	27.76	5.17	0.99	1.801E-01	0.03
H	59	23.79	4.61	0.60	1.846E-01	0.07
H	60	23.09	3.39	0.64	1.862E-01	0.06
H	61	25.11	-4.66	0.30	1.905E-01	0.05
H	62	23.84	-3.04	0.73	1.910E-01	0.05
H	63	23.67	3.54	0.75	1.903E-01	0.07
H	64	23.94	-7.08	0.32	2.409E-01	0.17
H	65	25.83	-5.40	0.55	1.822E-01	0.03
H	66	27.34	5.78	0.66	1.795E-01	0.02
H	67	27.31	7.49	0.60	1.804E-01	0.04
H	68	23.48	4.69	0.51	1.919E-01	0.07
H	69	23.91	4.50	0.52	1.896E-01	0.06
H	70	24.64	5.44	0.45	1.924E-01	0.06
H	71	23.98	4.53	0.55	1.923E-01	0.06
H	72	23.47	2.89	0.71	1.913E-01	0.08
H	73	26.36	18.18	0.18	2.658E-01	0.09
H	74	23.26	32.08	0.07	2.152E-01	0.12
H	75	23.82	26.68	0.35	2.223E-01	0.13
H	76	25.26	27.74	0.07	2.351E-01	0.12
H	77	20.90	29.29	0.14	1.768E-01	0.15
H	78	26.57	18.87	0.17	2.721E-01	0.09
H	79	18.13	27.81	0.08	1.267E-01	0.01

H	80	20.11	31.35	0.15	1.443E-01	0.03
H	81	27.27	9.96	0.41	2.256E-01	0.05
H	82	26.23	5.28	0.14	1.758E-01	0.07
H	83	27.29	7.29	0.33	1.761E-01	0.05
H	84	27.51	-5.73	0.91	1.753E-01	0.05
H	85	24.37	6.09	0.33	1.882E-01	0.07
H	86	23.25	-2.88	0.59	1.922E-01	0.05
H	87	23.32	-4.54	0.88	1.919E-01	0.08
H	88	23.35	-2.14	0.84	1.895E-01	0.06
H	89	16.83	29.81	0.13	1.507E-01	0.15
H	90	27.00	8.41	0.63	1.770E-01	0.05
H	91	29.48	9.03	0.40	1.828E-01	0.00
H	92	30.31	10.66	0.72	1.813E-01	0.02
H	93	29.50	7.71	0.36	1.867E-01	0.02
H	94	29.72	12.85	0.11	1.789E-01	0.01
H	95	27.48	10.14	0.31	1.818E-01	0.04
H	96	27.16	9.88	0.53	1.808E-01	0.06
H	97	22.18	-11.90	0.63	2.190E-01	0.17
H	98	25.95	4.45	0.75	1.749E-01	0.02
H	99	27.94	4.78	0.54	1.783E-01	0.03
H	100	28.37	7.36	0.96	1.801E-01	0.03
H	101	23.35	3.70	0.63	1.864E-01	0.07
H	102	23.86	3.09	0.62	1.885E-01	0.05
H	103	25.04	-4.34	0.30	1.887E-01	0.05
H	104	24.19	3.64	0.65	1.926E-01	0.05
H	105	24.67	-2.79	0.77	1.881E-01	0.07
H	106	19.23	17.73	0.58	1.852E-01	0.23
H	107	24.99	-5.81	0.43	1.762E-01	0.04
H	108	27.31	5.86	0.35	1.770E-01	0.03
H	109	26.47	8.93	0.37	1.801E-01	0.02
H	110	23.23	3.00	0.75	1.881E-01	0.07
H	111	23.48	3.65	0.10	1.911E-01	0.06
H	112	24.23	2.90	0.95	1.910E-01	0.06
H	113	24.50	6.38	0.36	1.899E-01	0.06
H	114	23.26	4.13	0.37	1.886E-01	0.07
H	115	24.14	11.68	0.38	1.998E-01	0.04
H	116	24.93	15.22	0.42	2.127E-01	0.02
H	117	20.14	24.30	0.46	1.570E-01	0.04
H	118	25.94	4.97	0.30	1.741E-01	0.07
H	119	26.41	8.60	0.64	1.720E-01	0.05
H	120	27.58	8.08	0.61	1.744E-01	0.05
H	121	25.38	7.20	0.38	1.880E-01	0.07
H	122	23.34	4.60	0.71	1.915E-01	0.07
H	123	23.98	-1.27	0.58	1.919E-01	0.07
H	124	22.42	4.13	0.71	1.789E-01	0.07
H	125	17.04	25.13	0.10	1.580E-01	0.16
H	126	26.47	11.39	0.43	1.750E-01	0.06
H	127	29.32	7.86	0.56	1.849E-01	0.01
H	128	30.86	10.56	0.99	1.815E-01	0.02
H	129	30.45	8.47	0.52	1.856E-01	0.01
H	130	30.70	11.65	0.31	1.795E-01	0.01
H	131	27.25	11.82	0.24	1.784E-01	0.04
H	132	27.31	9.73	0.54	1.811E-01	0.06

H	133	22.12	-12.05	0.85	2.184E-01	0.18
H	134	25.47	4.91	0.58	1.717E-01	0.01
H	135	28.94	6.71	0.49	1.767E-01	0.04
H	136	27.76	5.17	0.99	1.801E-01	0.03
H	137	23.79	4.61	0.60	1.846E-01	0.07
H	138	23.09	3.39	0.64	1.862E-01	0.06
H	139	25.11	-4.66	0.30	1.905E-01	0.05
H	140	23.84	-3.04	0.73	1.910E-01	0.05
H	141	23.67	3.54	0.75	1.903E-01	0.07
H	142	23.94	-7.08	0.32	2.409E-01	0.17
H	143	25.83	-5.40	0.55	1.822E-01	0.03
H	144	27.34	5.78	0.66	1.795E-01	0.02
H	145	27.31	7.49	0.60	1.804E-01	0.04
H	146	23.48	4.69	0.51	1.919E-01	0.07
H	147	23.91	4.50	0.52	1.896E-01	0.06
H	148	24.64	5.44	0.45	1.924E-01	0.06
H	149	23.98	4.53	0.55	1.923E-01	0.06
H	150	23.47	2.89	0.71	1.913E-01	0.08
H	151	26.36	18.18	0.18	2.658E-01	0.09
H	152	23.26	32.08	0.07	2.152E-01	0.12
H	153	23.82	26.68	0.35	2.223E-01	0.13
H	154	25.26	27.74	0.07	2.351E-01	0.12
H	155	20.90	29.29	0.14	1.768E-01	0.15
H	156	26.57	18.87	0.17	2.721E-01	0.09
C	1	118.38	23.41	0.94	2.817E+00	0.23
C	2	131.37	30.06	0.95	1.070E+00	0.66
C	3	48.52	175.44	0.64	1.819E+00	0.68
C	4	36.72	178.99	0.72	2.816E+00	0.15
C	5	53.46	150.14	0.71	2.137E+00	0.28
C	6	9.68	148.02	0.69	-3.057E+00	0.34
C	7	56.74	143.53	0.74	1.933E+00	0.27
C	8	37.88	170.25	0.80	2.692E+00	0.19
C	9	5.78	-122.41	0.77	2.687E+00	0.39
C	10	107.61	36.62	0.97	2.534E+00	0.33
C	11	143.06	-36.03	0.49	1.152E+00	0.65
C	12	150.97	-31.76	0.13	9.045E-01	0.78
C	13	124.50	46.46	0.84	2.858E+00	0.15
C	14	4.12	-122.57	0.84	3.140E+00	0.44
C	15	112.96	42.77	0.09	2.265E+00	0.72
C	16	129.93	27.96	0.34	8.650E-01	0.64
C	17	33.80	197.31	0.53	2.512E+00	0.47
C	18	38.94	174.76	0.83	2.730E+00	0.20
C	19	39.94	195.32	0.66	2.990E+00	0.09
C	20	43.03	196.17	0.65	2.934E+00	0.08
C	21	40.42	193.04	0.70	2.878E+00	0.15
C	22	41.97	178.50	0.74	2.645E+00	0.20
C	23	-1.78	124.22	0.69	3.237E+00	0.33
C	24	113.09	36.48	0.69	2.180E+00	0.51
C	25	130.73	25.31	0.57	9.192E-01	0.76
C	26	31.36	200.73	0.48	2.609E+00	0.39
C	27	38.70	168.71	0.88	2.628E+00	0.22
C	28	41.80	185.75	0.72	2.763E+00	0.19
C	29	42.60	187.19	0.68	2.718E+00	0.18

