Supplementary Material:

Applicability of medium-size basis sets in calculations of molecular dynamic polarisabilities

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Table 1: The CCS average electric polarizability and polarizability anisotropy for the investigated systems. Properties in atomic units, wavelengths in nm.

$\lambda=$	$\alpha_{ave}(\omega)$		$\alpha_{ani}(\omega)$	
	∞	632.8	∞	632.8
F ₂				
aVDZ	8.241	8.334	9.472	9.686
aVTZ	8.734	8.831	9.279	9.489
aVQZ	8.880	8.980	9.240	9.449
aV5Z	8.893	8.994	9.261	9.470
daVDZ	8.886	8.987	9.257	9.466
daVTZ	8.916	9.017	9.272	9.481
daVQZ	8.911	9.012	9.270	9.479
daV5Z	8.905	9.006	9.266	9.475
LPol-ds	8.908	9.009	9.297	9.508
LPol-dl	8.915	9.016	9.283	9.493
LPol-fs	8.904	9.005	9.287	9.496
LPol-fl	8.908	9.009	9.264	9.473
aug-pc-1	8.995	9.095	9.131	9.342
aug-pc-2	8.854	8.956	9.293	9.502
SVPD	8.707	8.804	9.154	9.362
TZVPD	8.882	8.983	9.231	9.440
N ₂				
aVDZ	12.050	12.180	5.577	5.677
aVTZ	12.285	12.422	5.445	5.539
aVQZ	12.312	12.451	5.402	5.494
aV5Z	12.310	12.450	5.400	5.492
daVDZ	12.269	12.407	5.442	5.534
daVTZ	12.318	12.458	5.417	5.510
daVQZ	12.314	12.454	5.405	5.498
daV5Z	12.310	12.450	5.403	5.495
LPol-ds	12.291	12.431	5.381	5.472
LPol-dl	12.299	12.439	5.361	5.452
LPol-fs	12.299	12.439	5.370	5.462
LPol-fl	12.304	12.444	5.377	5.468
aug-pc-1	12.355	12.493	5.377	5.466
aug-pc-2	12.247	12.387	5.448	5.539
SVPD	11.638	11.757	5.715	5.810
TZVPD	12.212	12.347	5.473	5.568
HF				
aVDZ	4.591	4.629	1.941	1.959
aVTZ	4.966	5.008	1.571	1.586
aVQZ	5.084	5.128	1.442	1.455
aV5Z	5.110	5.155	1.411	1.422

daVDZ	5.097	5.142	1.369	1.379
daVTZ	5.132	5.178	1.372	1.382
daVQZ	5.132	5.178	1.383	1.393
daV5Z	5.129	5.175	1.387	1.397
LPol-ds	5.120	5.166	1.393	1.404
LPol-dl	5.124	5.169	1.376	1.386
LPol-fs	5.132	5.179	1.375	1.384
LPol-fl	5.130	5.176	1.381	1.391
aug-pc-1	5.057	5.099	1.416	1.429
aug-pc-2	5.099	5.145	1.429	1.439
SVPD	4.926	4.966	1.465	1.479
TZVPD	5.070	5.114	1.406	1.418

CO

aVDZ	12.921	13.135	3.444	3.432
aVTZ	13.120	13.339	3.220	3.205
aVQZ	13.144	13.365	3.161	3.145
aV5Z	13.140	13.362	3.151	3.134
daVDZ	13.135	13.355	3.196	3.179
daVTZ	13.150	13.371	3.169	3.152
daVQZ	13.143	13.364	3.149	3.132
daV5Z	13.142	13.363	3.147	3.129
LPol-ds	13.124	13.344	3.137	3.120
LPol-dl	13.128	13.349	3.139	3.122
LPol-fs	13.133	13.353	3.138	3.121
LPol-fl	13.139	13.360	3.144	3.127
aug-pc-1	13.109	13.330	3.133	3.115
aug-pc-2	13.067	13.288	3.197	3.179
SVPD	13.017	13.233	3.004	2.980
TZVPD	13.113	13.332	3.167	3.151

CO₂

aVDZ	16.404	16.584	13.130	13.367
aVTZ	16.771	16.959	12.548	12.778
aVQZ	16.858	17.048	12.406	12.633
aV5Z	16.867	17.059	12.390	12.617
daVDZ	16.881	17.073	12.428	12.653
daVTZ	16.890	17.083	12.394	12.620
daVQZ	16.879	17.071	12.380	12.606
daV5Z	16.875	17.068	12.378	12.604
LPol-ds	16.868	17.060	12.421	12.649
LPol-dl	16.870	17.063	12.371	12.596
LPol-fs	16.883	17.076	12.374	12.599
LPol-fl	16.881	17.074	12.374	12.600
aug-pc-1	16.790	16.980	12.413	12.636
aug-pc-2	16.786	16.977	12.415	12.640
SVPD	16.602	16.787	12.395	12.622

