

Electronic Supplementary Information

Spectroscopic properties of open shell diatomic molecules using Piris Natural Orbital Functionals

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The potential energy surfaces, energy vs. distance corresponding to the nine heteronuclear diatomic molecules reported in the text, namely, BeO, CS, AlF, ClF, NH, NF, PH, CF and NO, calculated with CASSCF, CASPT2, PNOF7s, and NOF-MP2, are reported in this Supplementary material. In several cases, the grids are not the same because it was necessary to decrease the step size to assure that the molecule was in the correct state. Distances are in Å and energies in Hartrees. The tables are available upon request.

Table S1 Potential energy surface of BeO

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
5.000	-89.330754	5.000	-89.490744	5.000	-89.355717	4.998	-89.474363
4.900	-89.330758	4.900	-89.490767	4.900	-89.355836	4.993	-89.474386
4.800	-89.330763	4.800	-89.490793	4.800	-89.355984	4.988	-89.474409
4.700	-89.330769	4.700	-89.490820	4.700	-89.356166	4.983	-89.474433
4.600	-89.330776	4.600	-89.490854	4.600	-89.356391	4.978	-89.474457
4.500	-89.330784	4.500	-89.490881	4.500	-89.356667	4.973	-89.474481
4.400	-89.330794	4.400	-89.490923	4.400	-89.357004	4.968	-89.474506
4.300	-89.330806	4.300	-89.490975	4.300	-89.357414	4.963	-89.474531
4.200	-89.330821	4.200	-89.491021	4.200	-89.357908	4.958	-89.474556
4.100	-89.330839	4.100	-89.491089	4.100	-89.358501	4.953	-89.474582
4.000	-89.330862	4.000	-89.491171	4.000	-89.359211	4.948	-89.474608
3.900	-89.330891	3.900	-89.491272	3.900	-89.360057	4.943	-89.474633
3.800	-89.330927	3.800	-89.491408	3.800	-89.361059	4.938	-89.474659
3.700	-89.330974	3.700	-89.491578	3.700	-89.362243	4.933	-89.474686
3.600	-89.331033	3.600	-89.491799	3.600	-89.363638	4.928	-89.474712
3.500	-89.331111	3.500	-89.492094	3.500	-89.365279	4.923	-89.474739
3.400	-89.331212	3.400	-89.492488	3.400	-89.367211	4.918	-89.474765
3.300	-89.331347	3.300	-89.493017	3.300	-89.369488	4.913	-89.474792
3.200	-89.331527	3.200	-89.493727	3.200	-89.372177	4.908	-89.474819
3.100	-89.331770	3.100	-89.494698	3.100	-89.375364	4.903	-89.474845
3.000	-89.332101	3.000	-89.495990	3.000	-89.379153	4.898	-89.474872
2.900	-89.334643	2.900	-89.503121	2.900	-89.383673	4.893	-89.474899
2.800	-89.337427	2.800	-89.507739	2.800	-89.389076	4.888	-89.474926
2.700	-89.341989	2.700	-89.515435	2.700	-89.395529	4.883	-89.474953
2.600	-89.351010	2.600	-89.529113	2.600	-89.403197	4.878	-89.474980
2.500	-89.362642	2.500	-89.541077	2.500	-89.412217	4.873	-89.475007
2.400	-89.375552	2.400	-89.554241	2.400	-89.422661	4.868	-89.475034
2.300	-89.389674	2.300	-89.568800	2.300	-89.434536	4.863	-89.475062
2.200	-89.405063	2.200	-89.585022	2.200	-89.447761	4.858	-89.475089
2.100	-89.421957	2.100	-89.602954	2.100	-89.462157	4.853	-89.475117
2.000	-89.440566	2.000	-89.621372	2.000	-89.477426	4.848	-89.475145
1.900	-89.460830	1.900	-89.640630	1.900	-89.490297	4.843	-89.475173
1.800	-89.482591	1.800	-89.661005	1.880	-89.493688	4.838	-89.475201
1.700	-89.505349	1.700	-89.682261	1.860	-89.497061	4.833	-89.475230
1.600	-89.527952	1.600	-89.703483	1.840	-89.500408	4.828	-89.475259
1.500	-89.548189	1.500	-89.722646	1.820	-89.503722	4.823	-89.475288
1.490	-89.549953	1.490	-89.724332	1.800	-89.506995	4.818	-89.475317
1.480	-89.551652	1.480	-89.725953	1.780	-89.510220	4.813	-89.475347
1.470	-89.553281	1.470	-89.727509	1.760	-89.513385	4.808	-89.475377
1.460	-89.554834	1.460	-89.728994	1.740	-89.516481	4.803	-89.475408
1.450	-89.556307	1.450	-89.730404	1.720	-89.519497	4.798	-89.475439
1.440	-89.557691	1.440	-89.731731	1.700	-89.522418	4.793	-89.475470
1.430	-89.558983	1.430	-89.732970	1.680	-89.525232	4.788	-89.475502
1.420	-89.560174	1.420	-89.734115	1.660	-89.527923	4.783	-89.475535
1.410	-89.561257	1.410	-89.735158	1.640	-89.530474	4.778	-89.475567
1.400	-89.562226	1.400	-89.736093	1.620	-89.532866	4.773	-89.475600
1.390	-89.563073	1.390	-89.736911	1.600	-89.535079	4.768	-89.475634
1.380	-89.563790	1.380	-89.737605	1.580	-89.537090	4.763	-89.475668
1.370	-89.564367	1.370	-89.738166	1.560	-89.538875	4.758	-89.475702
1.360	-89.564797	1.360	-89.738586	1.540	-89.540405	4.753	-89.475737
1.350	-89.565070	1.350	-89.738846	1.520	-89.541650	4.748	-89.475772
1.349	-89.565088	1.349	-89.738871	1.500	-89.542579	4.743	-89.475807
1.348	-89.565105	1.348	-89.738881	1.480	-89.543154	4.738	-89.475843
1.347	-89.565120	1.347	-89.738902	1.460	-89.543334	4.733	-89.475879
1.346	-89.565133	1.346	-89.738909	1.440	-89.543076	4.728	-89.475916
1.345	-89.565145	1.345	-89.738927	1.420	-89.542330	4.723	-89.475952
1.344	-89.565154	1.344	-89.738931	1.400	-89.541044	4.718	-89.475990
1.343	-89.565162	1.343	-89.738946	1.300	-89.534024	4.713	-89.476027

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Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.342	-89.565169	1.342	-89.738947	1.280	-89.533177	4.708	-89.476065
1.341	-89.565173	1.341	-89.738958	1.260	-89.531333	4.703	-89.476103
1.340	-89.565176	1.340	-89.738955	1.240	-89.528374	4.698	-89.476142
1.339	-89.565177	1.339	-89.738963	1.220	-89.524171	4.693	-89.476181
1.338	-89.565176	1.338	-89.738957	1.200	-89.518583	4.688	-89.476220
1.337	-89.565174	1.337	-89.738961	1.180	-89.511452	4.683	-89.476260
1.336	-89.565169	1.336	-89.738951	1.160	-89.502606	4.678	-89.476300
1.335	-89.565163	1.335	-89.738952	1.140	-89.491853	4.673	-89.476340
1.334	-89.565155	1.334	-89.738939	1.120	-89.478983	4.668	-89.476381
1.333	-89.565146	1.333	-89.738937	1.100	-89.463763	4.663	-89.476422
1.332	-89.565134	1.332	-89.738923	1.080	-89.445932	4.658	-89.476464
1.331	-89.565120	1.331	-89.738917	1.060	-89.425206	4.653	-89.476506
1.330	-89.565105	1.330	-89.738909	1.040	-89.401270	4.648	-89.476548
1.329	-89.565088	1.329	-89.738890	1.020	-89.373775	4.643	-89.476591
1.328	-89.565068	1.328	-89.738878	1.000	-89.342337	4.638	-89.476634
1.327	-89.565047	1.327	-89.738853			4.633	-89.476678
1.326	-89.565024	1.326	-89.738837			4.628	-89.476722
1.325	-89.565000	1.325	-89.738808			4.623	-89.476766
1.324	-89.564973	1.324	-89.738789			4.618	-89.476811
1.323	-89.564944	1.323	-89.738756			4.613	-89.476857
1.322	-89.564913	1.322	-89.738732			4.608	-89.476903
1.321	-89.564881	1.321	-89.738696			4.603	-89.476949
1.320	-89.564846	1.320	-89.738669			4.598	-89.476996
1.319	-89.564809	1.319	-89.738628			4.593	-89.477044
1.318	-89.564770	1.318	-89.738597			4.588	-89.477091
1.317	-89.564730	1.317	-89.738553			4.583	-89.477140
1.316	-89.564687	1.316	-89.738518			4.578	-89.477189
1.315	-89.564642	1.315	-89.738470			4.573	-89.477238
1.314	-89.564595	1.314	-89.738431			4.568	-89.477288
1.313	-89.564547	1.313	-89.738379			4.563	-89.477338
1.312	-89.564495	1.312	-89.738336			4.558	-89.477389
1.311	-89.564443	1.311	-89.738280			4.553	-89.477440
1.310	-89.564387	1.310	-89.738233			4.548	-89.477491
1.309	-89.564330	1.309	-89.738173			4.543	-89.477543
1.308	-89.564271	1.308	-89.738122			4.538	-89.477596
1.307	-89.564209	1.307	-89.738057			4.533	-89.477648
1.306	-89.564145	1.306	-89.738002			4.528	-89.477701
1.305	-89.564080	1.305	-89.737934			4.523	-89.477755
1.304	-89.564012	1.304	-89.737874			4.518	-89.477808
1.303	-89.563941	1.303	-89.737802			4.513	-89.477862
1.302	-89.563869	1.302	-89.737738			4.508	-89.477917
1.301	-89.563794	1.301	-89.737661			4.503	-89.477972
1.300	-89.563718	1.300	-89.737593			4.498	-89.478027
1.290	-89.562824	1.290	-89.736728			4.493	-89.478082
1.280	-89.561694	1.280	-89.735641			4.488	-89.478138
1.270	-89.560313	1.270	-89.734309			4.483	-89.478194
1.260	-89.558666	1.260	-89.732720			4.478	-89.478250
1.250	-89.556739	1.250	-89.730858			4.473	-89.478307
1.240	-89.554516	1.240	-89.728707			4.468	-89.478364
1.230	-89.551979	1.230	-89.726250			4.463	-89.478422
1.220	-89.549111	1.220	-89.723470			4.458	-89.478480
1.210	-89.545893	1.210	-89.720348			4.453	-89.478538
1.200	-89.542307	1.200	-89.716864			4.448	-89.478597
1.180	-89.533943	1.180	-89.708730			4.443	-89.478657
1.160	-89.523843	1.160	-89.698893			4.438	-89.478717
1.140	-89.511811	1.140	-89.687158			4.433	-89.478777
1.120	-89.497632	1.120	-89.673311			4.428	-89.478838
1.100	-89.481068	1.100	-89.657116			4.423	-89.478899
1.080	-89.461856	1.080	-89.638312			4.418	-89.478961

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Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.060	-89.439707	1.060	-89.616611			4.413	-89.479024
1.040	-89.414303	1.040	-89.591697			4.408	-89.479087
1.020	-89.385292	1.020	-89.563221			4.403	-89.479150
1.000	-89.352287	1.000	-89.530799			4.398	-89.479215
						4.393	-89.479280
						4.388	-89.479345
						4.383	-89.479411
						4.378	-89.479478
						4.373	-89.479545
						4.368	-89.479613
						4.363	-89.479681
						4.358	-89.479750
						4.353	-89.479820
						4.348	-89.479890
						4.343	-89.479960
						4.338	-89.480032
						4.333	-89.480103
						4.328	-89.480176
						4.323	-89.480248
						4.318	-89.480322
						4.313	-89.480395
						4.308	-89.480470
						4.303	-89.480544
						4.298	-89.480620
						4.293	-89.480696
						4.288	-89.480772
						4.283	-89.480849
						4.278	-89.480926
						4.273	-89.481004
						4.268	-89.481082
						4.263	-89.481161
						4.258	-89.481240
						4.253	-89.481320
						4.248	-89.481400
						4.243	-89.481481
						4.238	-89.481563
						4.233	-89.481645
						4.228	-89.481728
						4.223	-89.481811
						4.218	-89.481895
						4.213	-89.481980
						4.208	-89.482065
						4.203	-89.482150
						4.198	-89.482237
						4.193	-89.482324
						4.188	-89.482411
						4.183	-89.482499
						4.178	-89.482588
						4.173	-89.482678
						4.168	-89.482768
						4.163	-89.482858
						4.158	-89.482950
						4.153	-89.483042
						4.148	-89.483134
						4.143	-89.483228
						4.138	-89.483322
						4.133	-89.483416
						4.128	-89.483511
						4.123	-89.483607

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Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						4.118	-89.483704
						4.113	-89.483801
						4.108	-89.483899
						4.103	-89.483997
						4.098	-89.484096
						4.093	-89.484196
						4.088	-89.484296
						4.083	-89.484397
						4.078	-89.484499
						4.073	-89.484602
						4.068	-89.484704
						4.063	-89.484808
						4.058	-89.484912
						4.053	-89.485017
						4.048	-89.485122
						4.043	-89.485228
						4.038	-89.485335
						4.033	-89.485442
						4.028	-89.485549
						4.023	-89.485658
						4.018	-89.485766
						4.013	-89.485876
						4.008	-89.485985
						4.003	-89.486096
						3.997	-89.486206
						3.992	-89.486318
						3.987	-89.486430
						3.982	-89.486542
						3.977	-89.486655
						3.972	-89.486768
						3.967	-89.486883
						3.962	-89.486997
						3.957	-89.487113
						3.952	-89.487229
						3.947	-89.487345
						3.942	-89.487462
						3.937	-89.487580
						3.932	-89.487699
						3.927	-89.487818
						3.922	-89.487938
						3.917	-89.488059
						3.912	-89.488180
						3.907	-89.488302
						3.902	-89.488425
						3.897	-89.488549
						3.892	-89.488674
						3.887	-89.488799
						3.882	-89.488925
						3.877	-89.489052
						3.872	-89.489179
						3.867	-89.489307
						3.862	-89.489436
						3.857	-89.489565
						3.852	-89.489695
						3.847	-89.489825
						3.842	-89.489956
						3.837	-89.490087
						3.832	-89.490219
						3.827	-89.490351

