Supplementary Material

to

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Z. Naturforsch, **59b**, pppp (2004).

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Table S1: HF calculated absolute ^{1}H shieldings of molecules **1** to **7**

	Basis Set	**1**	**2**	**3**	**4**	**5**		**6**			**7**
						H^1	H^2	H^2	H^1	H^3	
HF	STO-3G	32.762	32.745	27.411	31.128	32.714	32.710	27.561	27.716	26.732	25.684
	STO-6G	32.983	32.958	27.530	31.352	32.922	32.902	27.697	27.844	26.828	25.790
	3-21G	32.995	32.736	27.370	31.371	32.679	32.496	27.847	27.787	26.924	26.027
	6-31G	32.919	32.546	27.141	31.350	32.487	32.221	27.713	27.612	26.457	25.646
	6-31G*	32.294	31.853	27.018	30.850	31.818	31.496	27.526	27.416	26.243	25.189
	6-31+G*	32.276	31.788	26.902	30.709	31.751	31.422	27.447	27.235	25.880	25.034
	6-31++G*	32.260	31.783	26.913	30.730	31.743	31.432	27.467	27.244	25.871	25.029
	6-31G**	31.738	31.346	26.364	30.462	31.323	31.012	26.883	26.748	25.651	24.580
	6-31+G**	31.721	31.304	26.248	30.307	31.273	30.990	26.799	26.572	25.308	24.432
	6-31++G**	31.720	31.302	26.254	30.312	31.271	30.985	26.806	26.575	25.312	24.427
	6-311G	32.821	32.405	27.177	31.093	32.352	32.040	27.715	27.641	26.469	25.635
	6-311G*	32.184	31.699	26.917	30.860	31.667	31.362	27.400	27.256	26.057	25.044
	6-311+G*	32.160	31.671	26.828	30.786	31.642	31.327	27.374	27.155	25.821	24.945
	6-311++G*	32.173	31.676	26.843	30.806	31.644	31.327	27.376	27.174	25.815	24.955
	6-311G**	31.872	31.463	26.508	30.656	31.433	31.175	26.995	26.830	25.688	24.675
	6-311+G**	31.863	31.447	26.438	30.583	31.422	31.158	26.985	26.752	25.488	24.587
	6-311++G**	31.868	31.449	26.451	30.595	31.421	31.154	26.982	26.772	25.488	24.598
	cc-pVDZ	31.641	31.279	26.339	30.378	31.247	31.032	26.824	26.683	25.632	24.559
	cc-pVTZ	31.623	31.217	26.251	30.329	31.188	30.922	26.724	26.593	25.360	24.372
	cc-pVQZ	31.573	31.160	26.184	30.292	31.128	30.860	26.649	26.520	25.244	24.265
	cc-pV5Z	31.541	31.128	26.141	30.253	31.098	30.830	26.617	26.469	25.179	24.220
	aug-cc-pVDZ	31.719	31.269	26.248	30.357	31.230	30.979	26.732	26.590	25.329	24.426
	aug-cc-pVTZ	31.619	31.207	26.218	30.314	31.177	30.910	26.695	26.548	25.254	24.311
	aug-cc-pVQZ	31.572	31.156	26.170	30.282	31.125	30.856	26.645	26.493	25.199	24.247
	aug-cc-pV5Z	31.541	31.128	26.138	30.250	31.098	30.830	26.613	26.464	25.170	24.214
	range	*1.455*	*1.830*	*1.392*	*1.121*	*1.825*	*2.073*	*1.234*	*1.380*	*1.754*	*1.813*

Table S2: MP2 and B3LYP calculated absolute ^{1}H shieldings of molecules **1** to **7**

