SUPPLEMENTARY MATERIAL

to

On the convergence of zero-point vibrational corrections to nuclear shieldings and shielding anisotropies towards the complete basis set limit in water

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Tabel S1: HF: shieldings and shielding anisotropies

Basis sets	Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	347.957	31.380	30.588	19.730	353.748	31.817	30.163	20.332
pVTZ	335.625	30.836	42.408	20.709	343.690	31.457	41.938	21.581
pVQZ	331.477	30.609	51.084	20.853	340.135	31.241	50.488	21.795
pV5Z	328.635	30.506	55.182	20.919	337.360	31.128	54.612	21.868
pV6Z	327.957	30.481	56.718	20.939	336.738	31.101	56.059	21.888
aug-pVDZ	337.262	31.199	51.075	19.766	343.918	31.672	50.520	20.487
aug-pVTZ	328.803	30.751	56.138	20.587	336.700	31.335	55.657	21.425
aug-pVQZ	328.577	30.564	56.793	20.820	337.180	31.181	56.123	21.749
aug-pV5Z	327.909	30.505	57.255	20.907	336.662	31.125	56.569	21.852
aug-pV6Z	327.847	30.479	57.325	20.944	336.619	31.099	56.641	21.892
aug-pc-1	335.256	31.012	51.651	19.994	341.842	31.456	51.142	20.659
aug-pc-2	326.211	30.668	57.361	20.698	335.247	31.300	56.688	21.635
aug-pc-3	327.423	30.491	57.646	20.929	336.261	31.112	56.959	21.878
aug-pc-4	327.861	30.468	57.318	20.961	336.633	31.087	56.633	21.911
aug-pcS-1	326.009	30.521	58.403	20.513	332.390	30.938	58.220	21.202
aug-pcS-2	329.281	30.557	57.748	20.843	338.130	31.177	57.044	21.795
aug-pcS-3	327.848	30.466	57.365	20.962	336.617	31.084	56.675	21.913
aug-pcS-4	327.846	30.465	57.327	20.965	336.625	31.084	56.641	21.916

Tabel S2: B3LYP: shieldings and shielding anisotropies

Basis sets	Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	345.491	31.915	24.569	18.308	338.590	31.605	24.218	17.634
pVTZ	336.094	31.480	35.247	19.460	333.773	31.314	35.292	19.224
pVQZ	331.541	31.218	45.936	19.652	329.821	31.075	46.070	19.476
pV5Z	328.142	31.067	51.648	19.749	326.409	30.910	51.842	19.574
pV6Z	326.961	31.038	54.245	19.756	325.190	30.878	54.460	19.579
aug-pVDZ	336.410	31.649	50.225	18.573	332.335	31.342	50.340	18.143
aug-pVTZ	328.345	31.306	53.985	19.412	325.798	31.082	54.195	19.157
aug-pVQZ	327.851	31.123	54.895	19.639	325.943	30.950	55.113	19.447
aug-pV5Z	326.962	31.058	55.523	19.732	325.136	30.893	55.745	19.549
aug-pV6Z	326.795	31.033	55.649	19.767	324.991	30.869	55.870	19.586
aug-pc-1	335.158	31.463	49.819	18.829	330.237	31.103	49.979	18.336
aug-pc-2	326.407	31.218	55.282	19.492	324.318	31.035	55.535	19.287
aug-pc-3	326.619	31.045	55.690	19.749	324.802	30.881	55.916	19.568
aug-pc-4	326.737	31.021	55.679	19.784	324.930	30.858	55.904	19.604
aug-pcS-1	325.970	31.065	57.241	19.311	321.596	30.745	57.524	18.861
aug-pcS-2	328.422	31.106	56.136	19.654	326.578	30.935	56.370	19.472
aug-pcS-3	326.747	31.022	55.688	19.783	324.940	30.859	55.909	19.602
aug-pcS-4	326.753	31.018	55.668	19.788	324.955	30.855	55.890	19.609

Tabel S3: MP2: shieldings and shielding anisotropies

Basis sets	Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	363.215	31.602	17.982	19.531	360.091	31.474	17.622	19.131
pVTZ	352.760	31.002	28.654	20.602	352.132	30.994	28.376	20.509
pVQZ	349.399	30.628	37.754	20.896	349.263	30.643	37.645	20.873
pV5Z	346.870	30.456	42.337	21.018	346.603	30.443	42.274	20.979
pV6Z	346.141	30.410	44.413	21.051	345.782	30.385	44.363	21.001
aug-pVDZ	353.889	31.268	40.743	19.812	350.527	30.967	40.489	19.355
aug-pVTZ	346.471	30.803	44.194	20.595	344.862	30.658	44.029	20.385
aug-pVQZ	346.459	30.523	44.880	20.916	345.825	30.473	44.813	20.830
aug-pV5Z	346.022	30.435	45.312	21.026	345.571	30.400	45.265	20.965
aug-pV6Z	346.054	30.397	45.363	21.073	345.606	30.361	45.321	21.012
pCVDZ	362.085	31.591	18.041	19.539	359.307	31.488	17.621	19.173
pCVTZ	352.852	30.960	30.205	20.602	352.653	30.990	30.009	20.565
pCVQZ	348.828	30.593	37.859	20.891	349.004	30.632	37.787	20.910
pCV5Z	346.235	30.420	42.949	21.018	346.338	30.437	42.931	21.030
pCV6Z	345.746	30.375	44.734	21.053	345.759	30.378	44.724	21.055
aug-pCVDZ	352.265	31.253	41.599	19.819	349.123	30.974	41.338	19.391
aug-pCVTZ	346.222	30.765	44.727	20.597	345.012	30.656	44.624	20.440
aug-pCVQZ	345.915	30.488	45.414	20.913	345.613	30.465	45.382	20.872
aug-pCV5Z	345.730	30.400	45.696	21.027	345.647	30.394	45.685	21.015
aug-pCV6Z	345.713	30.362	45.773	21.075	345.640	30.356	45.766	21.065
aug-pc-1	353.674	31.104	40.141	20.078	350.035	30.784	39.897	19.612
aug-pc-2	344.536	30.741	45.430	20.710	343.916	30.689	45.383	20.630
aug-pc-3	345.415	30.465	45.863	21.001	345.052	30.443	45.806	20.951
aug-pc-4	345.952	30.407	45.397	21.067	345.574	30.382	45.343	21.014
aug-pcS-1	345.057	30.642	47.150	20.521	341.350	30.309	46.924	20.034
aug-pcS-2	346.959	30.610	46.150	20.857	346.318	30.551	46.117	20.773
aug-pcS-3	345.759	30.439	45.537	21.028	345.369	30.416	45.476	20.973
aug-pcS-4	345.942	30.404	45.394	21.070	345.572	30.379	45.341	21.018