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Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						3.822	-89.490483
						3.817	-89.490616
						3.812	-89.490749
						3.807	-89.490883
						3.802	-89.491016
						3.797	-89.491150
						3.792	-89.491284
						3.787	-89.491419
						3.782	-89.491554
						3.777	-89.491689
						3.772	-89.491825
						3.767	-89.491961
						3.762	-89.492097
						3.757	-89.492234
						3.752	-89.492372
						3.747	-89.492510
						3.742	-89.492649
						3.737	-89.492789
						3.732	-89.492929
						3.727	-89.493071
						3.722	-89.493213
						3.717	-89.493356
						3.712	-89.493500
						3.707	-89.493645
						3.702	-89.493790
						3.697	-89.493937
						3.692	-89.494085
						3.687	-89.494234
						3.682	-89.494384
						3.677	-89.494535
						3.672	-89.494687
						3.667	-89.494840
						3.662	-89.494994
						3.657	-89.495148
						3.652	-89.495304
						3.647	-89.495460
						3.642	-89.495617
						3.637	-89.495775
						3.632	-89.495933
						3.627	-89.496092
						3.622	-89.496252
						3.617	-89.496412
						3.612	-89.496573
						3.607	-89.496735
						3.602	-89.496897
						3.597	-89.497059
						3.592	-89.497222
						3.587	-89.497386
						3.582	-89.497549
						3.577	-89.497714
						3.572	-89.497879
						3.567	-89.498044
						3.562	-89.498210
						3.557	-89.498377
						3.552	-89.498544
						3.547	-89.498711
						3.542	-89.498880
						3.537	-89.499048
						3.532	-89.499217

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Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						3.527	-89.499387
						3.522	-89.499558
						3.517	-89.499728
						3.512	-89.499900
						3.507	-89.500072
						3.502	-89.500245
						3.497	-89.500418
						3.492	-89.500592
						3.487	-89.500766
						3.482	-89.500942
						3.477	-89.501117
						3.472	-89.501294
						3.467	-89.501471
						3.462	-89.501649
						3.457	-89.501828
						3.452	-89.502008
						3.447	-89.502188
						3.442	-89.502369
						3.437	-89.502551
						3.432	-89.502734
						3.427	-89.502918
						3.422	-89.503102
						3.417	-89.503288
						3.412	-89.503474
						3.407	-89.503662
						3.402	-89.503850
						3.397	-89.504039
						3.392	-89.504230
						3.387	-89.504421
						3.382	-89.504613
						3.377	-89.504806
						3.372	-89.505000
						3.367	-89.505194
						3.362	-89.505389
						3.357	-89.505585
						3.352	-89.505781
						3.347	-89.505978
						3.342	-89.506175
						3.337	-89.506372
						3.332	-89.506570
						3.327	-89.506768
						3.322	-89.506966
						3.317	-89.507164
						3.312	-89.507362
						3.307	-89.507560
						3.302	-89.507759
						3.297	-89.507957
						3.292	-89.508155
						3.287	-89.508352
						3.282	-89.508550
						3.277	-89.508748
						3.272	-89.508946
						3.267	-89.509144
						3.262	-89.509342
						3.257	-89.509541
						3.252	-89.509740
						3.247	-89.509939
						3.242	-89.510138
						3.237	-89.510338

Continued on next page

Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						3.232	-89.510538
						3.227	-89.510739
						3.222	-89.510941
						3.217	-89.511143
						3.212	-89.511345
						3.207	-89.511549
						3.202	-89.511753
						3.197	-89.511958
						3.192	-89.512164
						3.187	-89.512370
						3.182	-89.512578
						3.177	-89.512786
						3.172	-89.512996
						3.167	-89.513206
						3.162	-89.513417
						3.157	-89.513630
						3.152	-89.513843
						3.147	-89.514058
						3.142	-89.514273
						3.137	-89.514490
						3.132	-89.514708
						3.127	-89.514927
						3.122	-89.515147
						3.117	-89.515368
						3.112	-89.515590
						3.107	-89.515814
						3.102	-89.516039
						3.097	-89.516265
						3.092	-89.516493
						3.087	-89.516722
						3.082	-89.516952
						3.077	-89.517184
						3.072	-89.517418
						3.067	-89.517653
						3.062	-89.517889
						3.057	-89.518128
						3.052	-89.518367
						3.047	-89.518609
						3.042	-89.518853
						3.037	-89.519098
						3.032	-89.519345
						3.027	-89.519594
						3.022	-89.519845
						3.017	-89.520098
						3.012	-89.520354
						3.007	-89.520611
						3.002	-89.520870
						2.996	-89.521132
						2.991	-89.521396
						2.986	-89.521662
						2.981	-89.521930
						2.976	-89.522200
						2.971	-89.522472
						2.966	-89.522746
						2.961	-89.523021
						2.956	-89.523298
						2.951	-89.523577
						2.946	-89.523857
						2.941	-89.524138

Continued on next page

Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						2.936	-89.524421
						2.931	-89.524705
						2.926	-89.524990
						2.921	-89.525276
						2.916	-89.525564
						2.911	-89.525852
						2.906	-89.526141
						2.901	-89.526431
						2.896	-89.526722
						2.891	-89.527013
						2.886	-89.527305
						2.881	-89.527599
						2.876	-89.527893
						2.871	-89.528189
						2.866	-89.528486
						2.861	-89.528785
						2.856	-89.529086
						2.851	-89.529389
						2.846	-89.529693
						2.841	-89.530000
						2.836	-89.530309
						2.831	-89.530621
						2.826	-89.530935
						2.821	-89.531252
						2.816	-89.531571
						2.811	-89.531894
						2.806	-89.532220
						2.801	-89.532549
						2.796	-89.532882
						2.791	-89.533218
						2.786	-89.533558
						2.781	-89.533901
						2.776	-89.534248
						2.771	-89.534598
						2.766	-89.534951
						2.761	-89.535308
						2.756	-89.535669
						2.751	-89.536032
						2.746	-89.536399
						2.741	-89.536770
						2.736	-89.537143
						2.731	-89.537520
						2.726	-89.537901
						2.721	-89.538285
						2.716	-89.538672
						2.711	-89.539062
						2.706	-89.539455
						2.701	-89.539852
						2.696	-89.540252
						2.691	-89.540656
						2.686	-89.541062
						2.681	-89.541472
						2.676	-89.541885
						2.671	-89.542302
						2.666	-89.542722
						2.661	-89.543146
						2.656	-89.543573
						2.651	-89.544003
						2.646	-89.544437

Continued on next page

Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						2.641	-89.544875
						2.636	-89.545316
						2.631	-89.545761
						2.626	-89.546209
						2.621	-89.546662
						2.616	-89.547118
						2.611	-89.547577
						2.606	-89.548041
						2.601	-89.548508
						2.596	-89.548979
						2.591	-89.549454
						2.586	-89.549933
						2.581	-89.550416
						2.576	-89.550903
						2.571	-89.551393
						2.566	-89.551887
						2.561	-89.552385
						2.556	-89.552886
						2.551	-89.553391
						2.546	-89.553900
						2.541	-89.554413
						2.536	-89.554929
						2.531	-89.555449
						2.526	-89.555973
						2.521	-89.556500
						2.516	-89.557031
						2.511	-89.557565
						2.506	-89.558103
						2.501	-89.558644
						2.496	-89.559189
						2.491	-89.559737
						2.486	-89.560289
						2.481	-89.560845
						2.476	-89.561404
						2.471	-89.561966
						2.466	-89.562532
						2.461	-89.563101
						2.456	-89.563674
						2.451	-89.564250
						2.446	-89.564830
						2.441	-89.565413
						2.436	-89.566000
						2.431	-89.566590
						2.426	-89.567184
						2.421	-89.567781
						2.416	-89.568381
						2.411	-89.568985
						2.406	-89.569592
						2.401	-89.570203
						2.396	-89.570818
						2.391	-89.571435
						2.386	-89.572056
						2.381	-89.572681
						2.376	-89.573309
						2.371	-89.573940
						2.366	-89.574574
						2.361	-89.575211
						2.356	-89.575852
						2.351	-89.576496

Continued on next page

Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						2.346	-89.577143
						2.341	-89.577794
						2.336	-89.578447
						2.331	-89.579103
						2.326	-89.579763
						2.321	-89.580425
						2.316	-89.581091
						2.311	-89.581759
						2.306	-89.582431
						2.301	-89.583105
						2.296	-89.583782
						2.291	-89.584462
						2.286	-89.585145
						2.281	-89.585830
						2.276	-89.586519
						2.271	-89.587210
						2.266	-89.587903
						2.261	-89.588600
						2.256	-89.589298
						2.251	-89.590000
						2.246	-89.590704
						2.241	-89.591410
						2.236	-89.592119
						2.231	-89.592830
						2.226	-89.593543
						2.221	-89.594259
						2.216	-89.594977
						2.211	-89.595697
						2.206	-89.596419
						2.201	-89.597144
						2.196	-89.597871
						2.191	-89.598599
						2.186	-89.599330
						2.181	-89.600063
						2.176	-89.600798
						2.171	-89.601535
						2.166	-89.602274
						2.161	-89.603015
						2.156	-89.603758
						2.151	-89.604503
						2.146	-89.605250
						2.141	-89.605999
						2.136	-89.606750
						2.131	-89.607502
						2.126	-89.608257
						2.121	-89.609014
						2.116	-89.609772
						2.111	-89.610532
						2.106	-89.611294
						2.101	-89.612058
						2.096	-89.612824
						2.091	-89.613591
						2.086	-89.614360
						2.081	-89.615131
						2.076	-89.615903
						2.071	-89.616677
						2.066	-89.617452
						2.061	-89.618228
						2.056	-89.619005

Continued on next page

Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						2.051	-89.619783
						2.046	-89.620563
						2.041	-89.621343
						2.036	-89.622124
						2.031	-89.622905
						2.026	-89.623688
						2.021	-89.624470
						2.016	-89.625254
						2.011	-89.626037
						2.006	-89.626821
						2.001	-89.627605
						1.995	-89.628390
						1.990	-89.629174
						1.985	-89.629959
						1.980	-89.630744
						1.975	-89.631530
						1.970	-89.632316
						1.965	-89.633103
						1.960	-89.633891
						1.955	-89.634680
						1.950	-89.635470
						1.945	-89.636262
						1.940	-89.637054
						1.935	-89.637848
						1.930	-89.638644
						1.925	-89.639441
						1.920	-89.640240
						1.915	-89.641041
						1.910	-89.641844
						1.905	-89.642649
						1.900	-89.643457
						1.895	-89.644266
						1.890	-89.645078
						1.885	-89.645890
						1.880	-89.646703
						1.875	-89.647514
						1.870	-89.648325
						1.865	-89.649133
						1.860	-89.649939
						1.855	-89.650740
						1.850	-89.651537
						1.845	-89.652329
						1.840	-89.653114
						1.835	-89.653893
						1.830	-89.654664
						1.825	-89.655427
						1.820	-89.656180
						1.815	-89.656923
						1.810	-89.657656
						1.805	-89.658376
						1.800	-89.659085
						1.795	-89.659780
						1.790	-89.660465
						1.785	-89.661140
						1.780	-89.661808
						1.775	-89.662471
						1.770	-89.663132
						1.765	-89.663794
						1.760	-89.664457

Continued on next page

Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						1.755	-89.665124
						1.750	-89.665799
						1.745	-89.666482
						1.740	-89.667176
						1.735	-89.667884
						1.730	-89.668608
						1.725	-89.669349
						1.720	-89.670111
						1.715	-89.670895
						1.710	-89.671704
						1.705	-89.672540
						1.700	-89.673405
						1.695	-89.674301
						1.690	-89.675228
						1.685	-89.676185
						1.680	-89.677169
						1.675	-89.678181
						1.670	-89.679218
						1.665	-89.680279
						1.660	-89.681364
						1.655	-89.682470
						1.650	-89.683596
						1.645	-89.684742
						1.640	-89.685905
						1.635	-89.687085
						1.630	-89.688280
						1.625	-89.689489
						1.620	-89.690711
						1.615	-89.691945
						1.610	-89.693188
						1.605	-89.694440
						1.600	-89.695700
						1.595	-89.696966
						1.590	-89.698237
						1.585	-89.699512
						1.580	-89.700789
						1.575	-89.702067
						1.570	-89.703345
						1.565	-89.704621
						1.560	-89.705895
						1.555	-89.707164
						1.550	-89.708429
						1.545	-89.709686
						1.540	-89.710936
						1.535	-89.712176
						1.530	-89.713406
						1.525	-89.714625
						1.520	-89.715830
						1.515	-89.717021
						1.510	-89.718196
						1.505	-89.719354
						1.500	-89.720494
						1.495	-89.721614
						1.490	-89.722714
						1.485	-89.723792
						1.480	-89.724846
						1.475	-89.725875
						1.470	-89.726879
						1.465	-89.727855

Continued on next page

Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						1.460	-89.728803
						1.455	-89.729721
						1.450	-89.730608
						1.445	-89.731463
						1.440	-89.732283
						1.435	-89.733069
						1.430	-89.733819
						1.425	-89.734531
						1.420	-89.735204
						1.415	-89.735837
						1.410	-89.736429
						1.405	-89.736978
						1.400	-89.737483
						1.395	-89.737942
						1.390	-89.738356
						1.385	-89.738721
						1.380	-89.739037
						1.375	-89.739304
						1.370	-89.739528
						1.365	-89.739715
						1.360	-89.739865
						1.355	-89.739977
						1.350	-89.740048
						1.345	-89.740079
						1.340	-89.740068
						1.335	-89.740014
						1.330	-89.739916
						1.325	-89.739773
						1.320	-89.739582
						1.315	-89.739343
						1.310	-89.739055
						1.305	-89.738715
						1.300	-89.738323
						1.295	-89.737877
						1.290	-89.737376
						1.285	-89.736817
						1.280	-89.736199
						1.275	-89.735520
						1.270	-89.734778
						1.265	-89.733972
						1.260	-89.733099
						1.255	-89.732159
						1.250	-89.731148
						1.245	-89.730065
						1.240	-89.728908
						1.235	-89.727676
						1.230	-89.726367
						1.225	-89.724978
						1.220	-89.723508
						1.215	-89.721956
						1.210	-89.720319
						1.205	-89.718596
						1.200	-89.716784
						1.195	-89.714882
						1.190	-89.712886
						1.185	-89.710793
						1.180	-89.708598
						1.175	-89.706298
						1.170	-89.703889

Continued on next page

Table S1 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
						1.165	-89.701368
						1.160	-89.698729
						1.155	-89.695971
						1.150	-89.693088
						1.145	-89.690078
						1.140	-89.686935
						1.135	-89.683657
						1.130	-89.680240
						1.125	-89.676680
						1.120	-89.672973
						1.115	-89.669115
						1.110	-89.665102
						1.105	-89.660932
						1.100	-89.656599
						1.095	-89.652101
						1.090	-89.647433
						1.085	-89.642592
						1.080	-89.637576
						1.075	-89.632380
						1.070	-89.627001
						1.065	-89.621436
						1.060	-89.615681
						1.055	-89.609733
						1.050	-89.603589
						1.045	-89.597244
						1.040	-89.590697
						1.035	-89.583943
						1.030	-89.576979
						1.025	-89.569801
						1.020	-89.562407
						1.015	-89.554792
						1.010	-89.546953
						1.005	-89.538888
						1.000	-89.530592

