

Table S1. Cartesian Coordinates /Å of the optimized ground state geometries of compounds 1-7 at B3LYP/6-311G** level of theory in the gas phase.

1				2			
	x	y	z		x	y	z
N	1.48011	-0.00602	-0.78326	N	0.45341	0.22928	-0.11814
N	-0.77596	3.23395	-2.62331	N	2.22521	4.03706	-0.98379
C	0.23326	-4.96306	-1.9335	N	-8.78812	-2.84367	-1.16311
C	-0.57267	-3.8468	-2.59548	C	-4.20038	-0.76	-1.68617
N	-0.61045	-9.89409	-2.7087	C	-3.82876	0.62409	-1.15719
C	-0.43087	-2.48544	-2.4452	C	-2.61811	1.28211	-1.24538
H	0.33103	-2.09257	-1.78639	H	-1.78862	0.82033	-1.76494
C	-1.28678	-1.60626	-3.15683	C	-2.47311	2.57568	-0.69614
C	-2.27249	-2.1634	-4.00694	C	-3.59296	3.17758	-0.08421
H	-2.92909	-1.49386	-4.55181	H	-3.50447	4.16976	0.33941
C	-2.41832	-3.53212	-4.15833	C	-4.80659	2.51268	0.02139
H	-3.18366	-3.92775	-4.81586	H	-5.64333	2.99372	0.51496
C	-1.56414	-4.3837	-3.45008	C	-4.92938	1.2293	-0.51681
C	-1.47978	-5.83448	-3.40392	C	-6.0625	0.31305	-0.57441
C	-2.2254	-6.82552	-4.04965	C	-7.36992	0.42722	-0.09635
H	-3.02168	-6.56563	-4.73849	H	-7.69454	1.31407	0.43691
C	-1.92962	-8.16001	-3.81991	C	-8.26056	-0.61949	-0.2888
H	-2.49264	-8.93146	-4.32878	H	-9.2705	-0.54507	0.09339
C	-0.89497	-8.53386	-2.93547	C	-7.86904	-1.78894	-0.97086
C	-0.1487	-7.52978	-2.28672	C	-6.55086	-1.89531	-1.45463
H	0.64107	-7.8122	-1.60148	H	-6.24917	-2.79061	-1.9847
C	-0.43933	-6.19904	-2.52718	C	-5.66142	-0.85503	-1.24964
C	1.74158	-4.88833	-2.30987	C	-3.33029	-1.87846	-1.04224
H	2.15245	-3.97553	-1.86535	H	-3.66583	-2.83703	-1.45322
H	2.24917	-5.72291	-1.81414	H	-2.29924	-1.74291	-1.38566
C	2.06054	-4.91533	-3.80666	C	-3.34892	-1.94413	0.48671
H	1.60625	-4.07131	-4.33136	H	-4.35806	-2.11362	0.87044
H	1.70443	-5.83484	-4.27759	H	-2.96644	-1.02355	0.93328
H	3.14097	-4.85835	-3.96212	H	-2.71638	-2.76475	0.8344
C	0.11457	-4.92086	-0.38261	C	-4.04659	-0.8503	-3.23174
H	0.70904	-5.74874	0.01896	H	-2.98067	-0.75834	-3.46777
H	0.60009	-4.00266	-0.03498	H	-4.33709	-1.86151	-3.53686
C	-1.30608	-4.99298	0.18253	C	-4.84048	0.17475	-4.04539
H	-1.80691	-5.92068	-0.10492	H	-4.54877	1.19859	-3.79847
H	-1.9204	-4.1578	-0.16278	H	-5.91502	0.08063	-3.87103
H	-1.27899	-4.954	1.27452	H	-4.66271	0.02775	-5.11395
C	0.72458	-10.31954	-2.43701	C	-8.34703	-4.19879	-1.12436
C	1.78333	-9.90077	-3.25244	C	-7.51076	-4.6452	-0.09293
H	1.58244	-9.25033	-4.0952	H	-7.20226	-3.95268	0.68088
C	3.08252	-10.31988	-2.98273	C	-7.08149	-5.96842	-0.06184
H	3.89296	-9.98901	-3.62241	H	-6.43478	-6.29965	0.74291
C	3.34146	-11.1735	-1.91096	C	-7.49202	-6.86853	-1.04447
H	4.35337	-11.50356	-1.70744	H	-7.16145	-7.90009	-1.01361