Tabel S4: CCSD: shieldings and shielding anisotropies

Basis sets	Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	355.258	31.824	24.087	19.132	351.657	31.678	23.881	18.722
pVTZ	343.824	31.214	35.463	20.202	343.946	31.261	35.308	20.210
pVQZ	340.343	30.840	44.248	20.507	341.259	30.926	44.200	20.613
pV5Z	337.881	30.686	48.408	20.622	338.769	30.756	48.411	20.727
pV6Z	337.237	30.646	50.152	20.655	338.088	30.709	50.154	20.755
aug-pVDZ	346.104	31.527	45.502	19.399	342.860	31.271	45.509	19.011
aug-pVTZ	337.932	31.044	49.534	20.193	337.203	30.984	49.531	20.109
aug-pVQZ	337.736	30.756	50.366	20.522	338.231	30.793	50.365	20.581
aug-pV5Z	337.170	30.673	50.840	20.627	337.917	30.727	50.840	20.716
aug-pV6Z	337.146	30.637	50.909	20.670	337.931	30.694	50.912	20.764
pCVDZ	354.000	31.812	24.336	19.143	350.831	31.694	24.069	18.775
pCVTZ	343.852	31.175	36.919	20.205	344.489	31.259	36.799	20.273
pCVQZ	339.779	30.806	44.380	20.505	341.090	30.919	44.343	20.657
pCV5Z	337.332	30.652	48.958	20.625	338.676	30.753	48.962	20.784
pCV6Z	336.891	30.611	50.464	20.659	338.193	30.706	50.470	20.813
aug-pCVDZ	344.373	31.513	46.533	19.409	341.439	31.282	46.529	19.057
aug-pCVTZ	337.633	31.007	50.086	20.196	337.403	30.985	50.098	20.170
aug-pCVQZ	337.203	30.723	50.890	20.521	338.117	30.789	50.894	20.629
aug-pCV5Z	336.917	30.638	51.206	20.630	338.114	30.724	51.208	20.772
aug-pCV6Z	336.849	30.603	51.299	20.674	---	---	---	---
aug-pc-1	345.138	31.368	45.036	19.638	341.713	31.105	45.056	19.252
aug-pc-2	335.877	30.987	50.737	20.305	336.232	31.010	50.747	20.346
aug-pc-3	336.638	30.695	51.310	20.611	337.398	30.754	51.300	20.700
aug-pc-4	337.115	30.642	50.909	20.670	337.915	30.703	50.902	20.765
aug-pcS-1	336.207	30.902	52.022	20.087	332.731	30.626	52.075	19.682
aug-pcS-2	338.346	30.854	51.430	20.455	338.636	30.867	51.451	20.491
aug-pcS-3	336.998	30.670	50.993	20.637	337.730	30.728	50.982	20.723
aug-pcS-4	337.100	30.639	50.911	20.674	337.910	30.701	50.904	20.770

Tabel S5: CCSD(T): shieldings and shielding anisotropies

Basis sets	Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	355.139	31.876	23.325	19.047	350.802	31.697	22.997	18.555
pVTZ	344.597	31.250	34.143	20.149	343.671	31.224	33.893	20.034
pVQZ	341.310	30.864	42.874	20.468	341.036	30.865	42.786	20.433
pV5Z	338.867	30.703	47.099	20.590	338.495	30.680	47.067	20.544
pV6Z	338.201	30.660	48.914	20.623	337.757	30.628	48.900	20.570
aug-pVDZ	346.433	31.555	44.723	19.351	342.243	31.235	44.658	18.848
aug-pVTZ	338.787	31.061	48.407	20.159	336.819	30.905	48.340	19.930
aug-pVQZ	338.652	30.770	49.201	20.491	337.871	30.711	49.185	20.398
aug-pV5Z	338.108	30.686	49.659	20.596	337.555	30.644	49.651	20.530
aug-pV6Z	338.095	30.650	49.723	20.640	337.572	30.610	49.719	20.577
pCVDZ	353.893	31.865	23.559	19.057	349.979	31.711	23.165	18.605
pCVTZ	344.681	31.210	35.581	20.150	344.206	31.217	35.388	20.089
pCVQZ	340.776	30.831	42.974	20.465	340.850	30.855	42.907	20.471
pCV5Z	338.339	30.669	47.636	20.592	338.379	30.674	47.629	20.596
pCV6Z	337.883	30.626	49.202	20.626	337.853	30.622	49.207	20.624
aug-pCVDZ	344.735	31.542	45.756	19.360	340.834	31.244	45.680	18.890
aug-pCVTZ	338.538	31.024	48.930	20.161	337.005	30.901	48.903	19.985
aug-pCVQZ	338.153	30.737	49.702	20.489	337.741	30.703	49.703	20.440
aug-pCV5Z	337.886	30.652	50.006	20.598	337.744	30.638	50.015	20.582
aug-pCV6Z	337.827	30.616	50.094	20.643	337.720	30.604	50.105	20.631
aug-pc-1	345.391	31.396	44.375	19.588	341.123	31.078	44.332	19.106
aug-pc-2	336.616	31.007	49.644	20.265	335.773	30.944	49.635	20.168
aug-pc-3	337.561	30.710	50.151	20.577	337.046	30.676	50.127	20.515
aug-pc-4	338.052	30.655	49.728	20.639	337.556	30.621	49.711	20.579
aug-pcS-1	336.872	30.923	51.065	20.045	332.351	30.577	51.017	19.516
aug-pcS-2	339.141	30.872	50.298	20.415	338.244	30.799	50.305	20.311
aug-pcS-3	337.914	30.685	49.831	20.603	337.371	30.649	49.804	20.537
aug-pcS-4	338.038	30.653	49.729	20.642	337.552	30.619	49.713	20.583

Tabel S6: HF: vibrational corrections to shieldings and shielding anisotropies

Basis sets	Relative to the Experimental Geometry (ExpC)				Relative to the Optimized Geometry (ZPVC)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	-5.712	-0.073	-1.693	-0.337	-11.502	-0.509	-1.268	-0.939
pVTZ	-2.092	0.097	-1.569	-0.056	-10.156	-0.525	-1.099	-0.929
pVQZ	-1.665	0.113	-1.578	0.014	-10.323	-0.519	-0.981	-0.928
pV5Z	-1.605	0.106	-1.507	0.021	-10.330	-0.517	-0.937	-0.928
pV6Z	-1.634	0.103	-1.561	0.022	-10.415	-0.517	-0.903	-0.927
aug-pVDZ	-3.823	-0.050	-1.315	-0.172	-10.478	-0.524	-0.761	-0.893
aug-pVTZ	-2.231	0.056	-1.485	-0.068	-10.128	-0.528	-1.004	-0.906
aug-pVQZ	-1.717	0.098	-1.574	0.004	-10.320	-0.519	-0.904	-0.925
aug-pV5Z	-1.660	0.103	-1.587	0.016	-10.414	-0.517	-0.902	-0.928
aug-pV6Z	-1.630	0.100	-1.590	0.020	-10.410	-0.520	-0.906	-0.929
aug-pc-1	-4.349	-0.078	-1.508	-0.234	-10.935	-0.521	-1.000	-0.899
aug-pc-2	-1.538	0.109	-1.469	0.005	-10.574	-0.523	-0.796	-0.932
aug-pc-3	-1.587	0.104	-1.640	0.023	-10.425	-0.517	-0.953	-0.926
aug-pc-4	-1.549	0.101	-1.586	0.021	-10.320	-0.518	-0.901	-0.928
aug-pcS-1	-4.196	-0.086	-1.396	-0.233	-10.576	-0.502	-1.213	-0.923
aug-pcS-2	-1.551	0.109	-1.670	0.021	-10.399	-0.511	-0.965	-0.931
aug-pcS-3	-1.618	0.101	-1.594	0.021	-10.387	-0.517	-0.905	-0.929
aug-pcS-4	-1.606	0.102	-1.587	0.022	-10.385	-0.517	-0.901	-0.929