Table S2 Potential energy surface of CS

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
5.000	-435.220344	5.000	-435.411551	5.000	-435.255640	5.000	-435.437617
4.900	-435.220376	4.900	-435.411626	4.900	-435.255652	4.900	-435.437841
4.800	-435.220411	4.800	-435.411691	4.800	-435.255667	4.800	-435.438125
4.700	-435.220451	4.700	-435.411758	4.700	-435.255685	4.700	-435.438451
4.600	-435.220495	4.600	-435.411836	4.600	-435.255706	4.600	-435.438826
4.500	-435.220544	4.500	-435.411918	4.500	-435.255733	4.500	-435.439263
4.400	-435.220598	4.400	-435.412025	4.400	-435.255766	4.400	-435.439766
4.300	-435.220659	4.300	-435.412133	4.300	-435.255808	4.300	-435.440347
4.200	-435.220729	4.200	-435.412291	4.200	-435.255862	4.200	-435.441007
4.100	-435.220807	4.100	-435.412444	4.100	-435.255930	4.100	-435.441755
4.000	-435.220897	4.000	-435.412636	4.000	-435.256018	4.000	-435.442602
3.900	-435.221001	3.900	-435.412878	3.900	-435.256131	3.900	-435.443549
3.800	-435.221123	3.800	-435.413182	3.800	-435.256275	3.800	-435.444613
3.700	-435.221267	3.700	-435.413575	3.700	-435.256459	3.700	-435.445799
3.600	-435.221445	3.600	-435.414102	3.600	-435.256696	3.600	-435.447116
3.500	-435.221678	3.500	-435.414859	3.500	-435.256999	3.500	-435.448577
3.400	-435.222017	3.400	-435.416179	3.400	-435.257390	3.400	-435.450198
3.300	-435.222750	3.300	-435.422355	3.300	-435.257895	3.300	-435.451986
3.200	-435.224562	3.200	-435.429290	3.200	-435.258548	3.200	-435.453948

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Table S2 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
3.100	-435.227321	3.100	-435.434185	3.100	-435.259392	3.100	-435.456079
3.000	-435.231099	3.000	-435.439205	3.000	-435.260483	3.000	-435.458353
2.900	-435.236116	2.900	-435.445054	2.900	-435.261890	2.900	-435.460711
2.800	-435.242656	2.800	-435.452107	2.800	-435.263709	2.800	-435.463057
2.700	-435.251028	2.700	-435.460659	2.700	-435.266068	2.700	-435.465266
2.600	-435.261527	2.600	-435.471002	2.600	-435.269153	2.600	-435.467244
2.500	-435.274395	2.500	-435.483424	2.500	-435.273240	2.500	-435.469090
2.400	-435.289797	2.400	-435.498159	2.400	-435.278734	2.400	-435.471441
2.300	-435.307792	2.300	-435.515342	2.300	-435.286219	2.300	-435.475953
2.200	-435.328310	2.200	-435.534965	2.200	-435.296455	2.200	-435.485368
2.100	-435.351117	2.100	-435.556799	2.100	-435.310184	2.100	-435.502098
2.000	-435.375782	2.000	-435.580140	2.000	-435.327673	2.000	-435.526135
1.900	-435.401603	1.900	-435.604435	1.900	-435.348534	1.900	-435.555977
1.880	-435.406756	1.880	-435.609322	1.700	-435.391903	1.700	-435.631520
1.860	-435.411868	1.860	-435.614170	1.600	-435.411432	1.600	-435.648283
1.840	-435.416920	1.840	-435.618961	1.590	-435.412712	1.590	-435.649312
1.820	-435.421894	1.820	-435.623673	1.580	-435.413838	1.580	-435.650192
1.800	-435.426765	1.800	-435.628284	1.570	-435.414800	1.570	-435.650914
1.780	-435.431511	1.780	-435.632768	1.560	-435.415590	1.560	-435.651469
1.760	-435.436103	1.760	-435.637096	1.550	-435.416197	1.550	-435.651847
1.740	-435.440513	1.740	-435.641236	1.540	-435.416611	1.540	-435.652038
1.720	-435.444708	1.720	-435.645156	1.539	-435.416641	1.539	-435.652046
1.700	-435.448652	1.700	-435.648815	1.538	-435.416669	1.538	-435.652052
1.680	-435.452308	1.680	-435.652171	1.537	-435.416696	1.537	-435.652057
1.660	-435.455632	1.660	-435.655175	1.536	-435.416720	1.536	-435.652059
1.640	-435.458578	1.640	-435.657771	1.535	-435.416742	1.535	-435.652059
1.620	-435.460868	1.620	-435.658044	1.534	-435.416762	1.534	-435.652058
1.600	-435.463107	1.600	-435.659928	1.533	-435.416780	1.533	-435.652054
1.580	-435.464790	1.580	-435.661275	1.532	-435.416795	1.532	-435.652048
1.570	-435.465399	1.570	-435.661720	1.531	-435.416809	1.531	-435.652040
1.569	-435.465450	1.569	-435.661756	1.530	-435.416820	1.530	-435.652030
1.568	-435.465501	1.568	-435.661791	1.529	-435.416830	1.529	-435.652018
1.567	-435.465549	1.567	-435.661824	1.528	-435.416837	1.528	-435.652004
1.566	-435.465596	1.566	-435.661855	1.527	-435.416842	1.527	-435.651987
1.565	-435.465641	1.565	-435.661885	1.526	-435.416844	1.526	-435.651969
1.564	-435.465684	1.564	-435.661913	1.525	-435.416845	1.525	-435.651948
1.563	-435.465726	1.563	-435.661939	1.524	-435.416843	1.524	-435.651926
1.562	-435.465765	1.562	-435.661964	1.523	-435.416839	1.523	-435.651901
1.561	-435.465803	1.561	-435.661987	1.522	-435.416833	1.522	-435.651874
1.560	-435.465840	1.560	-435.662008	1.521	-435.416825	1.521	-435.651845
1.559	-435.465874	1.559	-435.662027	1.520	-435.416814	1.520	-435.651813
1.558	-435.465907	1.558	-435.662045	1.510	-435.416581	1.510	-435.651375
1.557	-435.465938	1.557	-435.662061	1.500	-435.416108	1.500	-435.650703
1.556	-435.465967	1.556	-435.662075	1.490	-435.415383	1.490	-435.649785
1.555	-435.465994	1.555	-435.662087	1.480	-435.414391	1.480	-435.648607
1.554	-435.466020	1.554	-435.662098	1.470	-435.413119	1.470	-435.647156
1.553	-435.466043	1.553	-435.662107	1.460	-435.411552	1.460	-435.645415
1.552	-435.466065	1.552	-435.662113	1.450	-435.409674	1.450	-435.643371
1.551	-435.466085	1.551	-435.662119	1.440	-435.407469	1.440	-435.641007
1.550	-435.466103	1.550	-435.662122	1.430	-435.404920	1.430	-435.638305
1.549	-435.466119	1.549	-435.662123	1.420	-435.402010	1.420	-435.635249
1.548	-435.466133	1.548	-435.662123	1.410	-435.398720	1.410	-435.631819
1.547	-435.466146	1.547	-435.662120	1.400	-435.395031	1.400	-435.627997
1.546	-435.466156	1.546	-435.662116	1.300	-435.331212	1.300	-435.563452
1.545	-435.466164	1.545	-435.662110	1.200	-435.198118	1.200	-435.430080
1.544	-435.466171	1.544	-435.662102				
1.543	-435.466176	1.543	-435.662092				
1.542	-435.466178	1.542	-435.662080				
1.541	-435.466179	1.541	-435.662066				

Continued on next page

Table S2 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.540	-435.466178	1.540	-435.662050				
1.539	-435.466174	1.539	-435.662032				
1.538	-435.466169	1.538	-435.662013				
1.537	-435.466162	1.537	-435.661992				
1.536	-435.466152	1.536	-435.661971				
1.535	-435.466141	1.535	-435.661943				
1.534	-435.466127	1.534	-435.661914				
1.533	-435.466112	1.533	-435.661888				
1.532	-435.466094	1.532	-435.661857				
1.531	-435.466075	1.531	-435.661823				
1.530	-435.466053	1.530	-435.661787				
1.529	-435.466029	1.529	-435.661749				
1.528	-435.466003	1.528	-435.661708				
1.527	-435.465975	1.527	-435.661666				
1.526	-435.465944	1.526	-435.661622				
1.525	-435.465912	1.525	-435.661575				
1.524	-435.465877	1.524	-435.661526				
1.523	-435.465841	1.523	-435.661475				
1.522	-435.465802	1.522	-435.661422				
1.521	-435.465760	1.521	-435.661367				
1.520	-435.465717	1.520	-435.661309				
1.519	-435.465671	1.519	-435.661250				
1.518	-435.465623	1.518	-435.661188				
1.517	-435.465573	1.517	-435.661124				
1.516	-435.465521	1.516	-435.661058				
1.515	-435.465466	1.515	-435.660989				
1.514	-435.465409	1.514	-435.660918				
1.513	-435.465350	1.513	-435.660845				
1.512	-435.465288	1.512	-435.660769				
1.511	-435.465224	1.511	-435.660692				
1.510	-435.465158	1.510	-435.660612				
1.509	-435.465089	1.509	-435.660529				
1.508	-435.465018	1.508	-435.660444				
1.507	-435.464945	1.507	-435.660357				
1.506	-435.464869	1.506	-435.660268				
1.505	-435.464791	1.505	-435.660176				
1.504	-435.464710	1.504	-435.660082				
1.503	-435.464627	1.503	-435.659985				
1.502	-435.464542	1.502	-435.659886				
1.501	-435.464454	1.501	-435.659784				
1.500	-435.464364	1.500	-435.659680				
1.480	-435.462014	1.480	-435.657061				
1.460	-435.458556	1.460	-435.653345				
1.440	-435.453866	1.440	-435.648405				
1.420	-435.447807	1.420	-435.642106				
1.400	-435.440233	1.400	-435.634298				
1.380	-435.430982	1.380	-435.624820				
1.360	-435.419874	1.360	-435.613495				
1.340	-435.406717	1.340	-435.600128				
1.320	-435.391296	1.320	-435.584507				
1.300	-435.373379	1.300	-435.566398				
1.280	-435.352710	1.280	-435.545546				
1.260	-435.329009	1.260	-435.521672				
1.240	-435.301968	1.240	-435.494467				
1.220	-435.271252	1.220	-435.463601				
1.200	-435.236494	1.200	-435.428705				

Table S3 Potential energy surface of AIF

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
5.000	-341.331284	5.000	-341.530801	5.000	-341.367113	5.000	-341.528167
4.900	-341.331331	4.900	-341.530864	4.900	-341.367145	4.900	-341.528220
4.800	-341.331386	4.800	-341.530940	4.700	-341.369610	4.700	-341.528529
4.700	-341.332800	4.700	-341.531035	4.600	-341.369648	4.600	-341.530011
4.600	-341.336424	4.600	-341.531152	4.500	-341.369689	4.500	-341.533924
4.500	-341.340269	4.500	-341.531302	4.400	-341.369732	4.400	-341.538041
4.400	-341.344343	4.400	-341.531501	4.300	-341.369777	4.300	-341.542375
4.300	-341.348652	4.300	-341.533400	4.200	-341.369826	4.200	-341.546942
4.200	-341.353203	4.200	-341.537876	4.100	-341.369878	4.100	-341.551747
4.100	-341.358005	4.100	-341.542621	4.000	-341.369934	4.000	-341.556828
4.000	-341.363068	4.000	-341.547646	3.900	-341.369994	3.900	-341.562173
3.900	-341.368406	3.900	-341.552961	3.800	-341.370062	3.800	-341.567823
3.800	-341.374037	3.800	-341.558585	3.700	-341.378297	3.700	-341.573805
3.700	-341.379982	3.700	-341.564543	3.600	-341.381028	3.600	-341.580151
3.600	-341.386270	3.600	-341.570858	3.500	-341.388998	3.500	-341.586896
3.500	-341.392933	3.500	-341.577566	3.400	-341.395443	3.400	-341.594080
3.400	-341.400010	3.400	-341.584706	3.300	-341.402313	3.300	-341.601745
3.300	-341.407542	3.300	-341.592320	3.200	-341.409660	3.200	-341.609937
3.200	-341.415576	3.200	-341.600454	3.100	-341.417537	3.100	-341.618702
3.100	-341.424160	3.100	-341.609159	3.000	-341.426006	3.000	-341.628077
3.000	-341.433343	3.000	-341.618484	2.900	-341.435704	2.900	-341.638090
2.900	-341.443173	2.900	-341.628478	2.800	-341.445519	2.800	-341.648755
2.800	-341.453693	2.800	-341.639182	2.700	-341.456091	2.700	-341.660083
2.700	-341.464938	2.700	-341.650628	2.600	-341.467449	2.600	-341.672099
2.600	-341.476924	2.600	-341.662828	2.500	-341.479603	2.500	-341.684816
2.500	-341.489647	2.500	-341.675771	2.400	-341.492534	2.400	-341.698226
2.400	-341.503059	2.400	-341.689411	2.300	-341.506179	2.300	-341.712257
2.300	-341.517062	2.300	-341.703642	2.200	-341.520405	2.200	-341.726737
2.200	-341.531472	2.200	-341.718282	2.100	-341.534955	2.100	-341.741380
2.100	-341.545974	2.100	-341.733022	2.000	-341.549383	2.000	-341.755707
2.080	-341.548845	2.080	-341.735941	1.990	-341.550793	1.990	-341.757095
2.060	-341.551694	2.060	-341.738840	1.970	-341.553586	1.970	-341.759836
2.040	-341.554516	2.040	-341.741712	1.950	-341.556332	1.950	-341.762521
2.020	-341.557304	2.020	-341.744551	1.930	-341.559024	1.930	-341.765141
2.000	-341.560050	2.000	-341.747348	1.910	-341.561651	1.910	-341.767843
1.980	-341.562747	1.980	-341.750099	1.890	-341.564224	1.890	-341.770298
1.960	-341.565386	1.960	-341.752793	1.870	-341.566687	1.870	-341.772656
1.940	-341.567956	1.940	-341.755421	1.850	-341.569047	1.850	-341.774899
1.920	-341.570448	1.920	-341.757972	1.830	-341.571287	1.830	-341.777013
1.900	-341.572850	1.900	-341.760435	1.810	-341.573395	1.810	-341.778981
1.880	-341.575147	1.880	-341.762796	1.790	-341.575346	1.790	-341.780783
1.860	-341.577327	1.860	-341.765041	1.770	-341.577122	1.770	-341.782398
1.840	-341.579372	1.840	-341.767155	1.750	-341.578697	1.750	-341.783804
1.820	-341.581266	1.820	-341.769121	1.730	-341.580047	1.730	-341.784973
1.800	-341.582989	1.800	-341.770919	1.710	-341.581140	1.710	-341.785878
1.780	-341.584520	1.780	-341.772528	1.690	-341.581946	1.690	-341.786487
1.760	-341.585834	1.760	-341.773925	1.670	-341.582429	1.670	-341.786763
1.740	-341.586907	1.740	-341.775084	1.669	-341.582444	1.669	-341.786767
1.720	-341.587709	1.720	-341.775977	1.668	-341.582458	1.668	-341.786771
1.700	-341.588208	1.700	-341.776571	1.667	-341.582471	1.667	-341.786773
1.680	-341.588370	1.680	-341.776833	1.666	-341.582484	1.666	-341.786775
1.679	-341.588369	1.679	-341.776837	1.665	-341.582495	1.665	-341.786775
1.678	-341.588366	1.678	-341.776840	1.664	-341.582505	1.664	-341.786775
1.677	-341.588363	1.677	-341.776842	1.663	-341.582515	1.663	-341.786774
1.676	-341.588358	1.676	-341.776842	1.662	-341.582523	1.662	-341.786771
1.675	-341.588353	1.675	-341.776842	1.661	-341.582531	1.661	-341.786768
1.674	-341.588347	1.674	-341.776841	1.660	-341.582537	1.660	-341.786764
1.673	-341.588340	1.673	-341.776839	1.659	-341.582543	1.659	-341.786759