	Basis Set	**1**	**2**	**3**	**4**	**5**		**6**			**7**
						H^1	H^2	H^2	H^1	H^3	
MP2	6-31G	32.607	32.109	27.535	31.388	32.011	31.668	27.940	27.833	26.821	25.784
	6-31G*	31.885	31.307	26.827	30.521	31.228	30.798	27.192	27.128	26.014	24.738
	6-31G**	31.645	31.121	26.528	30.411	31.054	30.653	26.904	26.804	25.755	24.448
	6-31++G**	31.616	31.051	26.353	30.209	30.978	30.598	26.763	26.577	25.379	24.237
	6-311G	32.527	31.958	27.480	31.180	31.865	31.480	27.845	27.768	26.728	25.674
	6-311G*	31.839	31.187	26.662	30.495	31.104	30.678	27.015	26.901	25.746	24.531
	6-311G**	31.779	31.212	26.563	30.550	31.132	30.772	26.916	26.778	25.678	24.443
	6-311++G**	31.769	31.194	26.485	30.474	31.110	30.750	26.878	26.700	25.484	24.339
	cc-pVDZ	31.514	31.007	26.386	30.246	30.930	30.613	26.746	26.634	25.622	24.360
	cc-pVTZ	31.429	30.874	26.144	30.191	30.792	30.428	26.503	26.396	25.194	23.981
	cc-pVQZ	31.318		25.985	30.094						
	aug-cc-pVDZ	31.603	31.000	26.271	30.276	30.908	30.570	26.635	26.521	25.302	24.197
	aug-cc-pVTZ	31.412	30.840	26.073	30.158	30.755	30.384				
	aug-cc-pVQZ	31.310			30.076						
	range	*1.297*	*1.270*	*1.550*	*1.312*	*1.256*	*1.285*	*1.438*	*1.437*	*1.627*	*1.802*
B3LYP	6-31G	32.616	32.058	27.017	31.565	31.971	31.555	27.573	27.468	26.357	25.636
	6-31G*	32.130	31.497	26.771	31.132	31.432	30.942	27.279	27.200	26.041	25.102
	6-31G**	31.679	31.065	26.139	30.694	31.012	30.516	26.662	26.556	25.437	24.480
	6-31++G**	31.652	30.992	25.978	30.422	30.939	30.476	26.519	26.359	25.095	24.281
	6-311G	32.638	32.027	27.089	31.349	31.941	31.531	27.574	27.520	26.402	25.639
	6-311G*	32.177	31.471	26.726	31.053	31.404	30.952	27.206	27.085	25.872	24.961
	6-311G**	31.911	31.252	26.308	30.870	31.190	30.765	26.793	26.652	25.492	24.568
	6-311++G**	31.899	31.231	26.242	30.791	31.169	30.744	26.742	26.610	25.303	24.484
	cc-pVDZ	31.500	30.895	25.996	30.490	30.840	30.423	26.490	26.385	25.303	24.383
	cc-pVTZ	31.593	30.946	25.968	30.542	30.888	30.456	26.439	26.339	25.077	24.176
	cc-pVQZ	31.541	30.884	25.891	30.480	30.823	30.395	26.357	26.257	24.949	24.059
	cc-pV5Z	31.502	30.849	25.845	30.442	30.791	30.362	26.321	26.206	24.880	24.010
	aug-cc-pVDZ	31.660	30.963	25.919	30.506	30.910	30.465	26.377	26.301	24.988	24.173
	aug-cc-pVTZ	31.592	30.929	25.923	30.494	30.867	30.434	26.411	26.296	24.961	24.088
	aug-cc-pVQZ	31.537	30.878	25.876	30.470	30.815	30.389	26.363	26.235	24.896	24.039
	aug-cc-pV5Z	31.496	30.851	25.845	30.436	30.797	30.379	26.331	26.205	24.856	
	range	*1.142*	*1.209*	*1.244*	*1.143*	*1.180*	*1.193*	*1.254*	*1.316*	*1.546*	*1.629*

Table S3: Statistical parameters of linear regressions of HF calculated absolute ^{1}H shieldings of molecules **1** to **7** with experimental σ_0 shieldings (10 values)