C	30	41.03	189.47	0.70	2.916E+00	0.11
C	31	39.82	183.56	0.73	2.662E+00	0.21
C	32	-10.82	109.10	0.74	3.528E+00	0.13
C	33	117.43	25.80	0.91	3.123E+00	0.25
C	34	135.26	31.45	0.71	1.194E+00	0.69
C	35	48.77	173.92	0.68	1.764E+00	0.78
C	36	36.10	174.32	0.73	2.871E+00	0.13
C	37	55.50	147.17	0.69	1.977E+00	0.27
C	38	8.69	151.57	0.63	-3.077E+00	0.33
C	39	55.92	148.81	0.71	1.988E+00	0.33
C	40	33.62	189.99	0.61	2.903E+00	0.03
C	41	5.19	-117.68	0.89	2.691E+00	0.31
C	42	108.30	-36.50	0.59	2.605E+00	0.40
C	43	142.60	-33.28	0.72	1.151E+00	0.74
C	44	153.25	-30.69	0.16	8.282E-01	0.78
C	45	124.52	49.79	0.84	3.085E+00	0.21
C	46	3.13	-119.90	0.94	3.202E+00	0.43
C	47	117.36	46.03	0.50	2.082E+00	0.88
C	48	136.88	27.53	0.06	5.765E-01	0.83
C	49	35.66	192.84	0.57	2.405E+00	0.60
C	50	41.12	175.02	0.80	2.719E+00	0.18
C	51	39.38	195.01	0.65	3.007E+00	0.07
C	52	41.56	197.84	0.65	2.988E+00	0.08
C	53	39.93	194.82	0.66	2.960E+00	0.10
C	54	39.81	179.98	0.70	2.681E+00	0.18
C	55	-0.08	120.88	0.82	3.203E+00	0.37
C	56	113.60	34.41	0.47	2.355E+00	0.47
C	57	135.48	27.48	0.31	8.364E-01	0.88
C	58	33.32	195.09	0.51	2.493E+00	0.45
C	59	40.07	175.48	0.81	2.590E+00	0.26
C	60	42.39	189.33	0.70	2.877E+00	0.12
C	61	44.51	193.09	0.70	2.874E+00	0.13
C	62	42.46	186.26	0.75	2.806E+00	0.18
C	63	39.92	170.70	0.79	2.699E+00	0.19
C	64	-12.57	111.31	0.71	3.559E+00	0.24
C	65	118.38	23.41	0.94	2.817E+00	0.23
C	66	131.37	30.06	0.95	1.070E+00	0.66
C	67	48.52	175.44	0.64	1.819E+00	0.68
C	68	36.72	178.99	0.72	2.816E+00	0.15
C	69	53.46	150.14	0.71	2.137E+00	0.28
C	70	9.68	148.02	0.69	-3.057E+00	0.34
C	71	56.74	143.53	0.74	1.933E+00	0.27
C	72	37.88	170.25	0.80	2.692E+00	0.19
C	73	5.78	-122.41	0.77	2.687E+00	0.39
C	74	107.61	36.62	0.97	2.534E+00	0.33
C	75	143.06	-36.03	0.49	1.152E+00	0.65
C	76	150.97	-31.76	0.13	9.045E-01	0.78
C	77	124.50	46.46	0.84	2.858E+00	0.15
C	78	4.12	-122.57	0.84	3.140E+00	0.44
C	79	112.96	42.77	0.09	2.265E+00	0.72
C	80	129.93	27.96	0.34	8.650E-01	0.64
C	81	33.80	197.31	0.53	2.512E+00	0.47
C	82	38.94	174.76	0.83	2.730E+00	0.20

C	83	39.94	195.32	0.66	2.990E+00	0.09
C	84	43.03	196.17	0.65	2.934E+00	0.08
C	85	40.42	193.04	0.70	2.878E+00	0.15
C	86	41.97	178.50	0.74	2.645E+00	0.20
C	87	-1.78	124.22	0.69	3.237E+00	0.33
C	88	113.09	36.48	0.69	2.180E+00	0.51
C	89	130.73	25.31	0.57	9.192E-01	0.76
C	90	31.36	200.73	0.48	2.609E+00	0.39
C	91	38.70	168.71	0.88	2.628E+00	0.22
C	92	41.80	185.75	0.72	2.763E+00	0.19
C	93	42.60	187.19	0.68	2.718E+00	0.18
C	94	41.03	189.47	0.70	2.916E+00	0.11
C	95	39.82	183.56	0.73	2.662E+00	0.21
C	96	-10.82	109.10	0.74	3.528E+00	0.13
C	97	117.43	25.80	0.91	3.123E+00	0.25
C	98	135.26	31.45	0.71	1.194E+00	0.69
C	99	48.77	173.92	0.68	1.764E+00	0.78
C	100	36.10	174.32	0.73	2.871E+00	0.13
C	101	55.50	147.17	0.69	1.977E+00	0.27
C	102	8.69	151.57	0.63	-3.077E+00	0.33
C	103	55.92	148.81	0.71	1.988E+00	0.33
C	104	33.62	189.99	0.61	2.903E+00	0.03
C	105	5.19	-117.68	0.89	2.691E+00	0.31
C	106	108.30	-36.50	0.59	2.605E+00	0.40
C	107	142.60	-33.28	0.72	1.151E+00	0.74
C	108	153.25	-30.69	0.16	8.282E-01	0.78
C	109	124.52	49.79	0.84	3.085E+00	0.21
C	110	3.13	-119.90	0.94	3.202E+00	0.43
C	111	117.36	46.03	0.50	2.082E+00	0.88
C	112	136.88	27.53	0.06	5.765E-01	0.83
C	113	35.66	192.84	0.57	2.405E+00	0.60
C	114	41.12	175.02	0.80	2.719E+00	0.18
C	115	39.38	195.01	0.65	3.007E+00	0.07
C	116	41.56	197.84	0.65	2.988E+00	0.08
C	117	39.93	194.82	0.66	2.960E+00	0.10
C	118	39.81	179.98	0.70	2.681E+00	0.18
C	119	-0.08	120.88	0.82	3.203E+00	0.37
C	120	113.60	34.41	0.47	2.355E+00	0.47
C	121	135.48	27.48	0.31	8.364E-01	0.88
C	122	33.32	195.09	0.51	2.493E+00	0.45
C	123	40.07	175.48	0.81	2.590E+00	0.26
C	124	42.39	189.33	0.70	2.877E+00	0.12
C	125	44.51	193.09	0.70	2.874E+00	0.13
C	126	42.46	186.26	0.75	2.806E+00	0.18
C	127	39.92	170.70	0.79	2.699E+00	0.19
C	128	-12.57	111.31	0.71	3.559E+00	0.24
N	1	181.77	29.03	0.49	1.536E+00	0.98
N	2	81.13	-158.85	0.64	-3.884E+00	0.14
N	3	103.17	-178.07	0.07	-3.551E+00	0.35
N	4	93.98	-161.23	0.17	-3.069E+00	0.52
N	5	181.19	39.45	0.51	1.049E+00	0.91
N	6	79.22	-152.72	0.56	-3.722E+00	0.12
N	7	103.41	-166.47	0.03	-3.743E+00	0.36