Continued on next page

Table S3 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.672	-341.588332	1.672	-341.776836	1.658	-341.582547	1.658	-341.786752
1.671	-341.588322	1.671	-341.776832	1.657	-341.582551	1.657	-341.786745
1.670	-341.588312	1.670	-341.776827	1.656	-341.582554	1.656	-341.786737
1.669	-341.588301	1.669	-341.776821	1.655	-341.582555	1.655	-341.786728
1.668	-341.588289	1.668	-341.776815	1.654	-341.582556	1.654	-341.786718
1.667	-341.588276	1.667	-341.776807	1.653	-341.582556	1.653	-341.786706
1.666	-341.588262	1.666	-341.776798	1.652	-341.582555	1.652	-341.786694
1.665	-341.588246	1.665	-341.776788	1.651	-341.582552	1.651	-341.786681
1.664	-341.588230	1.664	-341.776777	1.650	-341.582549	1.650	-341.786667
1.663	-341.588213	1.663	-341.776765	1.649	-341.582545	1.649	-341.786651
1.662	-341.588195	1.662	-341.776752	1.648	-341.582539	1.648	-341.786635
1.661	-341.588175	1.661	-341.776738	1.647	-341.582533	1.647	-341.786617
1.660	-341.588155	1.660	-341.776723	1.646	-341.582526	1.646	-341.786599
1.659	-341.588134	1.659	-341.776707	1.645	-341.582517	1.645	-341.786579
1.658	-341.588111	1.658	-341.776690	1.644	-341.582508	1.644	-341.786558
1.657	-341.588088	1.657	-341.776672	1.643	-341.582497	1.643	-341.786537
1.656	-341.588063	1.656	-341.776653	1.642	-341.582485	1.642	-341.786514
1.655	-341.588038	1.655	-341.776632	1.641	-341.582473	1.641	-341.786490
1.654	-341.588011	1.654	-341.776610	1.640	-341.582459	1.640	-341.786465
1.653	-341.587983	1.653	-341.776588	1.620	-341.581949	1.620	-341.785726
1.652	-341.587954	1.652	-341.776565	1.600	-341.580955	1.600	-341.784495
1.651	-341.587924	1.651	-341.776541	1.580	-341.579420	1.580	-341.782715
1.650	-341.587893	1.650	-341.776515	1.560	-341.577280	1.560	-341.780321
1.649	-341.587861	1.649	-341.776488	1.540	-341.574463	1.540	-341.777243
1.648	-341.587828	1.648	-341.776460	1.520	-341.570891	1.520	-341.773402
1.647	-341.587793	1.647	-341.776432	1.500	-341.566476	1.500	-341.768711
1.646	-341.587758	1.646	-341.776402	1.480	-341.561141	1.480	-341.763072
1.645	-341.587721	1.645	-341.776371	1.460	-341.554735	1.460	-341.756382
1.644	-341.587683	1.644	-341.776338	1.440	-341.547168	1.440	-341.748521
1.643	-341.587645	1.643	-341.776305	1.420	-341.538865	1.420	-341.739356
1.642	-341.587604	1.642	-341.776270	1.400	-341.528596	1.400	-341.728744
1.641	-341.587563	1.641	-341.776235	1.380	-341.516716	1.380	-341.716524
1.640	-341.587521	1.640	-341.776198	1.360	-341.503051	1.360	-341.702516
1.639	-341.587477	1.639	-341.776160	1.340	-341.487404	1.340	-341.686522
1.638	-341.587433	1.638	-341.776121	1.320	-341.469553	1.320	-341.668324
1.637	-341.587387	1.637	-341.776081	1.300	-341.449254	1.300	-341.647676
1.636	-341.587340	1.636	-341.776039	1.280	-341.426245	1.280	-341.624308
1.635	-341.587291	1.635	-341.775997	1.260	-341.400204	1.260	-341.597919
1.634	-341.587242	1.634	-341.775953	1.240	-341.370807	1.240	-341.568173
1.633	-341.587191	1.633	-341.775908	1.220	-341.337683	1.220	-341.534700
1.632	-341.587139	1.632	-341.775862	1.200	-341.300417	1.200	-341.497085
1.631	-341.587086	1.631	-341.775814				
1.630	-341.587032	1.630	-341.775766				
1.629	-341.586976	1.629	-341.775716				
1.628	-341.586919	1.628	-341.775665				
1.627	-341.586861	1.627	-341.775612				
1.626	-341.586802	1.626	-341.775559				
1.625	-341.586741	1.625	-341.775504				
1.624	-341.586680	1.624	-341.775448				
1.623	-341.586617	1.623	-341.775391				
1.622	-341.586552	1.622	-341.775332				
1.621	-341.586487	1.621	-341.775273				
1.620	-341.586420	1.620	-341.775211				
1.600	-341.584799	1.600	-341.773711				
1.580	-341.582600	1.580	-341.771637				
1.560	-341.579760	1.560	-341.768927				
1.540	-341.576206	1.540	-341.765508				
1.520	-341.571861	1.520	-341.761302				
1.500	-341.566636	1.500	-341.756221				

Continued on next page

Table S3 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.480	-341.560435	1.480	-341.750168				
1.460	-341.553150	1.460	-341.743035				
1.440	-341.544664	1.440	-341.734702				
1.420	-341.534844	1.420	-341.725040				
1.400	-341.523546	1.400	-341.713899				
1.380	-341.510607	1.380	-341.701118				
1.360	-341.495851	1.360	-341.686510				
1.340	-341.479080	1.340	-341.669873				
1.320	-341.460676	1.320	-341.651023				
1.300	-341.439479	1.300	-341.629676				
1.280	-341.415531	1.280	-341.605554				
1.260	-341.388527	1.260	-341.578353				
1.240	-341.358127	1.240	-341.547730				
1.220	-341.323956	1.220	-341.513312				
1.200	-341.285595	1.200	-341.474681				

Table S4 Potential energy surface of CIF

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
5.000	-558.954151	5.000	-559.261142	5.000	-558.945326	5.000	-559.231179
4.900	-558.954142	4.900	-559.261138	4.900	-558.945319	4.900	-559.231111
4.800	-558.954134	4.800	-559.261135	4.800	-558.945310	4.800	-559.231043
4.700	-558.954124	4.700	-559.261131	4.700	-558.945301	4.700	-559.230960
4.600	-558.954114	4.600	-559.261128	4.600	-558.945291	4.600	-559.230862
4.500	-558.954103	4.500	-559.261125	4.500	-558.945281	4.500	-559.230754
4.400	-558.954091	4.400	-559.261123	4.400	-558.945269	4.400	-559.230640
4.300	-558.954079	4.300	-559.261124	4.300	-558.945256	4.300	-559.230505
4.200	-558.954067	4.200	-559.261126	4.200	-558.945242	4.200	-559.230353
4.100	-558.954056	4.100	-559.261133	4.100	-558.945227	4.100	-559.230180
4.000	-558.954047	4.000	-559.261145	4.000	-558.945211	4.000	-559.229988
3.900	-558.954041	3.900	-559.261166	3.900	-558.945195	3.900	-559.229752
3.800	-558.954041	3.800	-559.261198	3.800	-558.945181	3.800	-559.229479
3.700	-558.954052	3.700	-559.261248	3.700	-558.945170	3.700	-559.229167
3.600	-558.954079	3.600	-559.261325	3.600	-558.945166	3.600	-559.228800
3.500	-558.954132	3.500	-559.261438	3.500	-558.945173	3.500	-559.228373
3.400	-558.954224	3.400	-559.261605	3.400	-558.945200	3.400	-559.227895
3.300	-558.954376	3.300	-559.261849	3.300	-558.945256	3.300	-559.227364
3.200	-558.954615	3.200	-559.262204	3.200	-558.945357	3.200	-559.226807
3.100	-558.954984	3.100	-559.262714	3.100	-558.945527	3.100	-559.226288
3.000	-558.955540	3.000	-559.263446	3.000	-558.945799	3.000	-559.225923
2.900	-558.956365	2.900	-559.264485	2.900	-558.946218	2.900	-559.225911
2.800	-558.957574	2.800	-559.265951	2.800	-558.946850	2.800	-559.226565
2.700	-558.959320	2.700	-559.267994	2.700	-558.947786	2.700	-559.228326
2.600	-558.961803	2.600	-559.270805	2.600	-558.949148	2.600	-559.231737
2.500	-558.965274	2.500	-559.274602	2.500	-558.951092	2.500	-559.237343
2.400	-558.970023	2.400	-559.279657	2.400	-558.953804	2.400	-559.245515
2.300	-558.976352	2.300	-559.286095	2.300	-558.957484	2.300	-559.256264
2.200	-558.984511	2.200	-559.294080	2.200	-558.962308	2.200	-559.269254
2.100	-558.994583	2.100	-559.303568	2.100	-558.968369	2.100	-559.283959
2.000	-559.006326	2.000	-559.314236	2.000	-558.975562	2.000	-559.299824
1.980	-559.008819	1.980	-559.316455	1.900	-558.983423	1.900	-559.316089
1.960	-559.011341	1.960	-559.318686	1.800	-558.990910	1.800	-559.331295
1.940	-559.013881	1.940	-559.320919	1.790	-558.991574	1.790	-559.332668
1.920	-559.016427	1.920	-559.323144	1.780	-558.992213	1.780	-559.334002
1.900	-559.018966	1.900	-559.325350	1.770	-558.992826	1.770	-559.335294
1.880	-559.021483	1.880	-559.327522	1.760	-558.993409	1.760	-559.336539
1.860	-559.023960	1.860	-559.329647	1.750	-558.993959	1.750	-559.337736

Continued on next page

Table S4 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.840	-559.026380	1.840	-559.331710	1.740	-558.994473	1.740	-559.338878
1.820	-559.028723	1.820	-559.333692	1.730	-558.994949	1.730	-559.339963
1.800	-559.030966	1.800	-559.335574	1.720	-558.995382	1.720	-559.340986
1.780	-559.033085	1.780	-559.337334	1.710	-558.995769	1.710	-559.341943
1.760	-559.035055	1.760	-559.338948	1.700	-558.996106	1.700	-559.342829
1.740	-559.036846	1.740	-559.340390	1.690	-558.996390	1.690	-559.343640
1.720	-559.038428	1.720	-559.341631	1.680	-558.996615	1.680	-559.344371
1.700	-559.039767	1.700	-559.342638	1.670	-558.996779	1.670	-559.345016
1.680	-559.040827	1.680	-559.343376	1.660	-558.996877	1.660	-559.345572
1.660	-559.041568	1.660	-559.343807	1.659	-558.996882	1.659	-559.345622
1.659	-559.041596	1.659	-559.343818	1.658	-558.996888	1.658	-559.345672
1.658	-559.041623	1.658	-559.343831	1.657	-558.996892	1.657	-559.345720
1.657	-559.041649	1.657	-559.343841	1.656	-558.996896	1.656	-559.345767
1.656	-559.041674	1.656	-559.343853	1.655	-558.996899	1.655	-559.345814
1.655	-559.041698	1.655	-559.343860	1.654	-558.996901	1.654	-559.345859
1.654	-559.041721	1.654	-559.343870	1.653	-558.996902	1.653	-559.345904
1.653	-559.041744	1.653	-559.343876	1.652	-558.996903	1.652	-559.345947
1.652	-559.041765	1.652	-559.343884	1.651	-558.996903	1.651	-559.345989
1.651	-559.041786	1.651	-559.343888	1.650	-558.996902	1.650	-559.346031
1.650	-559.041805	1.650	-559.343895	1.649	-558.996900	1.649	-559.346071
1.649	-559.041824	1.649	-559.343896	1.648	-558.996898	1.648	-559.346110
1.648	-559.041841	1.648	-559.343901	1.647	-558.996895	1.647	-559.346149
1.647	-559.041858	1.647	-559.343901	1.646	-558.996891	1.646	-559.346186
1.646	-559.041874	1.646	-559.343904	1.645	-558.996886	1.645	-559.346222
1.645	-559.041888	1.645	-559.343902	1.644	-558.996881	1.644	-559.346257
1.644	-559.041902	1.644	-559.343903	1.643	-558.996874	1.643	-559.346291
1.643	-559.041915	1.643	-559.343899	1.642	-558.996867	1.642	-559.346324
1.642	-559.041926	1.642	-559.343898	1.641	-558.996859	1.641	-559.346356
1.641	-559.041937	1.641	-559.343894	1.640	-558.996850	1.640	-559.346387
1.640	-559.041947	1.640	-559.343888	1.640	-558.996850	1.640	-559.346387
1.639	-559.041955	1.639	-559.343884	1.630	-558.996717	1.630	-559.346637
1.638	-559.041963	1.638	-559.343877	1.620	-558.996496	1.620	-559.346774
1.637	-559.041969	1.637	-559.343867	1.600	-558.995767	1.600	-559.346682
1.636	-559.041975	1.636	-559.343860	1.590	-558.995246	1.590	-559.346440
1.635	-559.041979	1.635	-559.343850	1.580	-558.994612	1.580	-559.346058
1.634	-559.041983	1.634	-559.343838	1.570	-558.993857	1.570	-559.345529
1.633	-559.041985	1.633	-559.343828	1.560	-558.992973	1.560	-559.344844
1.632	-559.041986	1.632	-559.343815	1.550	-558.991952	1.550	-559.343996
1.631	-559.041987	1.631	-559.343801	1.540	-558.990784	1.540	-559.342977
1.630	-559.041986	1.630	-559.343786	1.530	-558.989462	1.530	-559.341777
1.629	-559.041984	1.629	-559.343769	1.520	-558.987974	1.520	-559.340388
1.628	-559.041981	1.628	-559.343755	1.510	-558.986310	1.510	-559.338800
1.627	-559.041977	1.627	-559.343739	1.500	-558.984460	1.500	-559.337003
1.626	-559.041972	1.626	-559.343718	1.490	-558.982411	1.490	-559.334986
1.625	-559.041965	1.625	-559.343698	1.480	-558.980151	1.480	-559.332738
1.624	-559.041958	1.624	-559.343677	1.470	-558.977668	1.470	-559.330247
1.623	-559.041949	1.623	-559.343654	1.460	-558.974947	1.460	-559.327502
1.622	-559.041939	1.622	-559.343631	1.450	-558.971976	1.450	-559.324489
1.621	-559.041929	1.621	-559.343606	1.440	-558.968738	1.440	-559.321194
1.620	-559.041917	1.620	-559.343580	1.430	-558.965219	1.430	-559.317604
1.619	-559.041903	1.619	-559.343553	1.420	-558.961401	1.420	-559.313704
1.618	-559.041889	1.618	-559.343525	1.410	-558.957269	1.410	-559.309477
1.617	-559.041874	1.617	-559.343496	1.400	-558.952804	1.400	-559.304908
1.616	-559.041857	1.616	-559.343466			1.300	-559.235896
1.615	-559.041839	1.615	-559.343435				
1.614	-559.041820	1.614	-559.343402				
1.613	-559.041800	1.613	-559.343368				
1.612	-559.041779	1.612	-559.343334				
1.611	-559.041756	1.611	-559.343298				