	Basis Set	R	Rank	esd [ppm]	Rank	m	Rank	b [ppm]	Rank
HF	STO-3G	0.98782		0.438		0.8929		0.839	
	STO-6G	0.98848		0.426		0.8788		1.114	
	3-21G	0.99192		0.357		0.9231		-0.158	5
	6-31G	0.99558		0.264		0.9028		0.641	
	6-31G*	0.99795		0.180		0.9701	1	-0.925	
	6-31+G*	0.99796		0.180		0.9477		-0.153	4
	6-31++G*	0.99798		0.179		0.9484		-0.177	
	6-31G**	0.99786		0.184		0.9470		0.279	
	6-31+G**	0.99779		0.187		0.9242		1.036	
	6-31++G**	0.99785		0.184		0.9249		1.017	
	6-311G	0.99551		0.266		0.9290		-0.064	1
	6-311G*	0.99873	2	0.142	2	0.9652	2	-0.663	
	6-311+G*	0.99865	3	0.146	3	0.9498	4	-0.145	2
	6-311++G*	0.99874	1	0.141	1	0.9498	5	-0.152	3
	6-311G**	0.99812		0.173		0.9388		0.400	
	6-311+G**	0.99812		0.172		0.9257		0.830	
	6-311++G**	0.99820		0.169		0.9268		0.793	
	cc-pVDZ	0.99726		0.208		0.9515	3	0.195	
	cc-pVTZ	0.99809		0.174		0.9342		0.789	
	cc-pVQZ	0.99825	5	0.166	5	0.9278		1.036	
	cc-pV5Z	0.99823		0.167		0.9250		1.150	
	aug-cc-pVDZ	0.99811		0.173		0.9261		0.991	
	aug-cc-pVTZ	0.99817		0.170		0.9258		1.056	
	aug-cc-pVQZ	0.99826	4	0.166	4	0.9246		1.138	
	aug-cc-pV5Z	0.99822		0.168		0.9242		1.176	

Table S4: Statistical parameters of linear regressions of MP2 and B3LYP calculated absolute ^{1}H shieldings of molecules **1** to **7** with experimental σ_0 shieldings (10 values except where noted)

	Basis Set	R	Rank	esd [ppm]	Rank	m	Rank	b [ppm]	Rank
MP2	6-31G	0.99917		0.115		1.0178	5	-2.722	
	6-31G*	0.99904		0.124		1.0084	1	-1.633	
	6-31G**	0.99900		0.126		0.9874	2	-0.801	
	6-31++G**	0.99929		0.106		0.9591		0.158	1
	6-311G	0.99937	5	0.100	5	1.0297		-2.954	
	6-311G*	0.99954	2	0.086	2	0.9850	3	-0.813	
	6-311G**	0.99935		0.102		0.9646		-0.198	2
	6-311++G**	0.99950	3	0.089	3	0.9504		0.270	3
	cc-pVDZ	0.99883		0.136		0.9848	4	-0.602	5
	cc-pVTZ	0.99937	4	0.100	4	0.9478		0.651	
	aug-cc-pVDZ	0.99959	1	0.081	1	0.9513		0.423	4
	aug-cc-pVTZ [a]	0.99879	-	0.101	-	0.9457	-	0.754	-
B3LYP	6-31G	0.99781		0.186		0.9523	5	-0.609	4
	6-31G*	0.99898		0.127		0.9834	1	-1.100	
	6-31G**	0.99865		0.146		0.9493		0.389	2
	6-31++G**	0.99932	2	0.104	2	0.9281		1.135	
	6-311G	0.99850		0.154		0.9671	2	-1.032	
	6-311G*	0.99948	1	0.091	1	0.9643	3	-0.488	3
	6-311G**	0.99896		0.128		0.9320		0.737	5
	6-311++G**	0.99922	5	0.111	5	0.9211		1.100	
	cc-pVDZ	0.99859		0.149		0.9547	4	0.383	1
	cc-pVTZ	0.99912		0.118		0.9223		1.325	
	cc-pVQZ	0.99920		0.112		0.9153		1.593	
	cc-pV5Z	0.99920		0.112		0.9127		1.705	
	aug-cc-pVDZ	0.99918		0.114		0.9119		1.634	
	aug-cc-pVTZ	0.99931	3	0.104	3	0.9139		1.602	
	aug-cc-pVQZ	0.99923	4	0.110	4	0.9126		1.682	
	aug-cc-pV5Z [b]	0.99911		0.109		0.9027		2.006	