	N	8	93.36	-163.81	0.21	-3.457E+00	0.24
	N	9	181.77	29.03	0.49	1.536E+00	0.98
	N	10	81.13	-158.85	0.64	-3.884E+00	0.14
	N	11	103.17	-178.07	0.07	-3.551E+00	0.35
	N	12	93.98	-161.23	0.17	-3.069E+00	0.52
	N	13	181.19	39.45	0.51	1.049E+00	0.91
	N	14	79.22	-152.72	0.56	-3.722E+00	0.12
	N	15	103.41	-166.47	0.03	-3.743E+00	0.36
	N	16	93.36	-163.81	0.21	-3.457E+00	0.24
	O	1	152.69	119.00	0.35	-8.670E+00	0.52
	O	2	-73.67	607.18	0.46	8.754E+00	0.23
	O	3	-49.08	588.95	0.39	8.568E+00	0.23
	O	4	-19.12	481.03	0.38	8.802E+00	0.37
	O	5	-50.80	358.35	0.49	7.557E+00	0.43
	O	6	-5.73	327.94	0.64	7.978E+00	0.53
	O	7	161.21	114.21	0.62	-8.712E+00	0.55
	O	8	-57.08	582.20	0.43	8.351E+00	0.31
	O	9	-50.64	577.12	0.40	8.579E+00	0.23
	O	10	-29.38	517.25	0.29	8.310E+00	0.42
	O	11	-63.69	394.85	0.35	7.976E+00	0.31
	O	12	1.74	313.42	0.55	7.395E+00	0.66
	O	13	260.66	48.37	0.35	8.083E+00	0.85
	O	14	269.29	-31.27	0.78	7.836E+00	0.82
	O	15	252.89	-39.50	0.05	7.496E+00	0.93
	O	16	152.69	119.00	0.35	-8.670E+00	0.52
	O	17	-73.67	607.18	0.46	8.754E+00	0.23
	O	18	-49.08	588.95	0.39	8.568E+00	0.23
	O	19	-19.12	481.03	0.38	8.802E+00	0.37
	O	20	-50.80	358.35	0.49	7.557E+00	0.43
	O	21	-5.73	327.94	0.64	7.978E+00	0.53
	O	22	161.21	114.21	0.62	-8.712E+00	0.55
	O	23	-57.08	582.20	0.43	8.351E+00	0.31
	O	24	-50.64	577.12	0.40	8.579E+00	0.23
	O	25	-29.38	517.25	0.29	8.310E+00	0.42
	O	26	-63.69	394.85	0.35	7.976E+00	0.31
	O	27	1.74	313.42	0.55	7.395E+00	0.66
	O	28	260.66	48.37	0.35	8.083E+00	0.85
	O	29	269.29	-31.27	0.78	7.836E+00	0.82
	O	30	252.89	-39.50	0.05	7.496E+00	0.93

=====

GIPAW coordinates and calculated NMR parameters for fully dehydrated EM2-OH

xx

x	Element	Atom	Fractional coordinates of atoms x			
x		Number	u	v	w	x
x-----x						
x H		1	0.964592	-0.278313	0.175635	x
x H		2	0.933235	-0.096319	0.212692	x
x H		3	1.008840	-0.053684	0.190968	x
x H		4	0.886454	0.086873	0.137632	x
x H		5	0.994256	0.146647	0.107888	x
x H		6	1.005403	-0.118197	0.097190	x
x H		7	0.946566	-0.293895	0.017885	x
x H		8	0.910167	-0.254173	-0.079383	x
x H		9	0.883261	0.395807	-0.059324	x
x H		10	0.919202	0.354980	0.038069	x
x H		11	0.881462	0.240842	-0.139063	x
x H		12	0.819116	0.129306	0.059940	x
x H		13	0.705569	0.086071	-0.016133	x
x H		14	0.786356	-0.020292	-0.025101	x
x H		15	0.708302	-0.323143	-0.038735	x
x H		16	0.669252	-0.248677	0.014860	x
x H		17	0.754818	-0.478720	0.061762	x
x H		18	0.814060	-0.427914	0.019487	x
x H		19	0.735953	-0.157024	0.135944	x
x H		20	0.631355	0.168112	0.138741	x
x H		21	0.659817	-0.241511	0.199225	x
x H		22	0.596644	-0.058427	0.208849	x
x H		23	0.637577	-0.480701	0.128237	x
x H		24	0.560239	-0.618946	0.048804	x
x H		25	0.452352	-0.430027	0.008261	x
x H		26	0.423926	-0.098971	0.047790	x
x H		27	0.502625	0.041617	0.126978	x
x H		28	0.766331	-0.075378	0.232997	x
x H		29	0.799890	0.329079	0.282624	x
x H		30	0.786047	-0.070913	0.342342	x
x H		31	0.821991	0.163017	0.371454	x
x H		32	0.661227	-0.110760	0.315024	x
x H		33	0.543299	0.018998	0.316681	x
x H		34	0.527001	0.379153	0.346590	x
x H		35	0.629394	0.605975	0.372936	x
x H		36	0.747585	0.476252	0.369229	x
x H		37	0.035698	-0.165368	0.318621	x
x H		38	0.005908	0.078777	0.320707	x
x H		39	0.078260	0.026347	0.294333	x
x H		40	0.135829	0.104779	0.380853	x
x H		41	0.026607	0.210814	0.404302	x
x H		42	-0.001525	-0.047588	0.405171	x
x H		43	0.052311	-0.281972	0.479844	x
x H		44	0.080870	-0.292860	0.577307	x
x H		45	0.119130	0.358433	0.581842	x
x H		46	0.086848	0.370226	0.483950	x
x H		47	0.098973	-0.096910	0.654160	x