Tabel S7: B3LYP: vibrational corrections to shieldings and shielding anisotropies

Basis sets	Relative to the Experimental Geometry (ExpC)				Relative to the Optimized Geometry (ZPVC)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	-22.954	-0.827	-3.734	-1.813	-16.053	-0.517	-3.383	-1.139
pVTZ	-15.865	-0.688	-2.545	-1.319	-13.545	-0.522	-2.590	-1.083
pVQZ	-15.105	-0.657	-2.267	-1.239	-13.385	-0.514	-2.401	-1.063
pV5Z	-14.836	-0.667	-2.119	-1.223	-13.103	-0.510	-2.313	-1.048
pV6Z	-14.804	-0.671	-2.092	-1.222	-13.033	-0.510	-2.306	-1.045
aug-pVDZ	-17.035	-0.828	-1.924	-1.435	-12.960	-0.521	-2.039	-1.004
aug-pVTZ	-15.282	-0.745	-2.069	-1.281	-12.736	-0.521	-2.279	-1.026
aug-pVQZ	-14.918	-0.687	-1.970	-1.230	-13.009	-0.515	-2.188	-1.038
aug-pV5Z	-14.915	-0.677	-1.994	-1.225	-13.088	-0.512	-2.217	-1.043
aug-pV6Z	-14.955	-0.675	-2.046	-1.226	-13.151	-0.511	-2.268	-1.045
aug-pc-1	-18.347	-0.875	-2.206	-1.509	-13.426	-0.515	-2.365	-1.015
aug-pc-2	-15.246	-0.700	-1.818	-1.248	-13.157	-0.516	-2.071	-1.043
aug-pc-3	-14.965	-0.676	-1.993	-1.226	-13.148	-0.511	-2.219	-1.045
aug-pc-4	-14.699	-0.676	-2.657	-1.223	-12.892	-0.513	-2.882	-1.043
aug-pcS-1	-17.800	-0.823	-2.264	-1.489	-13.425	-0.502	-2.547	-1.040
aug-pcS-2	-14.937	-0.677	-2.025	-1.224	-13.092	-0.506	-2.259	-1.042
aug-pcS-3	-14.952	-0.674	-1.992	-1.226	-13.146	-0.511	-2.213	-1.046
aug-pcS-4	-14.935	-0.671	-2.048	-1.231	-13.138	-0.508	-2.270	-1.051

Tabel S8: MP2: vibrational corrections to shieldings and shielding anisotropies

Basis sets	Relative to the Experimental Geometry (ExpC)				Relative to the Optimized Geometry (ZPVC)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	-14.615	-0.628	-3.811	-1.434	-11.492	-0.501	-3.451	-1.034
pVTZ	-10.134	-0.525	-3.440	-1.078	-9.506	-0.517	-3.162	-0.985
pVQZ	-9.378	-0.499	-3.007	-0.999	-9.242	-0.514	-2.898	-0.976
pV5Z	-9.275	-0.526	-2.832	-1.005	-9.009	-0.513	-2.769	-0.966
pV6Z	-9.364	-0.539	-2.758	-1.010	-9.004	-0.514	-2.708	-0.960
aug-pVDZ	-12.598	-0.826	-2.890	-1.395	-9.236	-0.524	-2.636	-0.938
aug-pVTZ	-10.491	-0.666	-3.015	-1.148	-8.882	-0.521	-2.850	-0.938
aug-pVQZ	-9.604	-0.567	-2.753	-1.044	-8.970	-0.517	-2.686	-0.958
aug-pV5Z	-9.425	-0.550	-2.730	-1.024	-8.974	-0.516	-2.683	-0.963
aug-pV6Z	-9.406	-0.550	-2.713	-1.022	-8.958	-0.514	-2.671	-0.961
pCVDZ	-14.205	-0.606	-3.990	-1.399	-11.427	-0.502	-3.570	-1.033
pCVTZ	-9.851	-0.487	-3.297	-1.021	-9.652	-0.517	-3.101	-0.984
pCVQZ	-9.047	-0.475	-2.914	-0.956	-9.223	-0.514	-2.842	-0.975
pCV5Z	-8.922	-0.496	-2.718	-0.953	-9.024	-0.513	-2.700	-0.965
pCV6Z	---	---	---	---	---	---	---	---
aug-pCVDZ	-12.369	-0.804	-3.014	-1.369	-9.227	-0.525	-2.753	-0.941
aug-pCVTZ	-10.224	-0.631	-2.867	-1.097	-9.013	-0.522	-2.764	-0.940
aug-pCVQZ	-9.299	-0.540	-2.677	-0.999	-8.997	-0.517	-2.645	-0.958
aug-pCV5Z	-9.067	-0.521	-2.615	-0.973	-8.984	-0.515	-2.604	-0.961
aug-pCV6Z	-9.046	-0.521	-2.602	-0.972	-8.972	-0.515	-2.595	-0.962
aug-pc-1	-12.977	-0.836	-3.178	-1.407	-9.337	-0.517	-2.934	-0.941
aug-pc-2	-9.745	-0.572	-2.643	-1.041	-9.125	-0.519	-2.596	-0.961
aug-pc-3	-9.434	-0.536	-2.818	-1.013	-9.071	-0.514	-2.761	-0.963
aug-pc-4	-9.377	-0.539	-2.734	-1.018	-8.999	-0.514	-2.680	-0.965
aug-pcS-1	-13.030	-0.826	-3.364	-1.448	-9.324	-0.494	-3.138	-0.961
aug-pcS-2	-9.677	-0.563	-2.793	-1.043	-9.036	-0.504	-2.760	-0.959
aug-pcS-3	-9.439	-0.537	-2.798	-1.020	-9.049	-0.513	-2.737	-0.965
aug-pcS-4	-9.370	-0.538	-2.732	-1.017	-9.000	-0.514	-2.679	-0.965