[a] 6 values, [b] 9 values

Table S5: HF calculated absolute ^{13}C shieldings of molecules **1** to **7**

	Basis Set	**1**	**2**	**3**	**4**	**5**		**6**		**7**
						C^1	C^2	C^1	C^2	
HF	STO-3G	235.563	228.322	126.640	177.714	225.236	221.976	130.517	121.661	123.566
	STO-6G	236.199	227.913	118.081	173.978	224.609	220.587	122.302	112.433	114.021
	3-21G	211.767	205.889	92.489	141.994	198.662	200.127	98.335	83.417	92.113
	6-31G	207.323	200.004	77.357	132.794	191.544	192.969	84.391	65.610	75.532
	6-31G*	200.521	192.460	77.513	133.118	184.870	185.301	83.451	66.028	74.108
	6-31+G*	201.907	192.790	78.217	133.191	184.796	184.630	85.044	64.644	73.942
	6-31++G*	202.003	192.563	78.022	133.251	184.698	184.499	84.843	64.575	73.947
	6-31G**	202.499	193.792	78.066	133.225	186.131	186.143	84.343	65.926	74.396
	6-31+G**	203.549	194.047	78.573	133.287	185.976	185.573	85.803	64.450	74.188
	6-31++G**	203.826	193.911	78.481	133.418	185.919	185.427	85.599	64.400	74.210
	6-311G	203.547	193.585	66.097	118.665	185.017	184.552	74.760	53.338	64.007
	6-311G*	196.462	186.176	65.795	119.104	178.174	177.151	73.318	51.572	60.993
	6-311+G*	196.867	186.334	64.814	118.184	178.069	176.882	72.885	50.535	60.234
	6-311++G*	196.690	186.073	64.838	118.270	178.092	176.789	72.825	50.515	60.268
	6-311G**	197.051	186.426	64.021	118.433	178.276	177.187	71.842	50.256	59.930
	6-311+G**	196.926	186.322	62.829	117.544	178.032	176.864	71.300	49.076	59.261
	6-311++G**	197.139	186.292	62.909	117.625	178.102	176.887	71.296	49.049	59.280
	cc-pVDZ	205.204	194.818	76.567	131.923	186.917	185.529	83.309	63.010	71.822
	cc-pVTZ	196.665	185.866	63.315	118.535	177.590	176.364	71.421	49.092	58.918
	cc-pVQZ	195.487	184.163	59.968	116.429	175.877	174.362	68.417	45.445	55.788
	cc-pV5Z	194.728	183.345	58.100	114.946	174.968	173.466	66.711	43.406	53.813
	aug-cc-pVDZ	204.082	193.123	75.749	131.768	185.497	182.974	83.874	60.825	70.530
	aug-cc-pVTZ	197.161	185.811	63.160	118.628	177.610	176.059	71.568	48.574	58.624
	aug-cc-pVQZ	195.305	184.004	59.853	116.401	175.727	174.176	68.418	45.171	55.531
	aug-cc-pV5Z	194.697	183.323	58.082	114.970	174.928	173.433	66.695	43.368	53.742
	range	*41.501*	*44.999*	*68.558*	*62.767*	*50.308*	*48.543*	*63.821*	*78.293*	*69.825*

Table S6: MP2 and B3LYP calculated absolute ^{13}C shieldings of molecules **1** to **7**