Continued on next page

Table S4 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.610	-559.041732	1.610	-559.343260				
1.609	-559.041707	1.609	-559.343222				
1.608	-559.041681	1.608	-559.343182				
1.607	-559.041654	1.607	-559.343142				
1.606	-559.041625	1.606	-559.343100				
1.605	-559.041595	1.605	-559.343057				
1.604	-559.041564	1.604	-559.343012				
1.603	-559.041532	1.603	-559.342967				
1.602	-559.041498	1.602	-559.342920				
1.601	-559.041463	1.601	-559.342872				
1.600	-559.041427	1.600	-559.342822				
1.580	-559.040421	1.580	-559.341563				
1.560	-559.038838	1.560	-559.339743				
1.540	-559.036612	1.540	-559.337295				
1.520	-559.033670	1.520	-559.334146				
1.500	-559.029930	1.500	-559.330217				
1.480	-559.025306	1.480	-559.325419				
1.460	-559.019699	1.460	-559.319654				
1.440	-559.013003	1.440	-559.312816				
1.420	-559.005100	1.420	-559.304786				
1.400	-558.995860	1.400	-559.295435				
		1.380	-559.284617				
		1.360	-559.272173				
		1.340	-559.257923				
		1.320	-559.241671				
		1.300	-559.223198				

Table S5 Potential energy surface of NH

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
5.000	-54.897170	5.000	-55.008349	5.000	-54.902284	5.000	-54.984001
4.800	-54.897172	4.800	-55.008355	4.900	-54.902285	4.900	-54.984025
4.600	-54.897175	4.600	-55.008363	4.800	-54.902287	4.800	-54.984057
4.500	-54.897177	4.500	-55.008368	4.700	-54.902289	4.700	-54.984096
4.400	-54.897180	4.400	-55.008375	4.600	-54.902291	4.600	-54.984144
4.300	-54.897182	4.300	-55.008383	4.500	-54.902294	4.500	-54.984203
4.200	-54.897186	4.200	-55.008393	4.400	-54.902297	4.400	-54.984275
4.100	-54.897190	4.100	-55.008405	4.300	-54.902301	4.300	-54.984361
4.000	-54.897195	4.000	-55.008420	4.200	-54.902306	4.200	-54.984459
3.900	-54.897201	3.900	-55.008438	4.100	-54.902313	4.100	-54.984576
3.800	-54.897209	3.800	-55.008461	4.000	-54.902322	4.000	-54.984713
3.700	-54.897219	3.700	-55.008490	3.900	-54.902334	3.900	-54.984868
3.600	-54.897232	3.600	-55.008527	3.800	-54.902350	3.800	-54.985044
3.500	-54.897248	3.500	-55.008574	3.700	-54.902372	3.700	-54.985243
3.400	-54.897270	3.400	-55.008634	3.600	-54.902401	3.600	-54.985459
3.300	-54.897299	3.300	-55.008713	3.500	-54.902440	3.500	-54.985714
3.200	-54.897339	3.200	-55.008818	3.400	-54.902494	3.400	-54.985973
3.100	-54.897395	3.100	-55.008958	3.300	-54.902568	3.300	-54.986246
3.000	-54.897474	3.000	-55.009147	3.200	-54.902671	3.200	-54.986529
2.900	-54.897586	2.900	-55.009405	3.100	-54.902813	3.100	-54.986813
2.800	-54.897744	2.800	-55.009758	3.000	-54.903008	3.000	-54.987099
2.700	-54.897970	2.700	-55.010242	2.900	-54.903277	2.900	-54.987371
2.600	-54.898293	2.600	-55.010910	2.800	-54.903646	2.800	-54.987635
2.500	-54.898761	2.500	-55.011832	2.700	-54.904146	2.700	-54.987878
2.400	-54.899442	2.400	-55.013112	2.600	-54.904824	2.600	-54.988120
2.300	-54.900445	2.300	-55.014890	2.500	-54.905737	2.500	-54.988394
2.200	-54.901923	2.200	-55.017356	2.400	-54.906961	2.400	-54.988776

Continued on next page

Table S5 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
2.100	-54.904092	2.100	-55.020746	2.300	-54.908596	2.300	-54.989397
2.000	-54.907225	2.000	-55.025338	2.200	-54.910765	2.200	-54.990437
1.900	-54.911641	1.900	-55.031420	2.100	-54.913617	2.100	-54.992185
1.800	-54.917652	1.800	-55.039254	2.000	-54.917326	2.000	-54.995008
1.700	-54.925508	1.700	-55.049029	1.900	-54.922082	1.900	-54.999331
1.600	-54.935318	1.600	-55.060789	1.800	-54.928084	1.800	-55.005603
1.500	-54.946988	1.500	-55.074382	1.700	-54.935525	1.700	-55.014213
1.400	-54.960127	1.400	-55.089348	1.600	-54.944556	1.600	-55.025388
1.380	-54.962867	1.380	-55.092435	1.590	-54.945550	1.590	-55.026649
1.360	-54.965623	1.360	-55.095532	1.580	-54.946561	1.580	-55.027935
1.340	-54.968386	1.340	-55.098627	1.570	-54.947588	1.570	-55.029245
1.320	-54.971143	1.320	-55.101707	1.560	-54.948632	1.560	-55.030581
1.300	-54.973879	1.300	-55.104758	1.550	-54.949692	1.550	-55.031942
1.280	-54.976579	1.280	-55.107764	1.540	-54.950768	1.540	-55.033323
1.260	-54.979225	1.260	-55.110706	1.530	-54.951860	1.530	-55.034730
1.240	-54.981798	1.240	-55.113565	1.520	-54.952969	1.520	-55.036162
1.220	-54.984274	1.220	-55.116318	1.510	-54.954093	1.510	-55.037616
1.200	-54.986630	1.200	-55.118940	1.500	-54.955233	1.500	-55.039088
1.180	-54.988837	1.180	-55.121403	1.490	-54.956388	1.490	-55.040582
1.160	-54.990864	1.160	-55.123676	1.480	-54.957558	1.480	-55.042098
1.140	-54.992676	1.140	-55.125723	1.470	-54.958742	1.470	-55.043634
1.120	-54.994235	1.120	-55.127508	1.460	-54.959941	1.460	-55.045187
1.100	-54.995496	1.100	-55.128985	1.450	-54.961154	1.450	-55.046758
1.080	-54.996411	1.080	-55.130106	1.440	-54.962380	1.440	-55.048345
1.060	-54.996925	1.060	-55.130819	1.430	-54.963619	1.430	-55.049948
1.059	-54.996939	1.059	-55.130843	1.420	-54.964870	1.420	-55.051566
1.058	-54.996952	1.058	-55.130865	1.410	-54.966133	1.410	-55.053194
1.057	-54.996964	1.057	-55.130887	1.400	-54.967407	1.400	-55.054836
1.056	-54.996975	1.056	-55.130907	1.390	-54.968691	1.390	-55.056489
1.055	-54.996984	1.055	-55.130926	1.380	-54.969985	1.380	-55.058150
1.054	-54.996992	1.054	-55.130944	1.370	-54.971286	1.370	-55.059820
1.053	-54.996999	1.053	-55.130960	1.360	-54.972596	1.360	-55.061490
1.052	-54.997005	1.052	-55.130976	1.350	-54.973912	1.350	-55.063169
1.051	-54.997010	1.051	-55.130990	1.340	-54.975233	1.340	-55.064850
1.050	-54.997013	1.050	-55.131003	1.330	-54.976558	1.330	-55.066530
1.049	-54.997016	1.049	-55.131014	1.320	-54.977886	1.320	-55.068209
1.048	-54.997016	1.048	-55.131025	1.310	-54.979214	1.310	-55.069883
1.047	-54.997016	1.047	-55.131034	1.300	-54.980542	1.300	-55.071550
1.046	-54.997015	1.046	-55.131041	1.290	-54.981868	1.290	-55.073209
1.045	-54.997012	1.045	-55.131048	1.280	-54.983189	1.280	-55.074856
1.044	-54.997008	1.044	-55.131053	1.270	-54.984503	1.270	-55.076488
1.043	-54.997002	1.043	-55.131057	1.260	-54.985809	1.260	-55.078101
1.042	-54.996995	1.042	-55.131060	1.250	-54.987103	1.250	-55.079698
1.041	-54.996987	1.041	-55.131061	1.240	-54.988382	1.240	-55.081268
1.040	-54.996978	1.040	-55.131061	1.230	-54.989644	1.230	-55.082812
1.039	-54.996967	1.039	-55.131059	1.220	-54.990886	1.220	-55.084326
1.038	-54.996955	1.038	-55.131057	1.210	-54.992103	1.210	-55.085805
1.037	-54.996942	1.037	-55.131053	1.200	-54.993293	1.200	-55.087245
1.036	-54.996927	1.036	-55.131046	1.190	-54.994452	1.190	-55.088643
1.035	-54.996911	1.035	-55.131040	1.180	-54.995575	1.180	-55.089996
1.034	-54.996894	1.034	-55.131032	1.170	-54.996658	1.170	-55.091297
1.033	-54.996875	1.033	-55.131022	1.160	-54.997697	1.160	-55.092543
1.032	-54.996855	1.032	-55.131011	1.150	-54.998686	1.150	-55.093729
1.031	-54.996834	1.031	-55.130998	1.140	-54.999622	1.140	-55.094850
1.030	-54.996811	1.030	-55.130985	1.130	-55.000497	1.130	-55.095901
1.029	-54.996786	1.029	-55.130969	1.120	-55.001308	1.120	-55.096876
1.028	-54.996760	1.028	-55.130952	1.110	-55.002047	1.110	-55.097770
1.027	-54.996733	1.027	-55.130934	1.100	-55.002709	1.100	-55.098578
1.026	-54.996705	1.026	-55.130914	1.090	-55.003288	1.090	-55.099291

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Table S5 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.025	-54.996674	1.025	-55.130893	1.080	-55.003775	1.080	-55.099905
1.024	-54.996643	1.024	-55.130871	1.070	-55.004165	1.070	-55.100412
1.023	-54.996610	1.023	-55.130846	1.060	-55.004449	1.060	-55.100805
1.022	-54.996575	1.022	-55.130821	1.059	-55.004472	1.059	-55.100838
1.021	-54.996539	1.021	-55.130794	1.058	-55.004493	1.058	-55.100869
1.020	-54.996502	1.020	-55.130765	1.057	-55.004513	1.057	-55.100900
1.019	-54.996462	1.019	-55.130735	1.056	-55.004532	1.056	-55.100929
1.018	-54.996422	1.018	-55.130703	1.055	-55.004550	1.055	-55.100957
1.017	-54.996380	1.017	-55.130670	1.054	-55.004566	1.054	-55.100983
1.016	-54.996336	1.016	-55.130635	1.053	-55.004581	1.053	-55.101008
1.015	-54.996291	1.015	-55.130598	1.052	-55.004596	1.052	-55.101032
1.014	-54.996244	1.014	-55.130560	1.051	-55.004609	1.051	-55.101055
1.013	-54.996196	1.013	-55.130521	1.050	-55.004620	1.050	-55.101077
1.012	-54.996146	1.012	-55.130479	1.049	-55.004631	1.049	-55.101097
1.011	-54.996094	1.011	-55.130436	1.048	-55.004640	1.048	-55.101115
1.010	-54.996041	1.010	-55.130392	1.047	-55.004648	1.047	-55.101133
1.009	-54.995986	1.009	-55.130346	1.046	-55.004655	1.046	-55.101149
1.008	-54.995930	1.008	-55.130298	1.045	-55.004661	1.045	-55.101164
1.007	-54.995872	1.007	-55.130249	1.044	-55.004665	1.044	-55.101178
1.006	-54.995812	1.006	-55.130198	1.043	-55.004668	1.043	-55.101190
1.005	-54.995751	1.005	-55.130145	1.042	-55.004670	1.042	-55.101201
1.004	-54.995688	1.004	-55.130090	1.041	-55.004670	1.041	-55.101210
1.003	-54.995623	1.003	-55.130034	1.040	-55.004669	1.040	-55.101218
1.002	-54.995557	1.002	-55.129976	1.039	-55.004667	1.039	-55.101225
1.001	-54.995489	1.001	-55.129917	1.038	-55.004664	1.038	-55.101230
1.000	-54.995419	1.000	-55.129855	1.037	-55.004659	1.037	-55.101234
0.980	-54.993645	0.980	-55.128247	1.036	-55.004653	1.036	-55.101237
0.960	-54.991084	0.960	-55.125844	1.035	-55.004645	1.035	-55.101238
0.940	-54.987628	0.940	-55.122539	1.034	-55.004636	1.034	-55.101237
0.920	-54.983155	0.920	-55.118211	1.033	-55.004626	1.033	-55.101235
0.900	-54.977531	0.900	-55.112726	1.032	-55.004614	1.032	-55.101232
0.880	-54.970601	0.880	-55.105929	1.031	-55.004601	1.031	-55.101228
0.860	-54.962192	0.860	-55.097649	1.030	-55.004587	1.030	-55.101221
0.840	-54.952111	0.840	-55.087692	1.029	-55.004571	1.029	-55.101214
0.820	-54.940137	0.820	-55.075837	1.028	-55.004554	1.028	-55.101205
0.800	-54.926022	0.800	-55.061839	1.027	-55.004536	1.027	-55.101194
0.780	-54.909484	0.780	-55.045415	1.026	-55.004516	1.026	-55.101182
0.760	-54.890203	0.760	-55.026246	1.025	-55.004494	1.025	-55.101168
0.740	-54.867819	0.740	-55.003974	1.024	-55.004471	1.024	-55.101153
0.720	-54.841919	0.720	-54.978186	1.023	-55.004447	1.023	-55.101137
0.700	-54.812032	0.700	-54.948415	1.022	-55.004421	1.022	-55.101118
				1.021	-55.004394	1.021	-55.101098
				1.020	-55.004365	1.020	-55.101077
				1.019	-55.004334	1.019	-55.101054
				1.018	-55.004303	1.018	-55.101030
				1.017	-55.004269	1.017	-55.101004
				1.016	-55.004234	1.016	-55.100976
				1.015	-55.004198	1.015	-55.100947
				1.014	-55.004160	1.014	-55.100916
				1.013	-55.004120	1.013	-55.100883
				1.012	-55.004079	1.012	-55.100849
				1.011	-55.004036	1.011	-55.100814
				1.010	-55.003992	1.010	-55.100776
				1.000	-55.003459	1.000	-55.100308
				0.990	-55.002754	0.990	-55.099661
				0.980	-55.001865	0.980	-55.098825
				0.970	-55.000780	0.970	-55.097788
				0.960	-54.999485	0.960	-55.096536
				0.950	-54.997968	0.950	-55.095056