x H	48	0.190221	0.027447	0.468204	x
x H	49	0.304760	-0.134066	0.528241	x
x H	50	0.222055	-0.234263	0.533083	x
x H	51	0.284004	-0.547326	0.511608	x
x H	52	0.321902	-0.407886	0.465905	x
x H	53	0.224856	-0.534992	0.404179	x
x H	54	0.172643	-0.556534	0.452915	x
x H	55	0.245680	-0.169252	0.365571	x
x H	56	0.354766	0.149797	0.372089	x
x H	57	0.328013	-0.242013	0.303896	x
x H	58	0.389854	-0.050151	0.297233	x
x H	59	0.353196	-0.503287	0.368149	x
x H	60	0.434685	-0.667025	0.442358	x
x H	61	0.542999	-0.482934	0.485033	x
x H	62	0.566519	-0.132631	0.454427	x
x H	63	0.483299	0.033644	0.381996	x
x H	64	0.265101	-0.049243	0.250711	x
x H	65	0.184326	0.338519	0.232734	x
x H	66	0.253964	0.090035	0.156662	x
x H	67	0.200342	0.306146	0.138464	x
x H	68	0.369930	0.145217	0.222690	x
x H	69	0.471731	0.377649	0.243916	x
x H	70	0.461053	0.743826	0.215404	x
x H	71	0.347246	0.876843	0.167408	x
x H	72	0.244556	0.645466	0.148780	x
x H	73	-0.964592	0.221687	-0.175635	x
x H	74	-0.933235	0.403681	-0.212692	x
x H	75	-1.008840	0.446316	-0.190968	x
x H	76	-0.886454	0.586873	-0.137632	x
x H	77	-0.994256	0.646647	-0.107888	x
x H	78	-1.005403	0.381803	-0.097190	x
x H	79	-0.946566	0.206105	-0.017885	x
x H	80	-0.910167	0.245827	0.079383	x
x H	81	-0.883261	0.895807	0.059324	x
x H	82	-0.919202	0.854980	-0.038069	x
x H	83	-0.881462	0.740842	0.139063	x
x H	84	-0.819116	0.629306	-0.059940	x
x H	85	-0.705569	0.586071	0.016133	x
x H	86	-0.786356	0.479708	0.025101	x
x H	87	-0.708302	0.176857	0.038735	x
x H	88	-0.669252	0.251323	-0.014860	x
x H	89	-0.754818	0.021280	-0.061762	x
x H	90	-0.814060	0.072086	-0.019487	x
x H	91	-0.735953	0.342976	-0.135944	x
x H	92	-0.631355	0.668112	-0.138741	x
x H	93	-0.659817	0.258489	-0.199225	x
x H	94	-0.596644	0.441573	-0.208849	x
x H	95	-0.637577	0.019299	-0.128237	x
x H	96	-0.560239	-0.118946	-0.048804	x
x H	97	-0.452352	0.069973	-0.008261	x
x H	98	-0.423926	0.401029	-0.047790	x
x H	99	-0.502625	0.541617	-0.126978	x
x H	100	-0.766331	0.424622	-0.232997	x

x H	101	-0.799890	0.829079	-0.282624	x
x H	102	-0.786047	0.429087	-0.342342	x
x H	103	-0.821991	0.663017	-0.371454	x
x H	104	-0.661227	0.389240	-0.315024	x
x H	105	-0.543299	0.518998	-0.316681	x
x H	106	-0.527001	0.879153	-0.346590	x
x H	107	-0.629394	1.105975	-0.372936	x
x H	108	-0.747585	0.976252	-0.369229	x
x H	109	-0.035698	0.334632	-0.318621	x
x H	110	-0.005908	0.578777	-0.320707	x
x H	111	-0.078260	0.526347	-0.294333	x
x H	112	-0.135829	0.604779	-0.380853	x
x H	113	-0.026607	0.710814	-0.404302	x
x H	114	0.001525	0.452412	-0.405171	x
x H	115	-0.052311	0.218028	-0.479844	x
x H	116	-0.080870	0.207140	-0.577307	x
x H	117	-0.119130	0.858433	-0.581842	x
x H	118	-0.086848	0.870226	-0.483950	x
x H	119	-0.098973	0.403090	-0.654160	x
x H	120	-0.190221	0.527447	-0.468204	x
x H	121	-0.304760	0.365934	-0.528241	x
x H	122	-0.222055	0.265737	-0.533083	x
x H	123	-0.284004	-0.047326	-0.511608	x
x H	124	-0.321902	0.092114	-0.465905	x
x H	125	-0.224856	-0.034992	-0.404179	x
x H	126	-0.172643	-0.056534	-0.452915	x
x H	127	-0.245680	0.330748	-0.365571	x
x H	128	-0.354766	0.649797	-0.372089	x
x H	129	-0.328013	0.257987	-0.303896	x
x H	130	-0.389854	0.449849	-0.297233	x
x H	131	-0.353196	-0.003287	-0.368149	x
x H	132	-0.434685	-0.167025	-0.442358	x
x H	133	-0.542999	0.017066	-0.485033	x
x H	134	-0.566519	0.367369	-0.454427	x
x H	135	-0.483299	0.533644	-0.381996	x
x H	136	-0.265101	0.450757	-0.250711	x
x H	137	-0.184326	0.838519	-0.232734	x
x H	138	-0.253964	0.590035	-0.156662	x
x H	139	-0.200342	0.806146	-0.138464	x
x H	140	-0.369930	0.645217	-0.222690	x
x H	141	-0.471731	0.877649	-0.243916	x
x H	142	-0.461053	1.243826	-0.215404	x
x H	143	-0.347246	1.376843	-0.167408	x
x H	144	-0.244556	1.145466	-0.148780	x
x C	1	0.916350	-0.047757	0.129635	x
x C	2	0.966617	0.005656	0.092600	x
x C	3	0.936212	0.028443	0.034779	x
x C	4	0.931625	-0.142476	0.001203	x
x C	5	0.912088	-0.121607	-0.053270	x
x C	6	0.897337	0.074215	-0.075495	x
x C	7	0.896837	0.244750	-0.042071	x
x C	8	0.916796	0.220734	0.012360	x
x C	9	0.870277	-0.229499	0.106360	x