	Basis Set	**1**	**2**	**3**	**4**	**5**		**6**		**7**
						C^1	C^2	C^1	C^2	
MP2	6-31G	212.415	203.928	102.223	149.607	195.018	195.621	105.951	86.330	94.320
	6-31G*	209.176	199.136	94.845	144.411	190.654	189.737	98.737	80.169	88.133
	6-31G**	208.172	198.175	95.537	145.064	189.932	188.958	99.494	80.586	88.552
	6-31++G**	209.508	198.360	95.191	145.096	189.520	188.283	99.892	78.174	87.829
	6-311G	208.643	196.717	85.331	132.618	187.349	185.410	91.508	67.960	77.387
	6-311G*	205.613	192.716	79.675	129.294	183.401	180.712	85.783	61.911	71.872
	6-311G**	202.993	190.541	77.784	129.211	181.417	179.066	83.978	60.891	70.795
	6-311++G**	202.955	190.355	76.683	128.181	181.064	178.812	83.337	59.606	70.091
	cc-pVDZ	211.261	199.916	94.529	144.050	191.208	189.335	98.947	78.536	87.043
	cc-pVTZ	202.953	190.486	75.571	128.117	180.989	178.756	82.145	58.509	68.780
	cc-pVQZ	201.480		71.073	125.186					
	aug-cc-pVDZ	209.769	198.099	92.184	143.647	189.309	186.448	98.123	74.920	85.274
	aug-cc-pVTZ	203.355	190.518	75.285	128.027	181.003	178.627			
	aug-cc-pVQZ	201.380			125.081					
	range	*11.035*	*13.573*	*31.150*	*24.526*	*14.029*	*16.994*	*23.807*	*27.821*	*25.540*
B3LYP	6-31G	199.539	187.942	75.295	130.719	178.977	177.482	81.067	61.071	73.065
	6-31G*	194.647	182.527	72.998	129.054	174.111	172.086	78.205	59.044	69.963
	6-31G**	197.078	184.435	73.749	129.046	175.943	173.521	79.238	59.187	70.546
	6-31++G**	198.353	184.757	73.630	129.478	175.803	172.948	79.932	56.555	70.048
	6-311G	196.891	181.992	59.293	113.805	172.558	169.043	67.371	43.297	56.998
	6-311G*	191.408	176.307	56.234	112.717	167.051	163.344	63.897	38.916	52.342
	6-311G**	191.843	176.547	54.471	112.132	167.090	163.432	62.343	37.660	51.379
	6-311++G**	191.626	176.280	53.063	111.000	166.769	163.095	61.521	36.392	50.531
	cc-pVDZ	199.648	185.438	71.670	127.818	176.524	173.184	77.574	55.692	67.305
	cc-pVTZ	191.315	176.307	54.114	112.249	166.804	163.159	62.302	37.102	50.913
	cc-pVQZ	189.255	173.739	48.540	108.303	163.941	160.122	57.076	31.157	45.521
	cc-pV5Z	188.530	172.428	45.681	106.146	162.413	158.620	54.462	28.153	42.632
	aug-cc-pVDZ	198.386	184.840	69.703	128.102	176.163	171.668	77.526	52.636	66.340
	aug-cc-pVTZ	190.882	176.536	53.879	112.014	167.272	163.372	62.475	36.745	50.278
	aug-cc-pVQZ	189.019	173.566	48.246	108.212	163.700	160.067	57.278	30.958	45.081
	aug-cc-pV5Z	188.358	172.222	45.557	106.190	161.953	159.196	53.141	26.846	
	range	*11.290*	*15.720*	*29.738*	*24.573*	*17.024*	*18.862*	*27.926*	*34.225*	*30.433*

Table S7: Statistical parameters of linear regressions of HF calculated absolute ^{13}C shieldings of molecules **1** to **5** and **7** with experimental σ_0 shieldings (7 values)

	Basis Set	R	Rank	esd [ppm]	Rank	m	Rank	b [ppm]	Rank
HF	STO-3G	0.99714		4.716		1.1611		-85.696	
	STO-6G	0.99724		4.634		1.0717		-64.985	
	3-21G	0.99644		5.265		1.0575		-36.276	
	6-31G	0.99756		4.360		0.9758	4	-13.808	
	6-31G*	0.99817		3.773		1.0354		-18.591	
	6-31+G*	0.99881		3.041		1.0349		-18.755	
	6-31++G*	0.99883		3.013		1.0349		-18.686	
	6-31G**	0.99853		3.381		1.0262		-18.147	
	6-31+G**	0.99899		2.800		1.0256		-18.201	
	6-31++G**	0.99906		2.702		1.0255	5	-18.175	
	6-311G	0.99774		4.197		0.9300		1.489	5
	6-311G*	0.99903		2.751		0.9780	3	-1.048	3
	6-311+G*	0.99907		2.697		0.9699		0.427	2
	6-311++G*	0.99905		2.715		0.9713		0.275	1
	6-311G**	0.99903		2.753		0.9646		1.176	4
	6-311+G**	0.99896		2.843		0.9586		2.511	
	6-311++G**	0.99900		2.786		0.9584		2.474	
	cc-pVDZ	0.99923		2.451		0.9987	1	-13.801	
	cc-pVTZ	0.99918		2.523		0.9634		1.901	
	cc-pVQZ	0.99926	5	2.396	5	0.9514		5.650	
	cc-pV5Z	0.99926		2.401		0.9432		7.950	
	aug-cc-pVDZ	0.99936	1	2.233	1	1.0046	2	-13.390	
	aug-cc-pVTZ	0.99932	2	2.304	2	0.9613		2.224	
	aug-cc-pVQZ	0.99928	3	2.374	3	0.9514		5.793	
	aug-cc-pV5Z	0.99927	4	2.389	4	0.9431		7.982	