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Table S5 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
				0.940	-54.996213	0.940	-55.093334
				0.930	-54.994204	0.930	-55.091354
				0.920	-54.991925	0.920	-55.089100
				0.910	-54.989358	0.910	-55.086555
				0.900	-54.986485	0.900	-55.083699
				0.890	-54.983286	0.890	-55.080514
				0.880	-54.979740	0.880	-55.076980
				0.870	-54.975825	0.870	-55.073073
				0.860	-54.971517	0.860	-55.068770
				0.850	-54.966790	0.850	-55.064047
				0.840	-54.961620	0.840	-55.058877
				0.830	-54.955976	0.830	-55.053232
				0.820	-54.949830	0.820	-55.047082
				0.810	-54.943149	0.810	-55.040395
				0.800	-54.935899	0.800	-55.033137
				0.790	-54.928044	0.790	-55.025272
				0.780	-54.919546	0.780	-55.016762
				0.770	-54.910363	0.770	-55.007566
				0.760	-54.900451	0.760	-54.997640
				0.750	-54.889765	0.750	-54.986937
				0.740	-54.878255	0.740	-54.975408
				0.730	-54.865867	0.730	-54.963000
				0.720	-54.852545	0.720	-54.949656
				0.710	-54.838229	0.710	-54.935316
				0.700	-54.822853	0.700	-54.919915

Table S6 Potential energy surface of NF

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
5.000	-153.840244	5.000	-154.117010	5.000	-153.842956	5.000	-154.071152
4.900	-153.840245	4.900	-154.117013	4.900	-153.842956	4.900	-154.071139
4.800	-153.840245	4.800	-154.117015	4.800	-153.842957	4.800	-154.071130
4.700	-153.840246	4.700	-154.117018	4.700	-153.842959	4.700	-154.071125
4.600	-153.840247	4.600	-154.117023	4.600	-153.842961	4.600	-154.071123
4.500	-153.840249	4.500	-154.117028	4.500	-153.842963	4.500	-154.071128
4.400	-153.840252	4.400	-154.117035	4.400	-153.842967	4.400	-154.071141
4.300	-153.840256	4.300	-154.117045	4.300	-153.842972	4.300	-154.071179
4.200	-153.840261	4.200	-154.117062	4.200	-153.842979	4.200	-154.071208
4.100	-153.840267	4.100	-154.117077	4.100	-153.842987	4.100	-154.071260
4.000	-153.840275	4.000	-154.117106	4.000	-153.842997	4.000	-154.071321
3.900	-153.840285	3.900	-154.117131	3.900	-153.843009	3.900	-154.071394
3.800	-153.840298	3.800	-154.117162	3.800	-153.843023	3.800	-154.071483
3.700	-153.840313	3.700	-154.117201	3.700	-153.843041	3.700	-154.071588
3.600	-153.840333	3.600	-154.117250	3.600	-153.843062	3.600	-154.071720
3.500	-153.840357	3.500	-154.117312	3.500	-153.843091	3.500	-154.071879
3.400	-153.840388	3.400	-154.117391	3.400	-153.843129	3.400	-154.072054
3.300	-153.840430	3.300	-154.117495	3.300	-153.843182	3.300	-154.072258
3.200	-153.840486	3.200	-154.117631	3.200	-153.843256	3.200	-154.072494
3.100	-153.840563	3.100	-154.117813	3.100	-153.843361	3.100	-154.072749
3.000	-153.840670	3.000	-154.118059	3.000	-153.843510	3.000	-154.073027
2.900	-153.840818	2.900	-154.118395	2.900	-153.843720	2.900	-154.073323
2.800	-153.841026	2.800	-154.118859	2.800	-153.844018	2.800	-154.073636
2.700	-153.841322	2.700	-154.119504	2.700	-153.844437	2.700	-154.073973
2.600	-153.841749	2.600	-154.120415	2.600	-153.845023	2.600	-154.074367
2.500	-153.842382	2.500	-154.121713	2.500	-153.845838	2.500	-154.074883
2.400	-153.843351	2.400	-154.123627	2.400	-153.846975	2.400	-154.075675
2.300	-153.844883	2.300	-154.126363	2.300	-153.848558	2.300	-154.077016

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Table S6 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
2.200	-153.847360	2.200	-154.130323	2.200	-153.850748	2.200	-154.079378
2.100	-153.851380	2.100	-154.135946	2.100	-153.853736	2.100	-154.083433
2.000	-153.857712	2.000	-154.143642	2.000	-153.857733	2.000	-154.090030
1.900	-153.867051	1.900	-154.153720	1.900	-153.862942	1.900	-154.099968
1.800	-153.879574	1.800	-154.166285	1.800	-153.869483	1.800	-154.113492
1.700	-153.894668	1.700	-154.181061	1.700	-153.877257	1.700	-154.129863
1.600	-153.910945	1.600	-154.197144	1.600	-153.885752	1.600	-154.147194
1.500	-153.926271	1.500	-154.212776	1.590	-153.886604	1.590	-154.148884
1.480	-153.928969	1.480	-154.215616	1.580	-153.887451	1.580	-154.150560
1.460	-153.931476	1.460	-154.218295	1.570	-153.888292	1.570	-154.152208
1.440	-153.933758	1.440	-154.220780	1.560	-153.889124	1.560	-154.153821
1.420	-153.935775	1.420	-154.223032	1.550	-153.889947	1.550	-154.155420
1.400	-153.937487	1.400	-154.225010	1.540	-153.890757	1.540	-154.156987
1.380	-153.938845	1.380	-154.226667	1.530	-153.891554	1.530	-154.158515
1.360	-153.939797	1.360	-154.227952	1.520	-153.892334	1.520	-154.160014
1.340	-153.940284	1.340	-154.228806	1.510	-153.893097	1.510	-154.161469
1.339	-153.940295	1.339	-154.228836	1.500	-153.893839	1.500	-154.162877
1.338	-153.940304	1.338	-154.228865	1.490	-153.894558	1.490	-154.164250
1.337	-153.940313	1.337	-154.228893	1.480	-153.895251	1.480	-154.165571
1.336	-153.940320	1.336	-154.228919	1.470	-153.895916	1.470	-154.166836
1.335	-153.940325	1.335	-154.228945	1.460	-153.896549	1.460	-154.168043
1.334	-153.940329	1.334	-154.228969	1.450	-153.897146	1.450	-154.169189
1.333	-153.940332	1.333	-154.228991	1.440	-153.897705	1.440	-154.170268
1.332	-153.940334	1.332	-154.229013	1.430	-153.898221	1.430	-154.171273
1.331	-153.940334	1.331	-154.229033	1.420	-153.898690	1.420	-154.172212
1.330	-153.940332	1.330	-154.229051	1.410	-153.899106	1.410	-154.173063
1.329	-153.940330	1.329	-154.229069	1.400	-153.899465	1.400	-154.173829
1.328	-153.940325	1.328	-154.229085	1.390	-153.899760	1.390	-154.174501
1.327	-153.940320	1.327	-154.229099	1.380	-153.899986	1.380	-154.175075
1.326	-153.940313	1.326	-154.229113	1.370	-153.900135	1.370	-154.175539
1.325	-153.940304	1.325	-154.229125	1.360	-153.900201	1.360	-154.175895
1.324	-153.940294	1.324	-154.229135	1.350	-153.900175	1.350	-154.176129
1.323	-153.940283	1.323	-154.229145	1.349	-153.900164	1.349	-154.175659
1.322	-153.940270	1.322	-154.229152	1.348	-153.900172	1.348	-154.175696
1.321	-153.940255	1.321	-154.229159	1.347	-153.900179	1.347	-154.175732
1.320	-153.940239	1.320	-154.229164	1.346	-153.900185	1.346	-154.175767
1.319	-153.940222	1.319	-154.229167	1.345	-153.900190	1.345	-154.175801
1.318	-153.940203	1.318	-154.229169	1.344	-153.900195	1.344	-154.175833
1.317	-153.940182	1.317	-154.229170	1.343	-153.900198	1.343	-154.175865
1.316	-153.940160	1.316	-154.229170	1.342	-153.900201	1.342	-154.175895
1.315	-153.940137	1.315	-154.229167	1.341	-153.900203	1.341	-154.175924
1.314	-153.940112	1.314	-154.229164	1.340	-153.900203	1.340	-154.175952
1.313	-153.940085	1.313	-154.229158	1.339	-153.900203	1.339	-154.175978
1.311	-153.940027	1.311	-154.229144	1.338	-153.900202	1.338	-154.176004
1.310	-153.939995	1.310	-154.229134	1.337	-153.900200	1.337	-154.176028
1.309	-153.939962	1.309	-154.229123	1.336	-153.900197	1.336	-154.176051
1.308	-153.939927	1.308	-154.229110	1.335	-153.900193	1.335	-154.176072
1.307	-153.939891	1.307	-154.229096	1.334	-153.900188	1.334	-154.176093
1.306	-153.939853	1.306	-154.229080	1.333	-153.900182	1.333	-154.176112
1.305	-153.939813	1.305	-154.229062	1.332	-153.900175	1.332	-154.176129
1.304	-153.939772	1.304	-154.229043	1.331	-153.900167	1.331	-154.176146
1.303	-153.939729	1.303	-154.229023	1.330	-153.900158	1.330	-154.176161
1.302	-153.939684	1.302	-154.229001	1.329	-153.900149	1.329	-154.176175
1.301	-153.939637	1.301	-154.228977	1.328	-153.900138	1.328	-154.176188
1.300	-153.939589	1.300	-154.228952	1.327	-153.900126	1.327	-154.176199
1.299	-153.939539	1.299	-154.228924	1.326	-153.900113	1.326	-154.176209
1.298	-153.939488	1.298	-154.228896	1.325	-153.900099	1.325	-154.176218
1.297	-153.939435	1.297	-154.228865	1.324	-153.900083	1.324	-154.176225
1.296	-153.939379	1.296	-154.228833	1.323	-153.900067	1.323	-154.176230

Continued on next page

Table S6 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.295	-153.939323	1.295	-154.228800	1.322	-153.900050	1.322	-154.176232
1.294	-153.939264	1.294	-154.228764	1.321	-153.899816	1.321	-154.176204
1.293	-153.939204	1.293	-154.228727	1.320	-153.899465	1.320	-154.176032
1.292	-153.939141	1.292	-154.228689	1.310	-153.898985	1.310	-154.175708
1.291	-153.939077	1.291	-154.228648	1.300	-153.898367	1.300	-154.175223
1.290	-153.939011	1.290	-154.228606	1.290	-153.897600	1.290	-154.174566
1.289	-153.938944	1.289	-154.228562	1.280	-153.896671	1.280	-154.173727
1.288	-153.938874	1.288	-154.228516	1.270	-153.895568	1.270	-154.172695
1.287	-153.938803	1.287	-154.228469	1.260	-153.894278	1.260	-154.171459
1.286	-153.938730	1.286	-154.228419	1.250	-153.892786	1.250	-154.170004
1.285	-153.938654	1.285	-154.228368	1.240	-153.891077	1.240	-154.168320
1.284	-153.938577	1.284	-154.228315	1.230	-153.889135	1.230	-154.166390
1.283	-153.938498	1.283	-154.228261	1.220	-153.886944	1.220	-154.164199
1.282	-153.938417	1.282	-154.228204	1.210	-153.884485	1.210	-154.161732
1.281	-153.938335	1.281	-154.228146	1.200	-153.881740	1.200	-154.158970
1.280	-153.938250	1.280	-154.228086	1.190	-153.878688	1.190	-154.155895
1.260	-153.936126	1.260	-154.226473	1.180	-153.875307	1.180	-154.152486
1.240	-153.933112	1.240	-154.224005	1.170	-153.871574	1.170	-154.148722
1.220	-153.929085	1.220	-154.220562	1.160	-153.867466	1.160	-154.144581
1.200	-153.923909	1.200	-154.216006	1.150	-153.862957	1.150	-154.140038
1.180	-153.917429	1.180	-154.210183	1.140	-153.858018	1.140	-154.135066
1.160	-153.909469	1.160	-154.202917	1.130	-153.852622	1.130	-154.129638
1.140	-153.899832	1.140	-154.194007	1.120	-153.846737	1.120	-154.123724
1.120	-153.888292	1.120	-154.183228	1.110	-153.840330	1.110	-154.117292
1.100	-153.874596	1.100	-154.170325	1.100	-153.833366	1.100	-154.110309
		1.080	-154.155009			1.000	-154.000900
		1.060	-154.136951				
		1.040	-154.115780				
		1.020	-154.091078				
		1.000	-154.062369				

Table S7 Potential energy surface of PH

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
5.000	-341.215810	5.000	-341.312213	5.000	-341.218586	5.000	-341.284538
4.800	-341.215818	4.800	-341.312233	4.900	-341.218592	4.900	-341.284594
4.600	-341.215832	4.600	-341.312265	4.800	-341.218600	4.800	-341.284658
4.500	-341.215842	4.500	-341.312287	4.700	-341.218610	4.700	-341.284731
4.400	-341.215854	4.400	-341.312315	4.600	-341.218624	4.600	-341.284815
4.300	-341.215871	4.300	-341.312351	4.500	-341.218642	4.500	-341.284907
4.200	-341.215894	4.200	-341.312397	4.400	-341.218666	4.400	-341.285004
4.100	-341.215924	4.100	-341.312456	4.300	-341.218699	4.300	-341.285116
4.000	-341.215964	4.000	-341.312533	4.200	-341.218742	4.200	-341.285231
3.900	-341.216018	3.900	-341.312633	4.100	-341.218801	4.100	-341.285349
3.800	-341.216090	3.800	-341.312765	4.000	-341.218880	4.000	-341.285469
3.700	-341.216188	3.700	-341.312936	3.900	-341.218985	3.900	-341.285588
3.600	-341.216318	3.600	-341.313162	3.800	-341.219126	3.800	-341.285702
3.500	-341.216494	3.500	-341.313460	3.700	-341.219314	3.700	-341.285804
3.400	-341.216731	3.400	-341.313852	3.600	-341.219563	3.600	-341.285894
3.300	-341.217052	3.300	-341.314371	3.500	-341.219893	3.500	-341.285970
3.200	-341.217487	3.200	-341.315058	3.400	-341.220327	3.400	-341.286034
3.100	-341.218081	3.100	-341.315973	3.300	-341.220896	3.300	-341.286103
3.000	-341.218895	3.000	-341.317186	3.200	-341.221640	3.200	-341.286199
2.900	-341.220011	2.900	-341.318793	3.100	-341.222609	3.100	-341.286372
2.800	-341.221540	2.800	-341.320906	3.000	-341.223861	3.000	-341.286696
2.700	-341.223617	2.700	-341.323658	2.900	-341.225470	2.900	-341.287286
2.600	-341.226402	2.600	-341.327189	2.800	-341.227520	2.800	-341.288299