TZVPD	16.822	17.012	12.451	12.678
HCN				
aVDZ	17.503	17.787	9.473	9.677
aVTZ	17.813	18.111	9.106	9.296
aVQZ	17.852	18.154	9.048	9.234
aV5Z	17.853	18.155	9.056	9.242
daVDZ	17.830	18.132	9.034	9.216
daVTZ	17.861	18.164	9.060	9.245
daVQZ	17.857	18.160	9.056	9.241
daV5Z	17.856	18.159	9.054	9.239
LPol-ds	17.845	18.147	9.012	9.196
LPol-dl	17.853	18.156	8.997	9.180
LPol-fs	17.849	18.152	9.012	9.195
LPol-fl	17.855	18.158	9.021	9.205
aug-pc-1	17.701	18.000	8.944	9.118
aug-pc-2	17.786	18.088	9.088	9.273
SVPD	17.038	17.303	9.233	9.420
TZVPD	17.724	18.019	9.125	9.312
C ₂ H ₂				
aVDZ	24.370	24.935	13.750	14.101
aVTZ	24.908	25.508	13.125	13.433
aVQZ	24.981	25.593	13.039	13.329
aV5Z	24.989	25.603	13.020	13.307
daVDZ	24.940	25.553	12.998	13.281
daVTZ	25.004	25.621	13.034	13.317
daVQZ	24.996	25.613	13.024	13.308
daV5Z	24.994	25.611	13.021	13.304
LPol-ds	25.010	25.628	12.929	13.210
LPol-dl	25.026	25.645	12.932	13.213
LPol-fs	25.010	25.629	12.951	13.230
LPol-fl	25.019	25.638	12.980	13.262
aug-pc-1	24.772	25.367	12.696	12.954
aug-pc-2	24.884	25.497	13.085	13.367
SVPD	23.621	24.133	13.691	14.011
TZVPD	24.708	25.295	13.240	13.539

Table 2: The CC2 average electric polarizability and polarizability anisotropy for the investigated systems. Properties in atomic units, wavelengths in nm.

$\lambda=$	$\alpha_{ave}(\omega)$		$\alpha_{ani}(\omega)$	
	∞	632.8	∞	632.8
F ₂				
aVDZ	7.837	7.921	6.471	6.597
aVTZ	8.489	8.579	6.111	6.231
aVQZ	8.728	8.822	5.990	6.106
aV5Z	8.768	8.864	5.983	6.098
daVDZ	8.932	9.035	5.964	6.076
daVTZ	8.907	9.008	5.967	6.080
daVQZ	8.855	8.955	5.969	6.082
daV5Z	8.825	8.924	5.967	6.080
LPol-ds	8.905	9.007	5.999	6.115
LPol-dl	8.898	9.001	5.975	6.089
LPol-fs	8.963	9.065	5.961	6.074
LPol-fl	8.940	9.042	5.945	6.058
aug-pc-1	8.934	9.030	5.817	5.933
aug-pc-2	8.854	8.954	5.955	6.069
SVPD	8.657	8.749	5.995	6.116
TZVPD	8.784	8.881	5.949	6.064
N ₂				
aVDZ	11.557	11.706	4.348	4.429
aVTZ	11.623	11.773	4.164	4.237
aVQZ	11.587	11.737	4.132	4.204
aV5Z	11.557	11.707	4.120	4.191
daVDZ	11.712	11.867	4.302	4.378
daVTZ	11.649	11.801	4.168	4.241
daVQZ	11.593	11.744	4.139	4.210
daV5Z	11.561	11.712	4.124	4.195
LPol-ds	11.624	11.777	4.232	4.305
LPol-dl	11.586	11.738	4.226	4.299
LPol-fs	11.696	11.851	4.157	4.230
LPol-fl	11.663	11.816	4.155	4.227
aug-pc-1	11.782	11.937	4.158	4.230
aug-pc-2	11.565	11.718	4.191	4.261
SVPD	10.826	10.950	4.704	4.788
TZVPD	11.444	11.585	4.325	4.407
HF				
aVDZ	5.265	5.330	2.054	2.063
aVTZ	5.720	5.789	1.507	1.513
aVQZ	5.867	5.939	1.275	1.278
aV5Z	5.902	5.975	1.200	1.201