Tabel S9: CCSD: vibrational corrections to shieldings and shielding anisotropies

Basis sets	Relative to the Experimental Geometry (ExpC)				Relative to the Optimized Geometry (ZPVC)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	-16.656	-0.651	-3.098	-1.481	-13.056	-0.505	-2.892	-1.071
pVTZ	-10.953	-0.470	-2.553	-1.016	-11.074	-0.517	-2.398	-1.024
pVQZ	-9.988	-0.425	-2.137	-0.911	-10.904	-0.510	-2.089	-1.017
pV5Z	-9.869	-0.438	-1.964	-0.904	-10.757	-0.508	-1.967	-1.009
pV6Z	-9.921	-0.445	-1.919	-0.906	-10.772	-0.508	-1.921	-1.006
aug-pVDZ	-14.315	-0.776	-1.949	-1.371	-11.071	-0.520	-1.956	-0.983
aug-pVTZ	-11.375	-0.576	-2.111	-1.068	-10.646	-0.517	-2.108	-0.984
aug-pVQZ	-10.225	-0.475	-1.919	-0.943	-10.720	-0.512	-1.918	-1.002
aug-pV5Z	-9.994	-0.455	-1.909	-0.918	-10.741	-0.509	-1.909	-1.007
aug-pV6Z	-9.905	-0.448	-1.891	-0.908	-10.690	-0.505	-1.894	-1.002
pCVDZ	-16.149	-0.625	-3.250	-1.437	-12.980	-0.506	-2.983	-1.069
pCVTZ	-10.579	-0.432	-2.455	-0.956	-11.215	-0.517	-2.335	-1.024
pCVQZ	-9.555	-0.397	-2.071	-0.863	-10.866	-0.510	-2.034	-1.015
pCV5Z	-9.399	-0.407	-1.900	-0.849	-10.743	-0.508	-1.904	-1.008
pCV6Z	---	---	---	---	---	---	---	---
aug-pCVDZ	-13.991	-0.752	-2.049	-1.337	-11.058	-0.521	-2.045	-0.985
aug-pCVTZ	-10.995	-0.539	-2.008	-1.010	-10.765	-0.517	-2.020	-0.984
aug-pCVQZ	-9.813	-0.446	-1.874	-0.893	-10.727	-0.511	-1.878	-1.001
aug-pCV5Z	-9.528	-0.423	-1.835	-0.863	-10.725	-0.509	-1.837	-1.005
aug-pCV6Z	---	---	---	---	---	---	---	---
aug-pc-1	-14.706	-0.776	-2.235	-1.370	-11.280	-0.513	-2.255	-0.984
aug-pc-2	-10.591	-0.493	-1.883	-0.968	-10.946	-0.516	-1.893	-1.009
aug-pc-3	-10.100	-0.449	-1.999	-0.922	-10.860	-0.508	-1.989	-1.011
aug-pc-4	-9.972	-0.444	-1.948	-0.915	-10.772	-0.505	-1.941	-1.010
aug-pcS-1	-14.722	-0.767	-2.428	-1.412	-11.246	-0.491	-2.481	-1.007
aug-pcS-2	-10.538	-0.487	-2.037	-0.971	-10.828	-0.500	-2.058	-1.007
aug-pcS-3	-10.092	-0.449	-1.953	-0.926	-10.824	-0.506	-1.942	-1.012
aug-pcS-4	-10.009	-0.447	-1.981	-0.921	-10.819	-0.509	-1.974	-1.017

Tabel S10: CCSD(T): vibrational corrections to shieldings and shielding anisotropies

Basis sets	Relative to the Experimental Geometry (ExpC)				Relative to the Optimized Geometry (ZPVC)			
	Shielding		Anisotropy		Shielding		Anisotropy	
	O	H	O	H	O	H	O	H
pVDZ	-17.877	-0.685	-3.502	-1.591	-13.541	-0.506	-3.174	-1.099
pVTZ	-12.324	-0.543	-2.952	-1.165	-11.398	-0.517	-2.702	-1.050
pVQZ	-11.440	-0.510	-2.473	-1.076	-11.165	-0.511	-2.385	-1.041
pV5Z	-11.362	-0.532	-2.285	-1.077	-10.990	-0.508	-2.253	-1.031
pV6Z	-11.444	-0.542	-2.219	-1.081	-11.000	-0.510	-2.205	-1.028
aug-pVDZ	-15.554	-0.843	-2.244	-1.509	-11.364	-0.522	-2.179	-1.006
aug-pVTZ	-12.837	-0.673	-2.448	-1.234	-10.869	-0.517	-2.381	-1.005
aug-pVQZ	-11.723	-0.572	-2.209	-1.117	-10.942	-0.513	-2.193	-1.024
aug-pV5Z	-11.519	-0.553	-2.195	-1.094	-10.966	-0.511	-2.187	-1.028
aug-pV6Z	-11.494	-0.549	-2.170	-1.092	-10.971	-0.509	-2.166	-1.029
pCVDZ	-17.386	-0.661	-3.663	-1.550	-13.471	-0.507	-3.269	-1.098
pCVTZ	-12.023	-0.509	-2.843	-1.111	-11.548	-0.516	-2.650	-1.050
pCVQZ	-11.060	-0.487	-2.402	-1.033	-11.134	-0.511	-2.335	-1.039
pCV5Z	-10.937	-0.504	-2.203	-1.026	-10.977	-0.509	-2.196	-1.030
pCV6Z	---	---	---	---	---	---	---	---
aug-pCVDZ	-15.254	-0.821	-2.351	-1.477	-11.353	-0.523	-2.275	-1.007
aug-pCVTZ	-12.527	-0.640	-2.330	-1.183	-10.994	-0.518	-2.303	-1.007
aug-pCVQZ	-11.365	-0.546	-2.158	-1.072	-10.953	-0.513	-2.159	-1.023
aug-pCV5Z	-11.095	-0.525	-2.110	-1.044	-10.952	-0.511	-2.119	-1.028
aug-pCV6Z	-11.088	-0.525	-2.082	-1.044	-10.981	-0.514	-2.093	-1.032
aug-pc-1	-15.861	-0.832	-2.515	-1.488	-11.593	-0.515	-2.472	-1.006
aug-pc-2	-12.029	-0.580	-2.180	-1.127	-11.186	-0.517	-2.171	-1.030
aug-pc-3	-11.591	-0.542	-2.331	-1.094	-11.076	-0.508	-2.307	-1.032
aug-pc-4	-11.418	-0.535	-2.159	-1.086	-10.922	-0.501	-2.142	-1.026
aug-pcS-1	-16.019	-0.838	-2.784	-1.558	-11.498	-0.492	-2.736	-1.029
aug-pcS-2	-11.951	-0.574	-2.324	-1.131	-11.054	-0.501	-2.331	-1.027
aug-pcS-3	-11.611	-0.543	-2.275	-1.101	-11.068	-0.507	-2.248	-1.035
aug-pcS-4	-11.452	-0.541	-2.214	-1.090	-10.966	-0.507	-2.198	-1.031