Continued on next page

Table S7 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
2.500	-341.230062	2.500	-341.331639	2.700	-341.230107	2.700	-341.289936
2.400	-341.234742	2.400	-341.337129	2.600	-341.233332	2.600	-341.292429
2.300	-341.240539	2.300	-341.343744	2.500	-341.237297	2.500	-341.296024
2.200	-341.247480	2.200	-341.351510	2.400	-341.242095	2.400	-341.300932
2.100	-341.255506	2.100	-341.360375	2.300	-341.247799	2.300	-341.307297
2.000	-341.264462	2.000	-341.370193	2.200	-341.254442	2.200	-341.315155
1.900	-341.274077	1.900	-341.380693	2.100	-341.262004	2.100	-341.324414
1.880	-341.276045	1.880	-341.382841	2.000	-341.270390	2.000	-341.334842
1.860	-341.278019	1.860	-341.384995	1.900	-341.279398	1.900	-341.346082
1.840	-341.279994	1.840	-341.387152	1.800	-341.288688	1.800	-341.357664
1.820	-341.281965	1.820	-341.389305	1.700	-341.297725	1.700	-341.368998
1.800	-341.283926	1.800	-341.391450	1.600	-341.305675	1.600	-341.379170
1.780	-341.285873	1.780	-341.393581	1.440	-341.312336	1.440	-341.391757
1.760	-341.287797	1.760	-341.395690	1.430	-341.312404	1.430	-341.392053
1.740	-341.289692	1.740	-341.397770	1.429	-341.312407	1.429	-341.392073
1.720	-341.291550	1.720	-341.399815	1.428	-341.312409	1.428	-341.392092
1.700	-341.293364	1.700	-341.401815	1.427	-341.312411	1.427	-341.392108
1.680	-341.295123	1.680	-341.403762	1.426	-341.312411	1.426	-341.392123
1.660	-341.296818	1.660	-341.405646	1.425	-341.312411	1.425	-341.392137
1.640	-341.298438	1.640	-341.407455	1.424	-341.312410	1.424	-341.392147
1.620	-341.299973	1.620	-341.409179	1.423	-341.312409	1.423	-341.392154
1.600	-341.301408	1.600	-341.410805	1.422	-341.312406	1.422	-341.392159
1.580	-341.302730	1.580	-341.412319	1.421	-341.312403	1.421	-341.392169
1.560	-341.303925	1.560	-341.413706	1.420	-341.312399	1.420	-341.392189
1.540	-341.304976	1.540	-341.414949	1.400	-341.312152	1.400	-341.392140
1.520	-341.305865	1.520	-341.416032	1.390	-341.311902	1.390	-341.391970
1.500	-341.306574	1.500	-341.416935	1.380	-341.311562	1.380	-341.391702
1.480	-341.307082	1.480	-341.417638	1.370	-341.311127	1.370	-341.391335
1.460	-341.307366	1.460	-341.418117	1.360	-341.310593	1.360	-341.390866
1.440	-341.307401	1.440	-341.418349	1.350	-341.309956	1.350	-341.390291
1.439	-341.307396	1.439	-341.418355	1.340	-341.309211	1.340	-341.389606
1.438	-341.307390	1.438	-341.418359	1.330	-341.308352	1.330	-341.388807
1.437	-341.307384	1.437	-341.418362	1.320	-341.307374	1.320	-341.387888
1.436	-341.307376	1.436	-341.418364	1.310	-341.306271	1.310	-341.386844
1.435	-341.307368	1.435	-341.418366	1.300	-341.305039	1.300	-341.385670
1.434	-341.307360	1.434	-341.418367	1.200	-341.284093	1.200	-341.365282
1.433	-341.307350	1.433	-341.418368	1.100	-341.241475	1.100	-341.323050
1.432	-341.307340	1.432	-341.418367	1.000	-341.164863	1.000	-341.246402
1.431	-341.307329	1.431	-341.418366				
1.430	-341.307318	1.430	-341.418365				
1.429	-341.307306	1.429	-341.418362				
1.428	-341.307293	1.428	-341.418359				
1.427	-341.307279	1.427	-341.418355				
1.426	-341.307264	1.426	-341.418350				
1.425	-341.307249	1.425	-341.418345				
1.424	-341.307233	1.424	-341.418339				
1.423	-341.307217	1.423	-341.418332				
1.422	-341.307199	1.422	-341.418324				
1.421	-341.307181	1.421	-341.418316				
1.420	-341.307162	1.420	-341.418307				
1.419	-341.307142	1.419	-341.418297				
1.418	-341.307122	1.418	-341.418287				
1.417	-341.307101	1.417	-341.418275				
1.416	-341.307079	1.416	-341.418263				
1.415	-341.307056	1.415	-341.418250				
1.414	-341.307033	1.414	-341.418236				
1.413	-341.307008	1.413	-341.418222				
1.412	-341.306983	1.412	-341.418207				
1.411	-341.306957	1.411	-341.418191				

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Table S7 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.410	-341.306931	1.410	-341.418174				
1.409	-341.306903	1.409	-341.418156				
1.408	-341.306875	1.408	-341.418138				
1.407	-341.306846	1.407	-341.418118				
1.406	-341.306816	1.406	-341.418098				
1.405	-341.306785	1.405	-341.418077				
1.404	-341.306754	1.404	-341.418056				
1.403	-341.306721	1.403	-341.418033				
1.402	-341.306688	1.402	-341.418010				
1.401	-341.306654	1.401	-341.417986				
1.400	-341.306619	1.400	-341.417961				
1.380	-341.305741	1.380	-341.417277				
1.360	-341.304494	1.360	-341.416227				
1.340	-341.302841	1.340	-341.414769				
1.320	-341.300741	1.320	-341.412867				
1.300	-341.298151	1.300	-341.410472				
1.280	-341.295022	1.280	-341.407537				
1.260	-341.291304	1.260	-341.404011				
1.240	-341.286939	1.240	-341.399835				
1.200	-341.276018	1.200	-341.389285				
1.180	-341.269321	1.180	-341.382768				
1.160	-341.261697	1.160	-341.375318				
1.140	-341.253058	1.140	-341.366846				
1.120	-341.243308	1.120	-341.357254				
1.100	-341.232343	1.100	-341.346436				
1.000	-341.154785	1.000	-341.269429				

Table S8 Potential energy surface of CF

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
5.000	-137.148775	5.000	-137.382479	5.000	-137.176483	5.000	-137.408481
4.900	-137.148781	4.900	-137.382490	4.900	-137.176489	4.900	-137.408529
4.800	-137.148789	4.800	-137.382501	4.800	-137.176495	4.800	-137.408572
4.700	-137.148798	4.700	-137.382516	4.700	-137.176503	4.700	-137.408628
4.600	-137.148809	4.600	-137.382533	4.600	-137.176513	4.600	-137.408699
4.500	-137.148823	4.500	-137.382554	4.500	-137.176524	4.500	-137.408780
4.400	-137.148840	4.400	-137.382579	4.400	-137.176538	4.400	-137.408889
4.300	-137.148860	4.300	-137.382611	4.300	-137.176553	4.300	-137.409013
4.200	-137.148885	4.200	-137.382650	4.200	-137.176572	4.200	-137.409160
4.100	-137.148917	4.100	-137.382700	4.100	-137.176594	4.100	-137.409341
4.000	-137.148956	4.000	-137.382762	4.000	-137.176622	4.000	-137.409545
3.900	-137.149006	3.900	-137.382842	3.900	-137.176656	3.900	-137.409784
3.800	-137.149071	3.800	-137.382946	3.800	-137.176699	3.800	-137.410061
3.700	-137.149155	3.700	-137.383080	3.700	-137.176755	3.700	-137.410370
3.600	-137.149266	3.600	-137.383256	3.600	-137.176827	3.600	-137.410727
3.500	-137.149413	3.500	-137.383489	3.500	-137.176923	3.500	-137.411121
3.400	-137.149612	3.400	-137.383802	3.400	-137.177049	3.400	-137.411557
3.300	-137.149881	3.300	-137.384214	3.300	-137.177217	3.300	-137.412026
3.200	-137.150251	3.200	-137.384782	3.200	-137.177441	3.200	-137.412523
3.100	-137.150765	3.100	-137.385567	3.100	-137.177743	3.100	-137.413032
3.000	-137.151486	3.000	-137.386625	3.000	-137.178150	3.000	-137.413553
2.900	-137.152515	2.900	-137.388171	2.900	-137.178699	2.900	-137.414076
2.800	-137.154002	2.800	-137.390288	2.800	-137.179442	2.800	-137.414602
2.700	-137.156183	2.700	-137.393267	2.700	-137.180446	2.700	-137.415156
2.600	-137.159410	2.600	-137.397419	2.600	-137.181803	2.600	-137.415810
2.500	-137.164174	2.500	-137.403043	2.500	-137.183632	2.500	-137.416697
2.400	-137.171044	2.400	-137.410311	2.400	-137.186091	2.400	-137.418064

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Table S8 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
2.300	-137.180458	2.300	-137.419321	2.300	-137.189382	2.300	-137.420326
2.200	-137.192544	2.200	-137.430284	2.200	-137.193787	2.200	-137.424185
2.100	-137.207133	2.100	-137.443409	2.100	-137.199699	2.100	-137.430762
2.000	-137.223911	2.000	-137.458762	2.000	-137.207668	2.000	-137.441744
1.900	-137.242523	1.900	-137.476207	1.900	-137.218337	1.900	-137.458644
1.800	-137.262563	1.800	-137.495424	1.800	-137.232002	1.800	-137.480089
1.700	-137.283497	1.700	-137.515896	1.700	-137.248077	1.700	-137.502391
1.600	-137.304523	1.600	-137.536827	1.600	-137.265395	1.600	-137.523672
1.580	-137.308637	1.580	-137.540965	1.500	-137.282382	1.500	-137.542812
1.560	-137.312691	1.560	-137.545061	1.400	-137.296561	1.400	-137.557873
1.540	-137.316670	1.540	-137.549097	1.390	-137.297680	1.390	-137.559030
1.520	-137.320555	1.520	-137.553057	1.380	-137.298723	1.380	-137.560106
1.500	-137.324328	1.500	-137.556921	1.370	-137.299684	1.370	-137.561095
1.480	-137.327965	1.480	-137.560667	1.360	-137.300558	1.360	-137.561990
1.460	-137.331442	1.460	-137.564270	1.350	-137.301336	1.350	-137.562786
1.440	-137.334728	1.440	-137.567702	1.340	-137.302012	1.340	-137.563474
1.420	-137.337793	1.420	-137.570931	1.330	-137.302577	1.330	-137.564049
1.400	-137.340599	1.400	-137.573920	1.320	-137.303023	1.320	-137.564502
1.380	-137.343102	1.380	-137.576628	1.310	-137.303340	1.310	-137.564822
1.360	-137.345257	1.360	-137.579007	1.300	-137.303520	1.300	-137.565004
1.340	-137.347008	1.340	-137.581004	1.299	-137.303530	1.299	-137.565015
1.320	-137.348293	1.320	-137.582556	1.298	-137.303538	1.298	-137.565024
1.300	-137.349043	1.300	-137.583596	1.297	-137.303545	1.297	-137.565031
1.299	-137.349065	1.299	-137.583633	1.296	-137.303551	1.296	-137.565037
1.298	-137.349086	1.298	-137.583669	1.295	-137.303555	1.295	-137.565041
1.297	-137.349105	1.297	-137.583703	1.294	-137.303557	1.294	-137.565043
1.296	-137.349122	1.296	-137.583736	1.293	-137.303558	1.293	-137.565044
1.295	-137.349138	1.295	-137.583767	1.292	-137.303557	1.292	-137.565044
1.294	-137.349152	1.294	-137.583797	1.291	-137.303555	1.291	-137.565042
1.293	-137.349165	1.293	-137.583825	1.290	-137.303551	1.290	-137.565038
1.292	-137.349176	1.292	-137.583851	1.289	-137.303546	1.289	-137.565033
1.291	-137.349185	1.291	-137.583876	1.288	-137.303539	1.288	-137.565026
1.290	-137.349193	1.290	-137.583899	1.287	-137.303530	1.287	-137.565017
1.289	-137.349199	1.289	-137.583921	1.286	-137.303520	1.286	-137.565007
1.288	-137.349203	1.288	-137.583941	1.285	-137.303508	1.285	-137.564995
1.287	-137.349206	1.287	-137.583960	1.284	-137.303495	1.284	-137.564982
1.286	-137.349207	1.286	-137.583977	1.283	-137.303479	1.283	-137.564967
1.285	-137.349206	1.285	-137.583992	1.282	-137.303463	1.282	-137.564950
1.284	-137.349204	1.284	-137.584005	1.281	-137.303444	1.281	-137.564931
1.283	-137.349200	1.283	-137.584017	1.280	-137.303424	1.280	-137.564912
1.282	-137.349194	1.282	-137.584024	1.270	-137.303126	1.270	-137.564613
1.281	-137.349187	1.281	-137.584033	1.260	-137.302645	1.260	-137.564135
1.280	-137.349178	1.280	-137.584040	1.250	-137.301968	1.250	-137.563459
1.279	-137.349167	1.279	-137.584045	1.240	-137.301081	1.240	-137.562577
1.278	-137.349154	1.278	-137.584049	1.230	-137.299970	1.230	-137.561473
1.277	-137.349139	1.277	-137.584051	1.220	-137.298619	1.220	-137.560129
1.276	-137.349123	1.276	-137.584051	1.210	-137.297012	1.210	-137.558534
1.275	-137.349105	1.275	-137.584049	1.200	-137.295130	1.200	-137.556669
1.274	-137.349085	1.274	-137.584045	1.100	-137.256495	1.100	-137.518463
1.273	-137.349063	1.273	-137.584040	1.000	-137.159686	1.000	-137.423310
1.272	-137.349039	1.272	-137.584033				
1.271	-137.349014	1.271	-137.584024				
1.270	-137.348986	1.270	-137.584013				
1.269	-137.348957	1.269	-137.584000				
1.268	-137.348926	1.268	-137.583986				
1.267	-137.348893	1.267	-137.583970				
1.266	-137.348858	1.266	-137.583952				
1.265	-137.348821	1.265	-137.583932				
1.264	-137.348782	1.264	-137.583910				