daVDZ	6.057	6.137	1.159	1.154
daVTZ	6.036	6.115	1.118	1.113
daVQZ	5.983	6.060	1.128	1.124
daV5Z	5.955	6.031	1.133	1.129
LPol-ds	6.033	6.113	1.160	1.155
LPol-dl	6.021	6.100	1.144	1.139
LPol-fs	6.105	6.187	1.083	1.074
LPol-fl	6.069	6.149	1.113	1.107
aug-pc-1	5.938	6.012	1.216	1.217
aug-pc-2	6.010	6.088	1.181	1.177
SVPD	5.784	5.851	1.387	1.396
TZVPD	5.859	5.929	1.224	1.227

CO

aVDZ	13.327	13.586	4.255	4.289
aVTZ	13.432	13.694	3.990	4.015
aVQZ	13.397	13.660	3.923	3.944
aV5Z	13.365	13.627	3.901	3.922
daVDZ	13.552	13.818	4.052	4.079
daVTZ	13.470	13.735	3.947	3.971
daVQZ	13.403	13.666	3.910	3.931
daV5Z	13.371	13.633	3.897	3.917
LPol-ds	13.443	13.707	4.048	4.075
LPol-dl	13.409	13.672	4.068	4.097
LPol-fs	13.517	13.784	3.953	3.978
LPol-fl	13.492	13.757	3.958	3.983
aug-pc-1	13.526	13.792	3.983	4.010
aug-pc-2	13.375	13.639	3.963	3.985
SVPD	13.378	13.633	3.882	3.905
TZVPD	13.377	13.637	3.975	3.999

CO₂

aVDZ	18.297	18.596	17.209	17.697
aVTZ	18.628	18.933	16.529	17.008
aVQZ	18.668	18.974	16.374	16.849
aV5Z	18.648	18.954	16.344	16.819
daVDZ	18.905	19.221	16.506	16.984
daVTZ	18.803	19.115	16.358	16.834
daVQZ	18.711	19.020	16.337	16.811
daV5Z	18.667	18.975	16.326	16.800
LPol-ds	18.812	19.127	16.623	17.109
LPol-dl	18.793	19.108	16.588	17.072
LPol-fs	18.909	19.226	16.433	16.914
LPol-fl	18.875	19.191	16.432	16.914
aug-pc-1	18.864	19.178	16.566	17.043
aug-pc-2	18.693	19.003	16.403	16.878
SVPD	18.639	18.945	16.458	16.938

TZVPD	18.640	18.946	16.471	16.947
HCN				
aVDZ	16.676	16.982	8.834	9.066
aVTZ	16.816	17.129	8.409	8.624
aVQZ	16.761	17.073	8.345	8.555
aV5Z	16.719	17.029	8.337	8.546
daVDZ	16.973	17.296	8.465	8.678
daVTZ	16.864	17.181	8.380	8.592
daVQZ	16.772	17.085	8.351	8.561
daV5Z	16.728	17.038	8.333	8.542
LPol-ds	16.830	17.148	8.483	8.696
LPol-dl	16.789	17.104	8.476	8.689
LPol-fs	16.939	17.260	8.367	8.577
LPol-fl	16.901	17.220	8.372	8.582
aug-pc-1	16.800	17.119	8.253	8.452
aug-pc-2	16.754	17.069	8.397	8.607
SVPD	16.135	16.415	8.397	8.597
TZVPD	16.632	16.937	8.473	8.685
C ₂ H ₂				
aVDZ	22.407	22.944	12.821	13.218
aVTZ	22.699	23.251	12.172	12.532
aVQZ	22.632	23.186	12.114	12.462
aV5Z	22.580	23.132	12.094	12.439
daVDZ	22.926	23.507	12.128	12.462
daVTZ	22.789	23.357	12.097	12.436
daVQZ	22.654	23.212	12.092	12.433
daV5Z	22.594	23.147	12.085	12.427
LPol-ds	22.747	23.318	12.180	12.517
LPol-dl	22.692	23.259	12.193	12.530
LPol-fs	22.930	23.510	12.028	12.362
LPol-fl	22.863	23.437	12.061	12.398
aug-pc-1	22.593	23.152	11.573	11.868
aug-pc-2	22.572	23.133	12.156	12.489
SVPD	21.567	22.049	12.723	13.082
TZVPD	22.414	22.952	12.289	12.636

Table 3: The CC3 average electric polarizability and polarizability anisotropy for the investigated systems. Properties in atomic units, wavelengths in nm. Only the results not reported in Mol. Phys. **111**, 1462 (2013) are given.