Tabel S11: HF: extrapolated shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
Series	Used cardinal numbers	Shielding		Anisotropy		Shielding		Anisotropy	
		O	H	O	H	O	H	O	H
cc-pVXZ	D-T	330.433	30.607	47.385	21.121	339.455	31.306	46.896	22.107
	T-Q	328.450	30.444	57.414	20.959	337.542	31.083	56.726	21.951
	Q-5	325.653	30.397	59.483	20.988	334.448	31.009	58.940	21.944
	5-6	327.025	30.447	58.828	20.965	335.884	31.065	58.047	21.916
aug-cc-pVXZ	D-T	325.241	30.563	58.270	20.933	333.661	31.193	57.820	21.820
	T-Q	328.412	30.427	57.271	20.990	337.530	31.069	56.463	21.986
	Q-5	327.207	30.443	57.739	20.999	336.120	31.066	57.038	21.959
	5-6	327.763	30.443	57.423	20.994	336.560	31.062	56.740	21.949
aug-pc-n	1-2	322.402	30.523	59.765	20.994	332.470	31.234	59.023	22.046
	2-3	328.307	30.362	57.855	21.097	337.000	30.974	57.156	22.056
	3-4	328.321	30.444	56.973	20.995	337.023	31.061	56.290	21.945
aug-pcS-n	1-2	330.658	30.571	57.473	20.982	340.546	31.278	56.548	22.044
	2-3	326.802	30.400	57.084	21.050	335.513	31.017	56.406	21.998
	3-4	327.844	30.464	57.287	20.968	336.633	31.084	56.604	21.919

Tabel S12: B3LYP: extrapolated shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
Series	Used cardinal numbers	Shielding		Anisotropy		Shielding		Anisotropy	
		O	H	O	H	O	H	O	H
cc-pVXZ	D-T	332.138	31.297	39.744	19.945	331.745	31.192	39.955	19.894
	T-Q	328.219	31.026	53.735	19.792	326.938	30.900	53.934	19.660
	Q-5	324.576	30.909	57.641	19.851	322.830	30.737	57.898	19.677
	5-6	325.337	30.998	57.813	19.766	323.514	30.833	58.055	19.586
aug-cc-pVXZ	D-T	324.949	31.161	55.568	19.765	323.046	30.972	55.819	19.584
	T-Q	327.491	30.989	55.560	19.805	326.048	30.855	55.782	19.659
	Q-5	326.030	30.991	56.181	19.829	324.290	30.833	56.409	19.657
	5-6	326.565	30.997	55.822	19.815	324.792	30.837	56.042	19.637
aug-pc-n	1-2	322.723	31.115	57.582	19.771	321.826	31.006	57.874	19.688
	2-3	326.773	30.919	55.988	19.937	325.155	30.769	56.194	19.773
	3-4	326.860	30.996	55.668	19.821	325.064	30.834	55.892	19.641
aug-pcS-n	1-2	329.455	31.123	55.671	19.798	328.675	31.015	55.884	19.729
	2-3	325.524	30.961	55.361	19.876	323.745	30.803	55.573	19.697
	3-4	326.759	31.014	55.647	19.794	324.971	30.852	55.869	19.616

Tabel S13: MP2: extrapolated shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
Series	Used cardinal numbers	Shielding		Anisotropy		Shielding		Anisotropy	
		O	H	O	H	O	H	O	H
cc-pVXZ	D-T	348.358	30.749	33.147	21.053	348.781	30.792	32.904	21.089
	T-Q	346.946	30.355	44.395	21.111	347.169	30.387	44.409	21.139
	Q-5	344.217	30.276	47.145	21.146	343.812	30.233	47.131	21.090
	5-6	345.140	30.347	47.265	21.096	344.654	30.305	47.233	21.031
aug-cc-pVXZ	D-T	343.348	30.607	45.647	20.925	342.477	30.528	45.520	20.819
	T-Q	346.450	30.319	45.381	21.150	346.528	30.338	45.385	21.155
	Q-5	345.564	30.343	45.765	21.141	345.305	30.323	45.739	21.107
	5-6	346.098	30.345	45.433	21.138	345.654	30.307	45.398	21.077
cc-pCVXZ	D-T	348.964	30.694	35.327	21.050	349.851	30.780	35.225	21.151
	T-Q	345.892	30.325	43.444	21.102	346.341	30.371	43.463	21.162
	Q-5	343.514	30.238	48.289	21.151	343.541	30.232	48.328	21.156
	5-6	345.074	30.313	47.186	21.101	344.964	30.297	47.187	21.089
aug-cc-pCVXZ	D-T	343.678	30.560	46.044	20.925	343.281	30.522	46.008	20.882
	T-Q	345.691	30.286	45.915	21.144	346.052	30.326	45.935	21.187
	Q-5	345.536	30.308	45.992	21.147	345.683	30.320	46.003	21.165
	5-6	345.690	30.310	45.879	21.141	345.630	30.304	45.877	21.134
aug-pc-n	1-2	340.688	30.588	47.657	20.976	341.340	30.649	47.693	21.059
	2-3	346.056	30.264	46.179	21.213	345.881	30.263	46.115	21.185
	3-4	346.515	30.346	44.908	21.136	346.122	30.318	44.857	21.080
aug-pcS-n	1-2	347.760	30.597	45.729	20.998	348.410	30.653	45.777	21.084
	2-3	344.883	30.314	45.090	21.153	344.676	30.317	45.008	21.119
	3-4	346.134	30.367	45.244	21.114	345.785	30.340	45.199	21.065

Tabel S14: CCSD: extrapolated shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
Series	Used cardinal numbers	Shielding		Anisotropy		Shielding		Anisotropy	
		O	H	O	H	O	H	O	H
cc-pVXZ	D-T	339.010	30.957	40.253	20.653	340.699	31.085	40.119	20.837
	T-Q	337.803	30.567	50.659	20.730	339.298	30.682	50.689	20.907
	Q-5	335.298	30.524	52.773	20.743	336.157	30.578	52.829	20.847
	5-6	336.352	30.591	52.548	20.700	337.153	30.644	52.548	20.793
aug-cc-pVXZ	D-T	334.491	30.841	51.232	20.527	334.821	30.863	51.224	20.571
	T-Q	337.593	30.546	50.973	20.762	338.981	30.654	50.974	20.925
	Q-5	336.576	30.586	51.337	20.737	337.588	30.658	51.338	20.858
	5-6	337.113	30.588	51.004	20.729	337.950	30.649	51.011	20.830
cc-pCVXZ	D-T	339.579	30.907	42.217	20.652	341.819	31.076	42.159	20.904
	T-Q	336.807	30.537	49.825	20.724	338.610	30.671	49.848	20.937
	Q-5	334.765	30.490	53.761	20.751	336.143	30.579	53.808	20.917
	5-6	336.285	30.555	52.533	20.706	337.530	30.641	52.541	20.853
aug-cc-pCVXZ	D-T	334.795	30.794	51.582	20.527	335.704	30.860	51.601	20.639
	T-Q	336.889	30.516	51.477	20.758	338.638	30.646	51.475	20.964
	Q-5	336.617	30.549	51.538	20.744	338.111	30.656	51.537	20.922
	5-6	336.756	30.555	51.427	20.734	---	---	---	---
aug-pc-n	1-2	331.978	30.827	53.137	20.586	333.924	30.970	53.143	20.807
	2-3	337.193	30.482	51.728	20.834	338.249	30.567	51.704	20.958
	3-4	337.615	30.586	50.488	20.732	338.457	30.649	50.484	20.833
aug-pcS-n	1-2	339.247	30.834	51.181	20.610	341.122	30.968	51.188	20.832
	2-3	336.014	30.536	50.674	20.770	337.069	30.627	50.640	20.892
	3-4	337.207	30.606	50.825	20.713	338.099	30.673	50.822	20.819