Table S8: Statistical parameters of linear regressions of MP2 and B3LYP calculated absolute ^{13}C shieldings of molecules **1** to **5** and **7** with experimental σ_0 shieldings (7 values except where noted)

	Basis Set	R	Rank	esd [ppm]	Rank	m	Rank	b [ppm]	Rank
MP2	6-31G	0.99924		2.430		1.1477		-52.657	
	6-31G*	0.99957		1.831		1.1236		-42.750	
	6-31G**	0.99944		2.090		1.1396		-45.021	
	6-31++G**	0.99958		1.809		1.1312		-43.584	
	6-311G	0.99974		1.414		1.0418	5	-23.360	5
	6-311G*	0.99992	4	0.766	4	1.0278	2	-16.781	4
	6-311G**	0.99994	2	0.662	2	1.0360	4	-16.308	3
	6-311++G**	0.99995	1	0.605	1	1.0293	3	-14.773	2
	cc-pVDZ	0.99980	5	1.257	5	1.1063		-40.190	
	cc-pVTZ	0.99994	3	0.696	3	1.0192	1	-12.933	1
	aug-cc-pVDZ	0.99957		1.837		1.1066		-38.233	
	aug-cc-pVTZ [a]	0.99993		0.664		1.0157		-12.375	
B3LYP	6-31G	0.99933		2.287		1.0621		-18.814	
	6-31G*	0.99900		2.795		1.0868		-18.141	
	6-31G**	0.99935		2.253		1.0734		-17.594	
	6-31++G**	0.99929		2.351		1.0670		-16.793	
	6-311G	0.99950		1.972		0.9660		5.231	1
	6-311G*	0.99976	1	1.361	1	0.9831	1	7.282	2
	6-311G**	0.99968	3	1.571	3	0.9705	2	9.288	3
	6-311++G**	0.99963		1.687		0.9635		10.826	
	cc-pVDZ	0.99951		1.956		1.0374		-12.033	
	cc-pVTZ	0.99967	4	1.595	4	0.9704	3	9.572	4
	cc-pVQZ	0.99963		1.702		0.9481		15.934	
	cc-pV5Z	0.99962		1.713		0.9357		19.251	
	aug-cc-pVDZ	0.99904		2.740		1.0337	5	-10.559	
	aug-cc-pVTZ	0.99970	2	1.517	2	0.9667	4	10.152	5
	aug-cc-pVQZ	0.99964	5	1.671	5	0.9470		16.291	
	aug-cc-pV5Z [a]	0.99971		1.320		0.9229		21.401	