x C	10	0.778950	0.010350	0.056475	x
x C	11	0.745648	-0.028499	-0.001577	x
x C	12	0.717971	-0.248289	0.000039	x
x C	13	0.774855	-0.358498	0.039123	x
x C	14	0.724593	0.091921	0.086615	x
x C	15	0.666816	0.057647	0.162206	x
x C	16	0.624855	-0.120390	0.179508	x
x C	17	0.575479	-0.210170	0.132921	x
x C	18	0.591042	-0.395658	0.110362	x
x C	19	0.546901	-0.474575	0.065784	x
x C	20	0.486584	-0.368633	0.043244	x
x C	21	0.470699	-0.183085	0.065498	x
x C	22	0.514965	-0.104284	0.109965	x
x C	23	0.707829	0.182405	0.208888	x
x C	24	0.803846	0.160831	0.286374	x
x C	25	0.783393	0.097901	0.339109	x
x C	26	0.712176	0.173961	0.342216	x
x C	27	0.654170	0.047210	0.327295	x
x C	28	0.587737	0.120928	0.328125	x
x C	29	0.578555	0.321818	0.344620	x
x C	30	0.636279	0.449534	0.359576	x
x C	31	0.702463	0.376320	0.357970	x
x C	32	0.878987	0.094755	0.286395	x
x C	33	0.094158	-0.008438	0.379405	x
x C	34	0.043997	0.053893	0.415779	x
x C	35	0.069303	0.044286	0.474501	x
x C	36	0.068457	-0.141276	0.501836	x
x C	37	0.084267	-0.148374	0.556708	x
x C	38	0.101491	0.032406	0.586254	x
x C	39	0.105177	0.218170	0.559127	x
x C	40	0.088281	0.222820	0.504269	x
x C	41	0.122365	-0.228963	0.390949	x
x C	42	0.223694	-0.094434	0.457849	x
x C	43	0.259072	-0.215150	0.506703	x
x C	44	0.275253	-0.421062	0.483057	x
x C	45	0.211835	-0.461671	0.439277	x
x C	46	0.277460	0.010121	0.430897	x
x C	47	0.319641	0.042512	0.347061	x
x C	48	0.362385	-0.123409	0.325560	x
x C	49	0.413215	-0.225524	0.369461	x
x C	50	0.400253	-0.422673	0.387066	x
x C	51	0.446452	-0.514879	0.428617	x
x C	52	0.506618	-0.411467	0.452744	x
x C	53	0.519798	-0.214381	0.435525	x
x C	54	0.473053	-0.121604	0.394534	x
x C	55	0.270983	0.177253	0.306545	x
x C	56	0.199831	0.194400	0.216167	x
x C	57	0.238166	0.238804	0.170855	x
x C	58	0.299754	0.379955	0.185140	x
x C	59	0.364330	0.307381	0.211822	x
x C	60	0.421815	0.437511	0.223469	x
x C	61	0.415791	0.643363	0.207879	x
x C	62	0.351874	0.717690	0.181071	x

x C	63	0.294291	0.587746	0.170208	x
x C	64	0.133783	0.061883	0.197348	x
x C	65	-0.916350	0.452243	-0.129635	x
x C	66	-0.966617	0.505656	-0.092600	x
x C	67	-0.936212	0.528443	-0.034779	x
x C	68	-0.931625	0.357524	-0.001203	x
x C	69	-0.912088	0.378393	0.053270	x
x C	70	-0.897337	0.574215	0.075495	x
x C	71	-0.896837	0.744750	0.042071	x
x C	72	-0.916796	0.720734	-0.012360	x
x C	73	-0.870277	0.270501	-0.106360	x
x C	74	-0.778950	0.510350	-0.056475	x
x C	75	-0.745648	0.471501	0.001577	x
x C	76	-0.717971	0.251711	-0.000039	x
x C	77	-0.774855	0.141502	-0.039123	x
x C	78	-0.724593	0.591921	-0.086615	x
x C	79	-0.666816	0.557647	-0.162206	x
x C	80	-0.624855	0.379610	-0.179508	x
x C	81	-0.575479	0.289830	-0.132921	x
x C	82	-0.591042	0.104342	-0.110362	x
x C	83	-0.546901	0.025425	-0.065784	x
x C	84	-0.486584	0.131367	-0.043244	x
x C	85	-0.470699	0.316915	-0.065498	x
x C	86	-0.514965	0.395716	-0.109965	x
x C	87	-0.707829	0.682405	-0.208888	x
x C	88	-0.803846	0.660831	-0.286374	x
x C	89	-0.783393	0.597901	-0.339109	x
x C	90	-0.712176	0.673961	-0.342216	x
x C	91	-0.654170	0.547210	-0.327295	x
x C	92	-0.587737	0.620928	-0.328125	x
x C	93	-0.578555	0.821818	-0.344620	x
x C	94	-0.636279	0.949534	-0.359576	x
x C	95	-0.702463	0.876320	-0.357970	x
x C	96	-0.878987	0.594755	-0.286395	x
x C	97	-0.094158	0.491562	-0.379405	x
x C	98	-0.043997	0.553893	-0.415779	x
x C	99	-0.069303	0.544286	-0.474501	x
x C	100	-0.068457	0.358724	-0.501836	x
x C	101	-0.084267	0.351626	-0.556708	x
x C	102	-0.101491	0.532406	-0.586254	x
x C	103	-0.105177	0.718170	-0.559127	x
x C	104	-0.088281	0.722820	-0.504269	x
x C	105	-0.122365	0.271037	-0.390949	x
x C	106	-0.223694	0.405566	-0.457849	x
x C	107	-0.259072	0.284850	-0.506703	x
x C	108	-0.275253	0.078938	-0.483057	x
x C	109	-0.211835	0.038329	-0.439277	x
x C	110	-0.277460	0.510121	-0.430897	x
x C	111	-0.319641	0.542512	-0.347061	x
x C	112	-0.362385	0.376591	-0.325560	x
x C	113	-0.413215	0.274476	-0.369461	x
x C	114	-0.400253	0.077327	-0.387066	x
x C	115	-0.446452	-0.014879	-0.428617	x

x C	116	-0.506618	0.088533	-0.452744	x
x C	117	-0.519798	0.285619	-0.435525	x
x C	118	-0.473053	0.378396	-0.394534	x
x C	119	-0.270983	0.677253	-0.306545	x
x C	120	-0.199831	0.694400	-0.216167	x
x C	121	-0.238166	0.738804	-0.170855	x
x C	122	-0.299754	0.879955	-0.185140	x
x C	123	-0.364330	0.807381	-0.211822	x
x C	124	-0.421815	0.937511	-0.223469	x
x C	125	-0.415791	1.143363	-0.207879	x
x C	126	-0.351874	1.217690	-0.181071	x
x C	127	-0.294291	1.087746	-0.170208	x
x C	128	-0.133783	0.561883	-0.197348	x
x N	1	0.958996	-0.121353	0.180719	x
x N	2	0.809121	-0.191206	0.073822	x
x N	3	0.713027	-0.017142	0.128636	x
x N	4	0.756776	0.072772	0.241887	x
x N	5	0.051649	-0.013160	0.324442	x
x N	6	0.182389	-0.254036	0.425775	x
x N	7	0.276640	-0.049542	0.380499	x
x N	8	0.245076	0.087936	0.259407	x
x N	9	-0.958996	0.378647	-0.180719	x
x N	10	-0.809121	0.308794	-0.073822	x
x N	11	-0.713027	0.482858	-0.128636	x
x N	12	-0.756776	0.572772	-0.241887	x
x N	13	-0.051649	0.486840	-0.324442	x
x N	14	-0.182389	0.245964	-0.425775	x
x N	15	-0.276640	0.450458	-0.380499	x
x N	16	-0.245076	0.587936	-0.259407	x
x O	1	0.885111	0.091020	-0.128780	x
x O	2	0.893495	-0.406585	0.115609	x
x O	3	0.694432	0.254392	0.072015	x
x O	4	0.696494	0.366571	0.214673	x
x O	5	0.926528	0.192870	0.317596	x
x O	6	0.888959	-0.053401	0.257534	x
x O	7	0.113856	0.036005	0.639472	x
x O	8	0.088349	-0.375095	0.368037	x
x O	9	0.316706	0.141130	0.454762	x
x O	10	0.254284	0.350691	0.319090	x
x O	11	0.090427	0.044883	0.227788	x
x O	12	0.127179	-0.021096	0.152649	x
x O	13	-0.885111	0.591020	0.128780	x
x O	14	-0.893495	0.093415	-0.115609	x
x O	15	-0.694432	0.754392	-0.072015	x
x O	16	-0.696494	0.866571	-0.214673	x
x O	17	-0.926528	0.692870	-0.317596	x
x O	18	-0.888959	0.446599	-0.257534	x
x O	19	-0.113856	0.536005	-0.639472	x
x O	20	-0.088349	0.124905	-0.368037	x
x O	21	-0.316706	0.641130	-0.454762	x
x O	22	-0.254284	0.850691	-0.319090	x
x O	23	-0.090427	0.544883	-0.227788	x
x O	24	-0.127179	0.478904	-0.152649	x