Tabel S15: CCSD(T): extrapolated shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Experimental Geometry (ExpG)				Optimized Geometry (OptG)			
Series	Used cardinal numbers	Shielding		Anisotropy		Shielding		Anisotropy	
		O	H	O	H	O	H	O	H
cc-pVXZ	D-T	340.158	30.986	38.698	20.613	340.668	31.025	38.481	20.657
	T-Q	338.911	30.582	49.245	20.701	339.113	30.603	49.275	20.724
	Q-5	336.304	30.534	51.532	20.718	335.829	30.486	51.559	20.660
	5-6	337.286	30.601	51.407	20.668	336.743	30.557	51.418	20.606
aug-cc-pVXZ	D-T	335.568	30.853	49.958	20.499	334.535	30.766	49.890	20.386
	T-Q	338.553	30.558	49.780	20.733	338.639	30.569	49.802	20.740
	Q-5	337.537	30.598	50.140	20.706	337.223	30.574	50.140	20.668
	5-6	338.077	30.601	49.811	20.700	337.595	30.563	49.812	20.642
cc-pCVXZ	D-T	340.802	30.934	40.643	20.610	341.775	31.009	40.535	20.714
	T-Q	337.926	30.554	48.369	20.695	338.401	30.591	48.394	20.750
	Q-5	335.782	30.499	52.527	20.725	335.786	30.484	52.583	20.727
	5-6	337.257	30.567	51.353	20.673	337.130	30.551	51.375	20.662
aug-cc-pCVXZ	D-T	335.929	30.806	50.266	20.498	335.393	30.757	50.260	20.446
	T-Q	337.872	30.528	50.265	20.728	338.278	30.559	50.287	20.772
	Q-5	337.606	30.563	50.325	20.712	337.747	30.570	50.342	20.731
	5-6	337.746	30.567	50.215	20.705	337.687	30.557	50.229	20.698
aug-pc-n	1-2	332.921	30.843	51.863	20.550	333.520	30.888	51.868	20.615
	2-3	338.251	30.493	50.521	20.805	337.975	30.480	50.486	20.768
	3-4	338.567	30.597	49.284	20.704	338.091	30.563	49.275	20.646
aug-pcS-n	1-2	340.096	30.851	49.975	20.571	340.725	30.892	50.005	20.646
	2-3	337.019	30.549	49.490	20.740	336.734	30.540	49.438	20.702
	3-4	338.168	30.619	49.622	20.683	337.742	30.588	49.618	20.631

Tabel S16: HF: extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Zero-Point Vibrational Averaged (ZPVA)				Relative to the Optimized Geometry (ZPVC)				Relative to the Experimental Geometry (ExpC)			
Series	Used cardinal numbers	σ		$\Delta\sigma$		σ		$\Delta\sigma$		σ		$\Delta\sigma$	
		O	H	O	H	O	H	O	H	O	H	O	H
cc-pVXZ	D-T	329.865	30.774	45.868	21.183	-9.590	-0.531	-1.028	-0.925	-0.568	0.168	-1.517	0.062
	T-Q	327.097	30.569	55.831	21.023	-10.445	-0.514	-0.896	-0.928	-1.354	0.125	-1.583	0.065
	Q-5	324.111	30.495	58.050	21.017	-10.337	-0.515	-0.889	-0.927	-1.543	0.098	-1.433	0.028
	5-6	325.352	30.546	57.191	20.989	-10.532	-0.519	-0.856	-0.927	-1.673	0.099	-1.636	0.024
aug-cc-pVXZ	D-T	323.681	30.663	56.714	20.909	-9.980	-0.530	-1.106	-0.911	-1.560	0.100	-1.556	-0.024
	T-Q	327.070	30.557	55.631	21.047	-10.460	-0.512	-0.832	-0.939	-1.342	0.129	-1.640	0.056
	Q-5	325.606	30.551	56.138	21.028	-10.513	-0.515	-0.900	-0.931	-1.601	0.107	-1.601	0.029
	5-6	326.163	30.545	55.828	21.018	-10.396	-0.517	-0.912	-0.930	-1.600	0.102	-1.595	0.024
aug-pc-n	1-2	322.048	30.710	58.313	21.100	-10.422	-0.524	-0.710	-0.945	-0.354	0.187	-1.452	0.106
	2-3	326.685	30.462	56.089	21.133	-10.315	-0.512	-1.067	-0.923	-1.622	0.101	-1.766	0.036
	3-4	326.812	30.542	55.445	21.015	-10.211	-0.518	-0.846	-0.930	-1.509	0.099	-1.529	0.020
aug-pcS-n	1-2	330.222	30.763	55.687	21.110	-10.325	-0.515	-0.861	-0.934	-0.437	0.192	-1.786	0.128
	2-3	325.134	30.495	55.546	21.070	-10.378	-0.521	-0.861	-0.928	-1.667	0.095	-1.539	0.021
	3-4	326.250	30.567	55.706	20.991	-10.383	-0.517	-0.898	-0.928	-1.594	0.103	-1.580	0.023

Tabel S17: B3LYP: extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Zero-Point Vibrational Averaged (ZPVA)				Relative to the Optimized Geometry (ZPVC)				Relative to the Experimental Geometry (ExpC)			
Series	Used cardinal numbers	Σ		$\Delta\sigma$		σ		$\Delta\sigma$		σ		$\Delta\sigma$	
		O	H	O	H	O	H	O	H	O	H	O	H
cc-pVXZ	D-T	319.257	30.668	37.700	18.834	-12.488	-0.524	-2.256	-1.060	-12.881	-0.629	-2.044	-1.111
	T-Q	313.668	30.392	51.671	18.612	-13.269	-0.507	-2.263	-1.048	-14.551	-0.634	-2.065	-1.180
	Q-5	310.024	30.230	55.677	18.645	-12.806	-0.506	-2.221	-1.032	-14.552	-0.678	-1.964	-1.206
	5-6	310.577	30.323	55.758	18.546	-12.937	-0.510	-2.297	-1.040	-14.760	-0.676	-2.054	-1.220
aug-cc-pVXZ	D-T	310.405	30.451	53.439	18.548	-12.641	-0.521	-2.380	-1.036	-14.544	-0.711	-2.130	-1.216
	T-Q	312.839	30.344	53.661	18.612	-13.209	-0.510	-2.121	-1.047	-14.652	-0.645	-1.899	-1.193
	Q-5	311.119	30.325	54.162	18.609	-13.171	-0.508	-2.247	-1.048	-14.911	-0.666	-2.019	-1.220
	5-6	311.555	30.325	53.703	18.588	-13.237	-0.511	-2.338	-1.049	-15.010	-0.672	-2.118	-1.226
aug-pc-n	1-2	308.782	30.489	55.927	18.633	-13.044	-0.517	-1.947	-1.055	-13.941	-0.626	-1.655	-1.138
	2-3	312.013	30.261	53.867	18.727	-13.142	-0.508	-2.327	-1.046	-14.760	-0.658	-2.120	-1.209
	3-4	312.440	30.320	52.313	18.600	-12.624	-0.514	-3.579	-1.041	-14.420	-0.676	-3.355	-1.220
aug-pcS-n	1-2	315.724	30.506	53.747	18.686	-12.951	-0.508	-2.137	-1.043	-13.731	-0.616	-1.924	-1.113
	2-3	310.560	30.289	53.393	18.648	-13.185	-0.514	-2.180	-1.048	-14.964	-0.672	-1.968	-1.228
	3-4	311.842	30.347	53.541	18.558	-13.129	-0.505	-2.329	-1.057	-14.917	-0.667	-2.107	-1.236