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Table S8 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.263	-137.348741	1.263	-137.583886				
1.262	-137.348698	1.262	-137.583861				
1.261	-137.348653	1.261	-137.583833				
1.260	-137.348607	1.260	-137.583803				
1.259	-137.348558	1.259	-137.583772				
1.258	-137.348507	1.258	-137.583738				
1.257	-137.348454	1.257	-137.583703				
1.256	-137.348399	1.256	-137.583665				
1.255	-137.348342	1.255	-137.583626				
1.254	-137.348283	1.254	-137.583584				
1.253	-137.348222	1.253	-137.583541				
1.252	-137.348158	1.252	-137.583495				
1.251	-137.348093	1.251	-137.583448				
1.250	-137.348025	1.250	-137.583398				
1.249	-137.347956	1.249	-137.583346				
1.248	-137.347884	1.248	-137.583292				
1.247	-137.347810	1.247	-137.583236				
1.246	-137.347733	1.246	-137.583178				
1.245	-137.347655	1.245	-137.583117				
1.244	-137.347574	1.244	-137.583055				
1.243	-137.347491	1.243	-137.582990				
1.242	-137.347406	1.242	-137.582923				
1.241	-137.347318	1.241	-137.582854				
1.240	-137.347228	1.240	-137.582783				
1.230	-137.346201	1.230	-137.581941				
1.220	-137.344927	1.220	-137.580860				
1.210	-137.343391	1.210	-137.579519				
1.200	-137.341573	1.200	-137.577905				
1.190	-137.339456	1.190	-137.575996				
1.180	-137.337019	1.180	-137.573772				
1.170	-137.334241	1.170	-137.571213				
1.160	-137.331098	1.160	-137.568294				
1.150	-137.327568	1.150	-137.564993				
1.140	-137.323624	1.140	-137.561282				
1.130	-137.319240	1.130	-137.557134				
1.120	-137.314386	1.120	-137.552521				
1.110	-137.309032	1.110	-137.547412				
1.100	-137.303146	1.100	-137.541774				
1.090	-137.296692	1.090	-137.535571				
1.080	-137.289635	1.080	-137.528768				
1.070	-137.281935	1.070	-137.521324				
1.060	-137.273552	1.060	-137.513199				
1.050	-137.264440	1.050	-137.504348				
1.040	-137.254555	1.040	-137.494724				
1.030	-137.243845	1.030	-137.484276				
1.020	-137.232259	1.020	-137.472951				
1.010	-137.219741	1.010	-137.460693				
1.000	-137.206232	1.000	-137.447442				

Table S9 Potential energy surface of NO

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
5.000	-129.214715	5.000	-129.473269	5.000	-129.233463	5.000	-129.424282
4.900	-129.214716	4.900	-129.473272	4.900	-129.233465	4.900	-129.424296
4.800	-129.214717	4.800	-129.473277	4.800	-129.233467	4.800	-129.424284
4.700	-129.214719	4.700	-129.473282	4.700	-129.233469	4.700	-129.424335
4.600	-129.214721	4.600	-129.473289	4.600	-129.233473	4.600	-129.424362

Continued on next page

Table S9 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
4.500	-129.214724	4.500	-129.473298	4.500	-129.233477	4.500	-129.424415
4.400	-129.214728	4.400	-129.473312	4.400	-129.233482	4.400	-129.424487
4.300	-129.214733	4.300	-129.473326	4.300	-129.233488	4.300	-129.424584
4.200	-129.214739	4.200	-129.473343	4.200	-129.233496	4.200	-129.424709
4.100	-129.214746	4.100	-129.473372	4.100	-129.233504	4.100	-129.424867
4.000	-129.214755	4.000	-129.473397	4.000	-129.233513	4.000	-129.425064
3.900	-129.214764	3.900	-129.473427	3.900	-129.233523	3.900	-129.425323
3.800	-129.214775	3.800	-129.473466	3.800	-129.233535	3.800	-129.425614
3.700	-129.214788	3.700	-129.473510	3.700	-129.233549	3.700	-129.425963
3.600	-129.214802	3.600	-129.473565	3.600	-129.233566	3.600	-129.426377
3.500	-129.214820	3.500	-129.473632	3.500	-129.233590	3.500	-129.426867
3.400	-129.214842	3.400	-129.473719	3.400	-129.233621	3.400	-129.427438
3.300	-129.214871	3.300	-129.473826	3.300	-129.233666	3.300	-129.428104
3.200	-129.214909	3.200	-129.473967	3.200	-129.233728	3.200	-129.428870
3.100	-129.214959	3.100	-129.474147	3.100	-129.233816	3.100	-129.429744
3.000	-129.215026	3.000	-129.474382	3.000	-129.233938	3.000	-129.430724
2.900	-129.215114	2.900	-129.474693	2.900	-129.234107	2.900	-129.431819
2.800	-129.215232	2.800	-129.475109	2.800	-129.234338	2.800	-129.433014
2.700	-129.215392	2.700	-129.475670	2.700	-129.234650	2.700	-129.434313
2.600	-129.215619	2.600	-129.476439	2.600	-129.235074	2.600	-129.435716
2.500	-129.215962	2.500	-129.477515	2.500	-129.235654	2.500	-129.437236
2.400	-129.216515	2.400	-129.479048	2.400	-129.236454	2.400	-129.438920
2.300	-129.217453	2.300	-129.481275	2.300	-129.237565	2.300	-129.440855
2.200	-129.219098	2.200	-129.484550	2.200	-129.239114	2.200	-129.443214
2.100	-129.222010	2.100	-129.489394	2.100	-129.241283	2.100	-129.446297
2.000	-129.227096	2.000	-129.496548	2.000	-129.244353	2.000	-129.450594
1.900	-129.235656	1.900	-129.507032	1.900	-129.248762	1.900	-129.456848
1.800	-129.249243	1.800	-129.522131	1.800	-129.255191	1.800	-129.466114
1.700	-129.269205	1.700	-129.542998	1.700	-129.264626	1.700	-129.479835
1.600	-129.295991	1.600	-129.569891	1.600	-129.278320	1.600	-129.499876
1.500	-129.328570	1.500	-129.601809	1.500	-129.297457	1.500	-129.527895
1.480	-129.335574	1.480	-129.608620	1.400	-129.322133	1.400	-129.563249
1.460	-129.342677	1.460	-129.615521	1.390	-129.324832	1.390	-129.567043
1.440	-129.349845	1.440	-129.622481	1.380	-129.327556	1.380	-129.570852
1.420	-129.357040	1.420	-129.629469	1.370	-129.330301	1.370	-129.574678
1.400	-129.364219	1.400	-129.636446	1.360	-129.333059	1.360	-129.578506
1.380	-129.371334	1.380	-129.643368	1.350	-129.335824	1.350	-129.582330
1.360	-129.378332	1.360	-129.650186	1.340	-129.338589	1.340	-129.586138
1.340	-129.385150	1.340	-129.656843	1.330	-129.341344	1.330	-129.589922
1.320	-129.391722	1.320	-129.663275	1.320	-129.344082	1.320	-129.593670
1.300	-129.397969	1.300	-129.669406	1.310	-129.346793	1.310	-129.597372
1.280	-129.403804	1.280	-129.675154	1.300	-129.349466	1.300	-129.601012
1.260	-129.409128	1.260	-129.680418	1.290	-129.352090	1.290	-129.604581
1.240	-129.413829	1.240	-129.685095	1.280	-129.354654	1.280	-129.608063
1.220	-129.417781	1.220	-129.689056	1.270	-129.357144	1.270	-129.611445
1.200	-129.420841	1.200	-129.692161	1.260	-129.359546	1.260	-129.614709
1.180	-129.422850	1.180	-129.694250	1.250	-129.361846	1.250	-129.617841
1.179	-129.422919	1.179	-129.694325	1.240	-129.364028	1.240	-129.620824
1.178	-129.422986	1.178	-129.694397	1.230	-129.366075	1.230	-129.623640
1.177	-129.423049	1.177	-129.694465	1.220	-129.367969	1.220	-129.626269
1.176	-129.423109	1.176	-129.694531	1.210	-129.369690	1.210	-129.628692
1.175	-129.423167	1.175	-129.694593	1.200	-129.371218	1.200	-129.630887
1.174	-129.423220	1.174	-129.694653	1.190	-129.372530	1.190	-129.632834
1.173	-129.423271	1.173	-129.694709	1.180	-129.373604	1.180	-129.634509
1.172	-129.423319	1.172	-129.694762	1.170	-129.374415	1.170	-129.635887
1.171	-129.423363	1.171	-129.694812	1.160	-129.374935	1.160	-129.636943
1.170	-129.423404	1.170	-129.694858	1.159	-129.374970	1.159	-129.637030
1.169	-129.423441	1.169	-129.694902	1.158	-129.375002	1.158	-129.637113
1.168	-129.423475	1.168	-129.694942	1.157	-129.375031	1.157	-129.637193

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Table S9 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.167	-129.423506	1.167	-129.694979	1.156	-129.375056	1.156	-129.637269
1.166	-129.423533	1.166	-129.695012	1.155	-129.375078	1.155	-129.637342
1.165	-129.423557	1.165	-129.695043	1.154	-129.375097	1.154	-129.637411
1.164	-129.423578	1.164	-129.695070	1.153	-129.375112	1.153	-129.637476
1.163	-129.423595	1.163	-129.695093	1.152	-129.375124	1.152	-129.637538
1.162	-129.423609	1.162	-129.695113	1.151	-129.375133	1.151	-129.637596
1.161	-129.423619	1.161	-129.695130	1.150	-129.375138	1.150	-129.637650
1.160	-129.423625	1.160	-129.695143	1.149	-129.375139	1.149	-129.637700
1.159	-129.423628	1.159	-129.695152	1.148	-129.375138	1.148	-129.637746
1.158	-129.423627	1.158	-129.695159	1.147	-129.375132	1.147	-129.637789
1.157	-129.423623	1.157	-129.695161	1.146	-129.375123	1.146	-129.637828
1.156	-129.423615	1.156	-129.695160	1.145	-129.375111	1.145	-129.637863
1.155	-129.423603	1.155	-129.695156	1.144	-129.375094	1.144	-129.637894
1.154	-129.423587	1.154	-129.695147	1.143	-129.375075	1.143	-129.637921
1.153	-129.423568	1.153	-129.695135	1.142	-129.375051	1.142	-129.637944
1.152	-129.423545	1.152	-129.695120	1.141	-129.375024	1.141	-129.637963
1.151	-129.423518	1.151	-129.695101	1.140	-129.374993	1.140	-129.637978
1.150	-129.423488	1.150	-129.695077	1.130	-129.374469	1.130	-129.637898
1.149	-129.423453	1.149	-129.695050	1.120	-129.373533	1.120	-129.637378
1.148	-129.423415	1.148	-129.695019	1.110	-129.372149	1.110	-129.636384
1.147	-129.423372	1.147	-129.694985	1.100	-129.370280	1.100	-129.634881
1.146	-129.423326	1.146	-129.694946	1.090	-129.367887	1.090	-129.632831
1.145	-129.423276	1.145	-129.694904	1.080	-129.364928	1.080	-129.630193
1.144	-129.423221	1.144	-129.694858	1.070	-129.361359	1.070	-129.626925
1.143	-129.423163	1.143	-129.694808	1.060	-129.357133	1.060	-129.622983
1.142	-129.423101	1.142	-129.694754	1.050	-129.352201	1.050	-129.618318
1.141	-129.423034	1.141	-129.694696	1.040	-129.346511	1.040	-129.612880
1.140	-129.422964	1.140	-129.694633	1.030	-129.340007	1.030	-129.606616
1.139	-129.422889	1.139	-129.694567	1.020	-129.332631	1.020	-129.599468
1.138	-129.422810	1.138	-129.694497	1.010	-129.324321	1.010	-129.591376
1.137	-129.422727	1.137	-129.694422	1.000	-129.314175	1.000	-129.582276
1.136	-129.422639	1.136	-129.694344	0.990	-129.304032	0.990	-129.571896
1.135	-129.422547	1.135	-129.694261	0.980	-129.292743	0.980	-129.560548
1.136	-129.422639	1.136	-129.694344	0.970	-129.280227	0.970	-129.547975
1.135	-129.422547	1.135	-129.694261	0.960	-129.266403	0.960	-129.534095
1.134	-129.422451	1.134	-129.694174	0.950	-129.251183	0.950	-129.518822
1.133	-129.422351	1.133	-129.694082	0.940	-129.234473	0.940	-129.502061
1.132	-129.422246	1.132	-129.693987	0.930	-129.216174	0.930	-129.483716
1.131	-129.422137	1.131	-129.693887	0.920	-129.196180	0.920	-129.463681
1.130	-129.422023	1.130	-129.693783	0.910	-129.174381	0.910	-129.441845
1.129	-129.421905	1.129	-129.693674	0.900	-129.150656	0.900	-129.418089
1.128	-129.421783	1.128	-129.693561				
1.127	-129.421656	1.127	-129.693443				
1.126	-129.421524	1.126	-129.693321				
1.125	-129.421387	1.125	-129.693195				
1.124	-129.421247	1.124	-129.693063				
1.123	-129.421101	1.123	-129.692928				
1.122	-129.420951	1.122	-129.692787				
1.121	-129.420796	1.121	-129.692642				
1.120	-129.420636	1.120	-129.692493				
1.119	-129.420471	1.119	-129.692338				
1.118	-129.420302	1.118	-129.692179				
1.117	-129.420127	1.117	-129.692015				
1.116	-129.419948	1.116	-129.691846				
1.115	-129.419764	1.115	-129.691673				
1.114	-129.419575	1.114	-129.691494				
1.113	-129.419380	1.113	-129.691311				
1.112	-129.419181	1.112	-129.691122				
1.111	-129.418977	1.111	-129.690929				

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Table S9 – Continued from previous page

d (Å)	E CASSCF (Hartrees)	d (Å)	E CASPT2 (Hartrees)	d (Å)	E PNOF7s (Hartrees)	d (Å)	E NOF-MP2 (Hartrees)
1.110	-129.418767	1.110	-129.690730				
1.109	-129.418553	1.109	-129.690526				
1.108	-129.418333	1.108	-129.690318				
1.107	-129.418108	1.107	-129.690104				
1.106	-129.417878	1.106	-129.689885				
1.105	-129.417642	1.105	-129.689661				
1.104	-129.417401	1.104	-129.689431				
1.103	-129.417155	1.103	-129.689196				
1.102	-129.416903	1.102	-129.688956				
1.101	-129.416646	1.101	-129.688710				
1.100	-129.416383	1.100	-129.688459				
1.080	-129.409915	1.080	-129.682241				
1.060	-129.400905	1.060	-129.673505				
1.040	-129.388984	1.040	-129.661879				
1.020	-129.373738	1.020	-129.646944				
1.000	-129.354701	1.000	-129.628224				
0.980	-129.331345	0.980	-129.605186				
0.960	-129.303078	0.960	-129.577224				
0.940	-129.269228	0.940	-129.543659				
0.920	-129.229038	0.920	-129.503719				
0.900	-129.181648	0.900	-129.456534				