xx

Chemical Shielding and Electric Field Gradient Tensors						
Nucleus		Shielding tensor		EFG Tensor		
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
H	1	24.44	11.88	0.37	2.005E-01	0.03
H	2	18.78	32.78	0.17	1.317E-01	0.04
H	3	19.73	25.20	0.34	1.447E-01	0.04
H	4	25.96	-4.42	0.90	1.761E-01	0.07
H	5	26.67	6.91	0.96	1.785E-01	0.05
H	6	27.16	7.01	0.92	1.761E-01	0.06
H	7	24.68	6.31	0.30	1.880E-01	0.07
H	8	22.90	-5.45	0.10	1.862E-01	0.07
H	9	22.78	-3.75	0.76	1.888E-01	0.07
H	10	23.14	3.12	0.95	1.843E-01	0.07
H	11	18.43	28.91	0.23	1.791E-01	0.17
H	12	26.26	6.60	0.93	1.767E-01	0.06
H	13	29.65	8.25	0.30	1.828E-01	0.00
H	14	30.96	13.53	0.51	1.784E-01	0.02
H	15	29.90	8.96	0.18	1.856E-01	0.01
H	16	30.48	12.50	0.21	1.779E-01	0.00
H	17	26.06	14.38	0.18	1.714E-01	0.04
H	18	27.51	8.96	0.39	1.777E-01	0.06
H	19	24.85	-7.46	0.88	2.472E-01	0.17
H	20	26.38	3.93	0.30	1.732E-01	0.03
H	21	27.77	-5.79	0.90	1.731E-01	0.02
H	22	27.89	7.77	0.96	1.794E-01	0.02
H	23	22.96	4.67	0.96	1.840E-01	0.07
H	24	23.93	4.67	0.51	1.901E-01	0.05
H	25	25.33	-4.50	0.38	1.901E-01	0.06
H	26	24.35	3.15	0.67	1.913E-01	0.06
H	27	24.47	3.94	0.46	1.887E-01	0.07
H	28	24.48	-6.61	0.66	2.472E-01	0.19
H	29	25.20	-5.38	0.57	1.721E-01	0.03
H	30	27.58	6.74	0.47	1.770E-01	0.02
H	31	26.33	8.70	0.42	1.824E-01	0.01
H	32	23.54	4.25	0.65	1.885E-01	0.07
H	33	23.33	4.77	0.33	1.914E-01	0.07
H	34	24.84	6.06	0.76	1.885E-01	0.07
H	35	24.02	5.65	0.70	1.893E-01	0.06
H	36	23.28	4.18	0.69	1.879E-01	0.07
H	37	24.24	10.97	0.63	1.945E-01	0.04
H	38	18.10	26.39	0.29	1.247E-01	0.08
H	39	20.75	27.37	0.27	1.582E-01	0.04
H	40	26.28	5.97	0.38	1.753E-01	0.06
H	41	26.75	7.24	0.67	1.764E-01	0.04
H	42	27.39	-5.50	0.87	1.732E-01	0.05
H	43	24.83	7.09	0.29	1.893E-01	0.07
H	44	22.93	-2.99	0.94	1.922E-01	0.07

H	45	23.19	-3.49	0.59	1.924E-01	0.06
H	46	23.69	-2.84	0.29	1.906E-01	0.06
H	47	17.87	25.40	0.16	1.747E-01	0.15
H	48	27.21	10.94	0.43	1.756E-01	0.05
H	49	30.08	9.98	0.40	1.826E-01	0.01
H	50	30.39	10.17	0.86	1.806E-01	0.02
H	51	29.74	6.79	0.60	1.857E-01	0.03
H	52	30.04	13.93	0.08	1.780E-01	0.02
H	53	26.63	10.72	0.27	1.708E-01	0.06
H	54	27.18	11.41	0.53	1.806E-01	0.06
H	55	24.90	7.83	0.96	2.451E-01	0.17
H	56	25.76	4.59	0.82	1.729E-01	0.01
H	57	29.22	7.78	0.62	1.742E-01	0.04
H	58	27.46	5.05	0.56	1.805E-01	0.02
H	59	23.03	3.96	0.75	1.789E-01	0.07
H	60	23.10	3.52	0.55	1.868E-01	0.06
H	61	24.56	-4.14	0.26	1.887E-01	0.05
H	62	23.94	2.62	0.80	1.902E-01	0.05
H	63	23.28	4.63	0.28	1.895E-01	0.06
H	64	24.43	-9.50	0.26	2.426E-01	0.18
H	65	25.31	-3.00	0.53	1.747E-01	0.02
H	66	27.43	5.97	0.77	1.809E-01	0.02
H	67	26.55	9.86	0.86	1.814E-01	0.04
H	68	23.16	3.35	0.70	1.914E-01	0.07
H	69	23.82	2.78	0.93	1.888E-01	0.06
H	70	24.22	3.81	0.65	1.921E-01	0.06
H	71	23.19	-3.37	0.32	1.904E-01	0.06
H	72	22.77	-5.05	0.85	1.867E-01	0.06
H	73	24.44	11.88	0.37	2.005E-01	0.03
H	74	18.78	32.78	0.17	1.317E-01	0.04
H	75	19.73	25.20	0.34	1.447E-01	0.04
H	76	25.96	-4.42	0.90	1.761E-01	0.07
H	77	26.67	6.91	0.96	1.785E-01	0.05
H	78	27.16	7.01	0.92	1.761E-01	0.06
H	79	24.68	6.31	0.30	1.880E-01	0.07
H	80	22.90	-5.45	0.10	1.862E-01	0.07
H	81	22.78	-3.75	0.76	1.888E-01	0.07
H	82	23.14	3.12	0.95	1.843E-01	0.07
H	83	18.43	28.91	0.23	1.791E-01	0.17
H	84	26.26	6.60	0.93	1.767E-01	0.06
H	85	29.65	8.25	0.30	1.828E-01	0.00
H	86	30.96	13.53	0.51	1.784E-01	0.02
H	87	29.90	8.96	0.18	1.856E-01	0.01
H	88	30.48	12.50	0.21	1.779E-01	0.00
H	89	26.06	14.38	0.18	1.714E-01	0.04
H	90	27.51	8.96	0.39	1.777E-01	0.06
H	91	24.85	-7.46	0.88	2.472E-01	0.17
H	92	26.38	3.93	0.30	1.732E-01	0.03
H	93	27.77	-5.79	0.90	1.731E-01	0.02
H	94	27.89	7.77	0.96	1.794E-01	0.02
H	95	22.96	4.67	0.96	1.840E-01	0.07
H	96	23.93	4.67	0.51	1.901E-01	0.05
H	97	25.33	-4.50	0.38	1.901E-01	0.06