Tabel S18: MP2: extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Zero-Point Vibrational Averaged (ZPVA)				Relative to the Optimized Geometry (ZPVC)				Relative to the Experimental Geometry (ExpC)			
Series	Used cardinal numbers	σ		$\Delta\sigma$		σ		$\Delta\sigma$		σ		$\Delta\sigma$	
		O	H	O	H	O	H	O	H	O	H	O	H
cc-pVXZ	D-T	340.111	30.268	29.864	20.125	-8.670	-0.524	-3.040	-0.964	-8.247	-0.482	-3.284	-0.928
	T-Q	338.120	29.875	41.704	20.169	-9.049	-0.512	-2.705	-0.969	-8.826	-0.480	-2.691	-0.941
	Q-5	335.050	29.721	44.497	20.135	-8.762	-0.512	-2.634	-0.956	-9.167	-0.554	-2.648	-1.011
	5-6	335.653	29.790	44.608	20.079	-9.001	-0.515	-2.624	-0.952	-9.486	-0.557	-2.656	-1.017
aug-cc-pVXZ	D-T	333.744	30.009	42.579	19.881	-8.733	-0.519	-2.940	-0.938	-9.604	-0.599	-3.068	-1.044
	T-Q	337.494	29.824	42.819	20.182	-9.034	-0.514	-2.566	-0.973	-8.957	-0.495	-2.562	-0.968
	Q-5	336.326	29.811	43.059	20.138	-8.978	-0.513	-2.680	-0.968	-9.237	-0.532	-2.706	-1.003
	5-6	336.718	29.795	42.743	20.118	-8.936	-0.513	-2.655	-0.958	-9.380	-0.550	-2.690	-1.019
cc-pCVXZ	D-T	340.947	30.257	32.321	20.188	-8.905	-0.523	-2.904	-0.963	-8.018	-0.437	-3.005	-0.862
	T-Q	337.431	29.859	40.810	20.193	-8.910	-0.512	-2.653	-0.968	-8.460	-0.466	-2.635	-0.909
	Q-5	334.724	29.720	45.777	20.201	-8.817	-0.512	-2.551	-0.955	-8.791	-0.518	-2.512	-0.950
	5-6	---	---	---	---	---	---	---	---	---	---	---	---
aug-cc-pCVXZ	D-T	334.357	30.001	43.239	19.942	-8.924	-0.521	-2.769	-0.940	-9.321	-0.558	-2.805	-0.982
	T-Q	337.067	29.812	43.377	20.216	-8.985	-0.513	-2.558	-0.971	-8.624	-0.474	-2.538	-0.927
	Q-5	336.712	29.807	43.442	20.201	-8.970	-0.513	-2.561	-0.964	-8.824	-0.501	-2.550	-0.946
	5-6	336.672	29.789	43.295	20.170	-8.956	-0.515	-2.583	-0.963	-9.015	-0.521	-2.584	-0.971
aug-pc-n	1-2	332.304	30.127	45.239	20.089	-9.036	-0.520	-2.454	-0.969	-8.385	-0.459	-2.418	-0.887
	2-3	336.849	29.754	43.233	20.221	-9.032	-0.510	-2.881	-0.964	-9.207	-0.510	-2.946	-0.993
	3-4	337.198	29.804	42.262	20.113	-8.923	-0.514	-2.595	-0.967	-9.317	-0.542	-2.646	-1.023
aug-pcS-n	1-2	339.495	30.144	43.176	20.126	-8.915	-0.508	-2.601	-0.958	-8.265	-0.452	-2.553	-0.872
	2-3	335.618	29.796	42.288	20.150	-9.058	-0.520	-2.720	-0.969	-9.265	-0.516	-2.802	-1.003
	3-4	336.836	29.828	42.581	20.100	-8.949	-0.515	-2.618	-0.965	-9.298	-0.542	-2.663	-1.014