[a] 6 values

Table S9: Calculated relative ^{1}H chemical shifts

Basis Set	**1**	**2**	**3**	**4**	**5**		**6**			**7**
					H^1	H^2	H^2	H^1	H^3	
STO-3G	0.9949	1.0121	6.3466	2.6298	1.0433	1.0474	6.1965	6.0412	7.0256	8.0729
STO-6G	1.2016	1.2271	6.6547	2.8332	1.2627	1.2826	6.4884	6.3412	7.3575	8.3949
3-21G	0.8383	1.0970	6.4637	2.4628	1.1545	1.3373	5.9864	6.0465	6.9098	7.8063
6-31G	0.7595	1.1324	6.5376	2.3285	1.1916	1.4568	5.9648	6.0657	7.2213	8.0317
6-31G*	0.6092	1.0507	5.8859	2.0537	1.0855	1.4080	5.3774	5.4877	6.6607	7.7146
6-31+G*	0.5428	1.0315	5.9168	2.1096	1.0682	1.3970	5.3719	5.5838	6.9387	7.7855
6-31++G*	0.5588	1.0358	5.9052	2.0882	1.0755	1.3865	5.3514	5.5750	6.9474	7.7893
6-31G**	0.5975	0.9896	5.9721	1.8734	1.0127	1.3239	5.4531	5.5881	6.6851	7.7556
6-31+G**	0.5641	0.9809	6.0374	1.9784	1.0115	1.2950	5.4863	5.7134	6.9768	7.8534
6-31++G**	0.5714	0.9899	6.0374	1.9797	1.0204	1.3071	5.4856	5.7166	6.9794	7.8652
6-311G	0.8192	1.2354	6.4634	2.5472	1.2875	1.6001	5.9248	5.9988	7.1707	8.0048
6-311G*	0.6665	1.1512	5.9337	1.9907	1.1839	1.4881	5.4508	5.5942	6.7940	7.8063
6-311+G*	0.6392	1.1285	5.9710	2.0133	1.1573	1.4726	5.4257	5.6448	6.9789	7.8542
6-311++G*	0.6155	1.1125	5.9460	1.9823	1.1443	1.4613	5.4125	5.6144	6.9737	7.8339
6-311G**	0.6154	1.0248	5.9799	1.8315	1.0546	1.3126	5.4926	5.6575	6.7995	7.8126
6-311+G**	0.6012	1.0177	6.0264	1.8813	1.0423	1.3070	5.4796	5.7123	6.9768	7.8780
6-311++G**	0.5872	1.0058	6.0036	1.8600	1.0341	1.3011	5.4727	5.6828	6.9672	7.8569
range	*0.659*	*0.254*	*0.769*	*1.002*	*0.276*	*0.553*	*1.137*	*0.854*	*0.697*	*0.680*

Table S10: Calculated relative ^{13}C chemical shifts

Basis Set	**1**	**2**	**3**	**4**	**5**		**6**		**7**
					C^1	C^2	C^1	C^2	
STO-3G	13.8852	21.1262	122.8086	71.7349	27.4723	24.2128	118.9318	127.7877	125.8822
STO-6G	15.6539	23.9395	133.7721	77.8744	31.2658	27.2441	129.5502	139.4196	137.8320
3-21G	2.8893	8.7677	122.1682	72.6629	14.5294	15.9951	116.3222	131.2402	122.5439
6-31G	0.9135	8.2323	130.8791	75.4420	15.2667	16.6922	123.8454	142.6265	132.7038
6-31G*	1.2071	9.2689	124.2158	68.6103	16.4275	16.8584	118.2777	135.7005	127.6203
6-31+G*	-0.0609	9.0555	123.6287	68.6553	17.2163	17.0502	116.8023	137.2023	127.9035
6-31++G*	0.1000	9.5407	124.0809	68.8520	17.6042	17.4051	117.2605	137.5278	128.1564
6-31G**	0.6566	9.3632	125.0893	69.9305	17.0130	17.0249	118.8121	137.2300	128.7598
6-31+G**	-0.3774	9.1240	124.5988	69.8841	17.5988	17.1951	117.3686	138.7211	128.9833
6-31++G**	-0.3199	9.5947	125.0249	70.0879	18.0785	17.5867	117.9066	139.1057	129.2960
6-311G	-0.0032	9.9590	137.4471	84.8794	18.9921	18.5271	128.7840	150.2057	139.5369
6-311G*	-0.4729	9.8126	130.1942	76.8851	18.8382	17.8155	122.6706	144.4174	134.9957
6-311+G*	-0.9325	9.6010	131.1212	77.7508	19.0533	17.8655	123.0500	145.3996	135.7009
6-311++G*	-0.5402	10.0774	131.3120	77.8797	19.3607	18.0579	123.3247	145.6354	135.8817
6-311G**	-0.8344	9.7909	132.1951	77.7840	19.0293	17.9408	124.3742	145.9606	136.2862
6-311+G**	-1.0073	9.5972	133.0899	78.3743	19.0547	17.8868	124.6187	146.8428	136.6579
6-311++G**	-0.9570	9.8899	133.2734	78.5566	19.2945	18.0802	124.8860	147.1325	136.9016
range	*16.661*	*15.707*	*15.279*	*16.269*	*16.736*	*11.249*	*13.228*	*22.418*	*16.993*