$\lambda=$	$\alpha_{ave}(\omega)$		$\alpha_{ani}(\omega)$	
	∞	632.8	∞	632.8
F ₂				
aVDZ	7.516	7.596	6.322	6.452
aVTZ	8.109	8.194	6.022	6.146
aVQZ	8.315	8.403	5.944	6.066
aV5Z	8.343	8.433	5.947	6.068
daVDZ	8.453	8.547	5.927	6.047
daVTZ	8.442	8.535	5.929	6.048
daVQZ	8.402	8.494	5.943	6.064
LPol-ds	8.458	8.552	5.960	6.082
LPol-dl	8.455	8.550	5.943	6.065
LPol-fs	8.496	8.591	5.931	6.052
LPol-fl	8.476	8.570	5.912	6.032
aug-pc-1	8.485	8.574	5.797	5.920
aug-pc-2	8.387	8.479	5.914	6.033
SVPD	8.228	8.314	5.916	6.041
TZVPD	8.347	8.438	5.890	6.011
N ₂				
LPol-fl				4.762
aug-pc-1	11.999	12.162	4.684	4.774
aug-pc-2	11.746	11.907	4.700	4.788
SVPD	11.034	11.166	5.222	5.323
TZVPD	11.634	11.784	4.824	4.922
HF				
aug-pc-1	5.512	5.572	1.192	1.197
aug-pc-2	5.598	5.663	1.187	1.188
SVPD	5.400	5.457	1.329	1.340
TZVPD	5.500	5.560	1.203	1.209
CO				
LPol-fl	13.171	13.436	3.578	3.582
aug-pc-1	13.220	13.486	3.618	3.624
aug-pc-2	13.023	13.286	3.574	3.573
SVPD	13.060	13.315	3.564	3.569
TZVPD	13.035	13.294	3.593	3.596
CO ₂				
aVDZ	17.017	17.268	14.651	15.019
aVTZ	17.331	17.587	13.959	14.317
aVQZ	17.368	17.626	13.783	14.137
aV5Z	17.354	17.613	13.749	14.102

daVDZ	17.605	17.872	13.985	14.344
daVTZ	17.492	17.755	13.793	14.148
daVQZ	17.403	17.664	13.748	14.101
LPol-ds	17.550	17.818	14.045	14.409
LPol-dl	17.538	17.805	13.999	14.361
LPol-fs	17.617	17.885	13.886	14.246
LPol-fl	17.580	17.847	13.872	14.232
aug-pc-1	17.571	17.836	13.998	14.353
aug-pc-2	17.369	17.630	13.813	14.166
SVPD	17.366	17.624	13.931	14.292
TZVPD	17.343	17.601	13.883	14.239

HCN

aVDZ	16.634	16.945	8.906	9.145
aVTZ	16.792	17.110	8.475	8.698
aVQZ	16.769	17.089	8.414	8.634
aV5Z	16.742	17.060	8.412	8.631
daVDZ	16.943	17.271	8.519	8.737
daVTZ	16.841	17.164	8.440	8.659
daVQZ	16.777	17.097	8.420	8.639
LPol-ds	16.853	17.179	8.530	8.751
LPol-dl	16.826	17.151	8.519	8.739
LPol-fs	16.943	17.271	8.430	8.648
LPol-fl	16.914	17.241	8.433	8.652
aug-pc-1	16.839	17.166	8.320	8.525
aug-pc-2	16.729	17.050	8.453	8.670
SVPD	16.156	16.443	8.555	8.767
TZVPD	16.615	16.926	8.533	8.753

C₂H₂

aVDZ	22.340	22.896	12.535	12.944
aVTZ	22.688	23.265	11.918	12.292
aVQZ	22.676	23.259	11.860	12.222
aV5Z	22.649	23.231	11.841	12.200
daVDZ	22.863	23.463	11.837	12.183
daVTZ	22.777	23.370	11.840	12.193
daVQZ	22.694	23.281	11.842	12.198
LPol-ds	22.778	23.375	11.882	12.232
LPol-dl	22.750	23.346	11.893	12.242
LPol-fs	22.920	23.524	11.761	12.109
LPol-fl	22.868	23.468	11.791	12.142
aug-pc-1	22.683	23.271	11.325	11.633
aug-pc-2	22.594	23.181	11.890	12.237
SVPD	21.579	22.082	12.497	12.871
TZVPD	22.408	22.971	12.032	12.392