Tabel S19: CCSD: extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Zero-Point Vibrational Averaged (ZPVA)				Relative to the Optimized Geometry (ZPVC)				Relative to the Experimental Geometry (ExpC)			
Series	σ	$\Delta\sigma$		σ		σ		$\Delta\sigma$		σ		σ	
		O	H	O	H	O	H	O	H	O	H	O	H
cc-pVXZ	D-T	330.458	30.563	37.929	19.832	-10.241	-0.522	-2.190	-1.004	-8.552	-0.394	-2.324	-0.820
	T-Q	328.519	30.175	48.825	19.895	-10.779	-0.507	-1.864	-1.012	-9.284	-0.392	-1.833	-0.834
	Q-5	325.554	30.073	50.990	19.846	-10.603	-0.505	-1.839	-1.001	-9.744	-0.452	-1.782	-0.897
	5-6	326.360	30.136	50.690	19.792	-10.793	-0.508	-1.858	-1.002	-9.992	-0.455	-1.857	-0.909
aug-cc-pVXZ	D-T	324.354	30.349	49.052	19.587	-10.467	-0.514	-2.172	-0.984	-10.137	-0.492	-2.179	-0.940
	T-Q	328.207	30.145	49.194	19.910	-10.774	-0.509	-1.779	-1.015	-9.386	-0.401	-1.779	-0.852
	Q-5	326.825	30.152	49.439	19.845	-10.763	-0.506	-1.900	-1.012	-9.752	-0.434	-1.899	-0.892
	5-6	327.330	30.149	49.138	19.835	-10.620	-0.500	-1.873	-0.995	-9.783	-0.438	-1.866	-0.894
cc-pCVXZ	D-T	331.345	30.556	40.097	19.899	-10.473	-0.520	-2.062	-1.005	-8.234	-0.351	-2.120	-0.753
	T-Q	327.999	30.165	48.034	19.929	-10.611	-0.506	-1.814	-1.008	-8.808	-0.371	-1.791	-0.795
	Q-5	325.529	30.073	52.041	19.917	-10.614	-0.506	-1.768	-1.001	-9.235	-0.417	-1.721	-0.834
	5-6	---	---	50.749	19.555	---	---	-1.792	-1.298	---	---	-1.784	-1.150
aug-cc-pCVXZ	D-T	325.062	30.345	49.591	19.655	-10.642	-0.515	-2.009	-0.984	-9.734	-0.449	-1.991	-0.872
	T-Q	327.939	30.138	49.700	19.951	-10.699	-0.508	-1.774	-1.013	-8.950	-0.378	-1.776	-0.808
	Q-5	327.388	30.150	49.743	19.913	-10.723	-0.506	-1.794	-1.009	-9.229	-0.399	-1.794	-0.832
	5-6	---	---	---	---	---	---	---	---	---	---	---	---
aug-pc-n	1-2	323.119	30.453	51.403	19.787	-10.805	-0.517	-1.741	-1.020	-8.859	-0.374	-1.735	-0.799
	2-3	327.452	30.065	49.644	19.946	-10.797	-0.502	-2.059	-1.012	-9.742	-0.417	-2.084	-0.888
	3-4	327.778	30.148	48.594	19.824	-10.680	-0.502	-1.891	-1.009	-9.838	-0.439	-1.894	-0.908
aug-pcS-n	1-2	330.470	30.465	49.308	19.825	-10.652	-0.504	-1.880	-1.007	-8.776	-0.369	-1.872	-0.785
	2-3	326.248	30.116	48.782	19.877	-10.821	-0.510	-1.857	-1.016	-9.767	-0.420	-1.892	-0.893
	3-4	327.285	30.161	48.815	19.797	-10.814	-0.512	-2.008	-1.022	-9.922	-0.446	-2.010	-0.916

Tabel S20: CCSD(T): extrapolated vibrational corrections to shieldings using the inverse-third-power functions and specified basis sets

Basis sets		Zero-Point Vibrational Averaged (ZPVA)				Relative to the Optimized Geometry (ZPVC)				Relative to the Experimental Geometry (ExpC)			
Series	$\Delta\sigma$	σ		σ		$\Delta\sigma$		σ		σ		$\Delta\sigma$	
		O	H	O	H	O	H	O	H	O	H	O	H
cc-pVXZ	D-T	330.172	30.503	35.978	19.627	-10.496	-0.522	-2.503	-1.029	-9.986	-0.483	-2.720	-0.986
	T-Q	328.116	30.096	47.122	19.690	-10.997	-0.507	-2.154	-1.034	-10.795	-0.486	-2.123	-1.011
	Q-5	325.024	29.979	49.444	19.640	-10.805	-0.507	-2.115	-1.021	-11.280	-0.555	-2.088	-1.078
	5-6	325.730	30.045	49.279	19.582	-11.014	-0.511	-2.139	-1.024	-11.557	-0.556	-2.128	-1.086
aug-cc-pVXZ	D-T	323.875	30.252	47.424	19.381	-10.661	-0.514	-2.466	-1.005	-11.693	-0.601	-2.534	-1.118
	T-Q	327.643	30.059	47.746	19.702	-10.995	-0.510	-2.056	-1.038	-10.910	-0.498	-2.035	-1.032
	Q-5	326.232	30.065	47.959	19.636	-10.991	-0.509	-2.181	-1.032	-11.305	-0.533	-2.180	-1.070
	5-6	326.617	30.057	47.675	19.611	-10.978	-0.506	-2.137	-1.030	-11.460	-0.544	-2.136	-1.089
cc-pCVXZ	D-T	331.037	30.489	38.145	19.684	-10.738	-0.520	-2.389	-1.030	-9.765	-0.445	-2.498	-0.926
	T-Q	327.569	30.083	46.289	19.719	-10.832	-0.507	-2.105	-1.031	-10.357	-0.471	-2.080	-0.976
	Q-5	324.974	29.977	50.533	19.707	-10.812	-0.507	-2.050	-1.021	-10.808	-0.522	-1.994	-1.019
	5-6	---	---	---	---	---	---	---	---	---	---	---	---
aug-cc-pCVXZ	D-T	324.550	30.242	47.945	19.439	-10.843	-0.514	-2.315	-1.007	-11.379	-0.564	-2.321	-1.059
	T-Q	327.355	30.050	48.233	19.737	-10.923	-0.508	-2.054	-1.035	-10.517	-0.477	-2.032	-0.991
	Q-5	326.794	30.060	48.265	19.698	-10.953	-0.510	-2.077	-1.033	-10.812	-0.503	-2.060	-1.015
	5-6	326.668	30.039	48.171	19.661	-11.019	-0.518	-2.057	-1.037	-11.078	-0.527	-2.044	-1.044
aug-pc-n	1-2	322.506	30.370	49.824	19.575	-11.015	-0.518	-2.044	-1.040	-10.416	-0.473	-2.039	-0.975
	2-3	326.979	29.979	48.080	19.735	-10.996	-0.501	-2.406	-1.033	-11.271	-0.514	-2.441	-1.070
	3-4	327.331	30.070	47.306	19.626	-10.760	-0.494	-1.969	-1.020	-11.236	-0.528	-1.979	-1.078
aug-pcS-n	1-2	329.858	30.388	47.845	19.620	-10.867	-0.505	-2.160	-1.026	-10.238	-0.463	-2.130	-0.951
	2-3	325.656	30.028	47.251	19.661	-11.078	-0.511	-2.187	-1.041	-11.363	-0.520	-2.239	-1.079
	3-4	326.883	30.081	47.472	19.604	-10.859	-0.507	-2.146	-1.027	-11.285	-0.539	-2.150	-1.078

Tabel S21: HF: extrapolated shieldings using the exponential function and specified basis sets

Basis sets		Optimized Geometry (OptG)		Zero-Point Vibrational Averaged (ZPVA)	
Series	Used cardinal numbers	Shielding		Shielding	
		O	H	O	H
aug-cc-pVXZ	D-Q	337.150	31.052	326.848	30.556
	T-5	336.931	31.093	326.664	30.575
	Q-6	336.615	31.075	326.210	30.557
aug-pcS-n	2-4	336.932	31.110	326.533	30.597
	3-5	336.625	31.084	326.239	30.567

Tabel S22: CCSD(T): extrapolated shieldings using the exponential function and specified basis sets

Basis sets		Optimized Geometry (OptG)		Zero-Point Vibrational Averaged (ZPVA)	
Series	Used cardinal numbers	Shielding		Shielding	
		O	H	O	H
aug-cc-pCVXZ	D-Q	337.622	30.433	326.646	29.932
	T-5	337.744	30.606	326.791	30.095
	Q-6	337.741	30.567	326.788	30.039
aug-pcS-n	2-4	337.484	30.709	326.412	30.208
	3-5	337.521	30.612	326.518	30.105