H	98	24.35	3.15	0.67	1.913E-01	0.06
H	99	24.47	3.94	0.46	1.887E-01	0.07
H	100	24.48	-6.61	0.66	2.472E-01	0.19
H	101	25.20	-5.38	0.57	1.721E-01	0.03
H	102	27.58	6.74	0.47	1.770E-01	0.02
H	103	26.33	8.70	0.42	1.824E-01	0.01
H	104	23.54	4.25	0.65	1.885E-01	0.07
H	105	23.33	4.77	0.33	1.914E-01	0.07
H	106	24.84	6.06	0.76	1.885E-01	0.07
H	107	24.02	5.65	0.70	1.893E-01	0.06
H	108	23.28	4.18	0.69	1.879E-01	0.07
H	109	24.24	10.97	0.63	1.945E-01	0.04
H	110	18.10	26.39	0.29	1.247E-01	0.08
H	111	20.75	27.37	0.27	1.582E-01	0.04
H	112	26.28	5.97	0.38	1.753E-01	0.06
H	113	26.75	7.24	0.67	1.764E-01	0.04
H	114	27.39	-5.50	0.87	1.732E-01	0.05
H	115	24.83	7.09	0.29	1.893E-01	0.07
H	116	22.93	-2.99	0.94	1.922E-01	0.07
H	117	23.19	-3.49	0.59	1.924E-01	0.06
H	118	23.69	-2.84	0.29	1.906E-01	0.06
H	119	17.87	25.40	0.16	1.747E-01	0.15
H	120	27.21	10.94	0.43	1.756E-01	0.05
H	121	30.08	9.98	0.40	1.826E-01	0.01
H	122	30.39	10.17	0.86	1.806E-01	0.02
H	123	29.74	6.79	0.60	1.857E-01	0.03
H	124	30.04	13.93	0.08	1.780E-01	0.02
H	125	26.63	10.72	0.27	1.708E-01	0.06
H	126	27.18	11.41	0.53	1.806E-01	0.06
H	127	24.90	7.83	0.96	2.451E-01	0.17
H	128	25.76	4.59	0.82	1.729E-01	0.01
H	129	29.22	7.78	0.62	1.742E-01	0.04
H	130	27.46	5.05	0.56	1.805E-01	0.02
H	131	23.03	3.96	0.75	1.789E-01	0.07
H	132	23.10	3.52	0.55	1.868E-01	0.06
H	133	24.56	-4.14	0.26	1.887E-01	0.05
H	134	23.94	2.62	0.80	1.902E-01	0.05
H	135	23.28	4.63	0.28	1.895E-01	0.06
H	136	24.43	-9.50	0.26	2.426E-01	0.18
H	137	25.31	-3.00	0.53	1.747E-01	0.02
H	138	27.43	5.97	0.77	1.809E-01	0.02
H	139	26.55	9.86	0.86	1.814E-01	0.04
H	140	23.16	3.35	0.70	1.914E-01	0.07
H	141	23.82	2.78	0.93	1.888E-01	0.06
H	142	24.22	3.81	0.65	1.921E-01	0.06
H	143	23.19	-3.37	0.32	1.904E-01	0.06
H	144	22.77	-5.05	0.85	1.867E-01	0.06
C	1	118.77	-29.85	0.90	2.793E+00	0.28
C	2	129.80	29.19	0.81	1.197E+00	0.57
C	3	49.17	174.43	0.63	1.761E+00	0.70
C	4	34.70	180.76	0.69	2.785E+00	0.17
C	5	54.32	150.01	0.66	2.088E+00	0.23
C	6	9.61	147.92	0.67	-3.077E+00	0.30

C	7	56.53	151.64	0.63	1.973E+00	0.25
C	8	33.89	180.77	0.68	2.772E+00	0.14
C	9	2.89	-116.92	0.97	2.819E+00	0.32
C	10	107.25	-33.23	0.97	2.576E+00	0.36
C	11	143.48	-34.85	0.42	1.213E+00	0.70
C	12	153.09	-28.46	0.20	7.587E-01	0.80
C	13	124.16	47.04	0.78	3.151E+00	0.29
C	14	2.88	-119.60	0.93	3.168E+00	0.46
C	15	112.26	42.15	0.31	2.439E+00	0.60
C	16	134.43	28.29	0.08	8.274E-01	0.66
C	17	32.50	197.35	0.52	2.507E+00	0.50
C	18	37.70	179.39	0.76	2.900E+00	0.09
C	19	39.41	193.96	0.67	2.998E+00	0.08
C	20	44.30	189.67	0.71	2.782E+00	0.16
C	21	41.44	189.12	0.74	2.791E+00	0.17
C	22	43.42	174.37	0.80	2.525E+00	0.26
C	23	3.08	-122.29	0.89	3.120E+00	0.50
C	24	116.42	36.50	0.97	2.099E+00	0.61
C	25	128.83	20.21	0.52	7.929E-01	0.76
C	26	31.44	200.04	0.48	2.555E+00	0.42
C	27	39.53	168.30	0.88	2.623E+00	0.23
C	28	41.82	184.66	0.73	2.749E+00	0.20
C	29	43.46	189.22	0.68	2.775E+00	0.13
C	30	40.23	186.99	0.74	2.831E+00	0.14
C	31	39.51	180.09	0.74	2.636E+00	0.21
C	32	-10.11	108.96	0.70	3.544E+00	0.21
C	33	117.93	-26.71	0.94	2.778E+00	0.29
C	34	130.51	27.32	0.84	1.103E+00	0.62
C	35	50.09	173.40	0.64	1.749E+00	0.65
C	36	36.24	180.06	0.69	2.754E+00	0.17
C	37	54.52	147.96	0.65	1.896E+00	0.29
C	38	8.62	150.34	0.61	-3.007E+00	0.40
C	39	55.18	145.29	0.71	1.973E+00	0.30
C	40	35.11	172.17	0.77	2.679E+00	0.22
C	41	5.21	-119.99	0.86	2.736E+00	0.34
C	42	108.23	34.39	0.79	2.643E+00	0.35
C	43	140.95	-32.28	0.59	1.218E+00	0.58
C	44	151.73	-31.83	0.35	1.030E+00	0.71
C	45	123.82	49.11	0.74	3.062E+00	0.18
C	46	4.51	-125.59	0.85	3.147E+00	0.50
C	47	115.16	47.89	0.14	2.253E+00	0.71
C	48	135.47	21.73	0.27	6.214E-01	0.77
C	49	34.21	195.35	0.55	2.443E+00	0.56
C	50	39.07	179.67	0.75	2.825E+00	0.10
C	51	39.10	194.60	0.67	2.950E+00	0.09
C	52	41.20	196.52	0.65	2.911E+00	0.09
C	53	40.04	193.00	0.68	2.889E+00	0.12
C	54	39.72	179.24	0.71	2.617E+00	0.21
C	55	1.83	-123.81	0.93	3.139E+00	0.44
C	56	115.25	49.66	0.57	2.435E+00	0.61
C	57	134.02	27.59	0.39	-8.466E-01	0.77
C	58	28.16	203.95	0.45	2.721E+00	0.31
C	59	40.26	171.83	0.85	2.546E+00	0.28

C	60	42.23	188.96	0.74	2.865E+00	0.13
C	61	43.54	191.76	0.71	2.726E+00	0.17
C	62	41.40	186.32	0.77	2.744E+00	0.22
C	63	40.52	174.54	0.79	2.737E+00	0.13
C	64	-8.93	101.86	0.79	3.498E+00	0.16
C	65	118.77	-29.85	0.90	2.793E+00	0.28
C	66	129.80	29.19	0.81	1.197E+00	0.57
C	67	49.17	174.43	0.63	1.761E+00	0.70
C	68	34.70	180.76	0.69	2.785E+00	0.17
C	69	54.32	150.01	0.66	2.088E+00	0.23
C	70	9.61	147.92	0.67	-3.077E+00	0.30
C	71	56.53	151.64	0.63	1.973E+00	0.25
C	72	33.89	180.77	0.68	2.772E+00	0.14
C	73	2.89	-116.92	0.97	2.819E+00	0.32
C	74	107.25	-33.23	0.97	2.576E+00	0.36
C	75	143.48	-34.85	0.42	1.213E+00	0.70
C	76	153.09	-28.46	0.20	7.587E-01	0.80
C	77	124.16	47.04	0.78	3.151E+00	0.29
C	78	2.88	-119.60	0.93	3.168E+00	0.46
C	79	112.26	42.15	0.31	2.439E+00	0.60
C	80	134.43	28.29	0.08	8.274E-01	0.66
C	81	32.50	197.35	0.52	2.507E+00	0.50
C	82	37.70	179.39	0.76	2.900E+00	0.09
C	83	39.41	193.96	0.67	2.998E+00	0.08
C	84	44.30	189.67	0.71	2.782E+00	0.16
C	85	41.44	189.12	0.74	2.791E+00	0.17
C	86	43.42	174.37	0.80	2.525E+00	0.26
C	87	3.08	-122.29	0.89	3.120E+00	0.50
C	88	116.42	36.50	0.97	2.099E+00	0.61
C	89	128.83	20.21	0.52	7.929E-01	0.76
C	90	31.44	200.04	0.48	2.555E+00	0.42
C	91	39.53	168.30	0.88	2.623E+00	0.23
C	92	41.82	184.66	0.73	2.749E+00	0.20
C	93	43.46	189.22	0.68	2.775E+00	0.13
C	94	40.23	186.99	0.74	2.831E+00	0.14
C	95	39.51	180.09	0.74	2.636E+00	0.21
C	96	-10.11	108.96	0.70	3.544E+00	0.21
C	97	117.93	-26.71	0.94	2.778E+00	0.29
C	98	130.51	27.32	0.84	1.103E+00	0.62
C	99	50.09	173.40	0.64	1.749E+00	0.65
C	100	36.24	180.06	0.69	2.754E+00	0.17
C	101	54.52	147.96	0.65	1.896E+00	0.29
C	102	8.62	150.34	0.61	-3.007E+00	0.40
C	103	55.18	145.29	0.71	1.973E+00	0.30
C	104	35.11	172.17	0.77	2.679E+00	0.22
C	105	5.21	-119.99	0.86	2.736E+00	0.34
C	106	108.23	34.39	0.79	2.643E+00	0.35
C	107	140.95	-32.28	0.59	1.218E+00	0.58
C	108	151.73	-31.83	0.35	1.030E+00	0.71
C	109	123.82	49.11	0.74	3.062E+00	0.18
C	110	4.51	-125.59	0.85	3.147E+00	0.50
C	111	115.16	47.89	0.14	2.253E+00	0.71
C	112	135.47	21.73	0.27	6.214E-01	0.77

C	113	34.21	195.35	0.55	2.443E+00	0.56
C	114	39.07	179.67	0.75	2.825E+00	0.10
C	115	39.10	194.60	0.67	2.950E+00	0.09
C	116	41.20	196.52	0.65	2.911E+00	0.09
C	117	40.04	193.00	0.68	2.889E+00	0.12
C	118	39.72	179.24	0.71	2.617E+00	0.21
C	119	1.83	-123.81	0.93	3.139E+00	0.44
C	120	115.25	49.66	0.57	2.435E+00	0.61
C	121	134.02	27.59	0.39	-8.466E-01	0.77
C	122	28.16	203.95	0.45	2.721E+00	0.31
C	123	40.26	171.83	0.85	2.546E+00	0.28
C	124	42.23	188.96	0.74	2.865E+00	0.13
C	125	43.54	191.76	0.71	2.726E+00	0.17
C	126	41.40	186.32	0.77	2.744E+00	0.22
C	127	40.52	174.54	0.79	2.737E+00	0.13
C	128	-8.93	101.86	0.79	3.498E+00	0.16
N	1	186.09	29.07	0.52	1.469E+00	0.67
N	2	82.65	-151.18	0.60	-3.751E+00	0.12
N	3	101.48	-175.13	0.26	-3.813E+00	0.19
N	4	111.13	-145.99	0.20	-4.006E+00	0.18
N	5	185.65	26.57	0.58	1.466E+00	0.51
N	6	80.58	-152.85	0.58	-3.746E+00	0.10
N	7	101.85	-165.58	0.18	-3.859E+00	0.22
N	8	102.78	-146.03	0.08	-3.777E+00	0.15
N	9	186.09	29.07	0.52	1.469E+00	0.67
N	10	82.65	-151.18	0.60	-3.751E+00	0.12
N	11	101.48	-175.13	0.26	-3.813E+00	0.19
N	12	111.13	-145.99	0.20	-4.006E+00	0.18
N	13	185.65	26.57	0.58	1.466E+00	0.51
N	14	80.58	-152.85	0.58	-3.746E+00	0.10
N	15	101.85	-165.58	0.18	-3.859E+00	0.22
N	16	102.78	-146.03	0.08	-3.777E+00	0.15
O	1	162.72	112.31	0.62	-8.702E+00	0.58
O	2	-55.06	586.32	0.42	8.353E+00	0.29
O	3	-58.83	585.38	0.40	8.716E+00	0.22
O	4	-68.19	557.23	0.43	9.121E+00	0.14
O	5	-18.22	298.19	0.69	6.099E+00	0.90
O	6	-15.84	385.42	0.52	8.082E+00	0.44
O	7	159.91	120.41	0.59	-8.866E+00	0.58
O	8	-53.07	584.29	0.44	8.270E+00	0.29
O	9	-52.42	601.71	0.39	8.583E+00	0.21
O	10	-54.37	544.33	0.38	8.734E+00	0.22
O	11	-19.16	285.67	0.67	7.101E+00	0.69
O	12	-46.21	386.80	0.56	8.501E+00	0.35
O	13	162.72	112.31	0.62	-8.702E+00	0.58
O	14	-55.06	586.32	0.42	8.353E+00	0.29
O	15	-58.83	585.38	0.40	8.716E+00	0.22
O	16	-68.19	557.23	0.43	9.121E+00	0.14
O	17	-18.22	298.19	0.69	6.099E+00	0.90
O	18	-15.84	385.42	0.52	8.082E+00	0.44
O	19	159.91	120.41	0.59	-8.866E+00	0.58
O	20	-53.07	584.29	0.44	8.270E+00	0.29
O	21	-52.42	601.71	0.39	8.583E+00	0.21

	O	22	-54.37	544.33	0.38	8.734E+00	0.22
	O	23	-19.16	285.67	0.67	7.101E+00	0.69
	O	24	-46.21	386.80	0.56	8.501E+00	0.35

---