C 2.28711 -11.60085 -1.10555	C -8.33336 -6.42931 -2.06545
H 2.47662 -12.26194 -0.26742	H -8.65636 -7.11828 -2.83785
C 0.987 -11.17336 -1.35922	C -8.75375 -5.10339 -2.11305
H 0.17047 -11.49969 -0.72652	H -9.39945 -4.76313 -2.91353
C -1.64921 -10.87094 -2.72705	C -10.16468 -2.57128 -1.40728
C -1.46663 -12.07914 -3.41108	C -10.54507 -1.57404 -2.31521
H -0.53658 -12.25902 -3.93648	H -9.78271 -1.00669 -2.83504
C -2.47162 -13.04171 -3.41295	C -11.89209 -1.31483 -2.54825
H -2.31622 -13.97257 -3.94667	H -12.17043 -0.54049 -3.25442
C -3.67468 -12.8096 -2.74816	C -12.87862 -2.05394 -1.89677
H -4.45748 -13.55893 -2.75606	H -13.92678 -1.85418 -2.08597
C -3.8604 -11.60537 -2.07046	C -12.50272 -3.05376 -1.00102
H -4.78767 -11.41674 -1.54115	H -13.25953 -3.63295 -0.48389
C -2.85434 -10.64435 -2.04984	C -11.158 -3.30839 -0.74957
H -2.99698 -9.71654 -1.50926	H -10.87084 -4.07945 -0.04507
C -1.23658 -0.16889 -3.08502	C -1.20761 3.31549 -0.78394
H -1.97533 0.33525 -3.70058	C -1.28472 4.80895 -0.9603
C -0.42648 0.68417 -2.38144	H -1.60589 5.28027 -0.0255
C 0.62368 0.29118 -1.50133	H -2.02162 5.06601 -1.72338
C -0.61826 2.09381 -2.51399	H -0.32343 5.24206 -1.23047
	C 0.02316 2.71098 -0.69826
	C 0.2289 1.3315 -0.38482
	C 1.23522 3.45353 -0.8571
3	4
N 1.64178 0.02422 -0.99251	N 5.79608 -0.19954 -0.07664
N -0.76668 3.25876 -2.63875	C 4.42164 -0.51848 -0.17165
C 0.28531 -4.93684 -1.99701	C 6.25799 1.09956 -0.43517
C -0.57425 -3.82197 -2.59052	C 6.73139 -1.16689 0.38861
N -0.62764 -9.86819 -2.67274	C 7.96107 -1.33286 -0.26267
C -0.41761 -2.46057 -2.46014	C 8.88093 -2.26819 0.20214
H 0.40022 -2.06606 -1.87325	C 8.58584 -3.06218 1.30976
C -1.33181 -1.5825 -3.09766	C 7.36014 -2.90377 1.95583
C -2.39005 -2.14225 -3.85411	C 6.44154 -1.95932 1.50776
H -3.09136 -1.47397 -4.34192	C 7.15934 1.78427 0.39037
C -2.55086 -3.51114 -3.98534	C 7.61847 3.04829 0.03115
H -3.37211 -3.90832 -4.57053	C 7.1762 3.65471 -1.14396
C -1.63847 -4.36173 -3.35157	C 6.27443 2.97769 -1.96466
C -1.55215 -5.81132 -3.30634	C 5.82361 1.70664 -1.62113
C -2.35212 -6.80543 -3.87892	C 4.01691 -1.80193 -0.5871
H -3.20593 -6.54815 -4.49623	C 2.67132 -2.13257 -0.67854
C -2.03911 -8.13882 -3.66989	C 1.70592 -1.17224 -0.36685
H -2.64598 -8.91098 -4.12395	C 2.10332 0.11574 0.0402
C -0.92948 -8.51218 -2.87869	C 3.44387 0.44356 0.14553
C -0.12804 -7.50377 -2.30382	C 0.24792 -1.22951 -0.37176
H 0.71945 -7.78274 -1.69018	C -0.25264 0.02286 0.03604
C -0.43868 -6.17447 -2.52332	C 0.88826 0.994 0.33464

C	1.75462	-4.86649	-2.5051	C	-0.63341	-2.26854	-0.69521
H	2.20443	-3.95223	-2.10323	C	-1.99951	-2.05046	-0.6106
H	2.30273	-5.6997	-2.05197	C	-2.51993	-0.80274	-0.20344
C	1.94017	-4.90155	-4.02406	C	-1.61584	0.23368	0.12034
H	1.44225	-4.05939	-4.5108	C	-3.9434	-0.53034	-0.09984
H	1.5425	-5.8228	-4.45675	C	-4.9617	-1.38033	-0.36108
H	3.00272	-4.84715	-4.27479	C	-6.36428	-1.05788	-0.24011
C	0.30372	-4.88743	-0.44199	O	-7.14789	-2.12241	-0.59215
H	0.93004	-5.71461	-0.09047	C	-8.50338	-2.03028	-0.54957
H	0.81895	-3.96842	-0.14249	C	-9.11863	-0.89144	-0.16057
C	-1.06189	-4.95492	0.24606	C	-8.35278	0.26208	0.22223
H	-1.58688	-5.88313	0.00762	C	-6.93833	0.11533	0.16159
H	-1.70314	-4.12033	-0.04791	C	-9.16392	-3.29638	-0.971
H	-0.93911	-4.91117	1.33133	C	-8.9655	1.45638	0.63003
C	0.72032	-10.29035	-2.45894	C	-10.37493	1.58075	0.68377
C	1.73945	-9.89909	-3.33436	N	-11.53025	1.66959	0.72329
H	1.50204	-9.26813	-4.18271	C	0.85293	1.96693	-2.09451
C	3.04738	-10.32074	-3.12228	C	0.8428	2.24522	-0.58938
H	3.8214	-10.00841	-3.81604	C	0.91235	0.38253	2.87898
C	3.38037	-11.1546	-2.04849	C	0.86434	1.47963	1.81265
C	2.34958	-11.5517	-1.19062	C	-8.19641	2.58527	1.00348
H	2.57411	-12.20143	-0.35086	N	-7.5505	3.49948	1.30539
C	1.03975	-11.12343	-1.38257	H	8.19124	-0.72691	-1.13054
H	0.25834	-11.43978	-0.70193	H	9.82782	-2.38431	-0.31321
C	-1.65823	-10.85571	-2.65228	H	9.3018	-3.79377	1.66546
C	-1.51263	-12.04421	-3.37508	H	7.12099	-3.50823	2.82367
H	-0.61686	-12.20512	-3.96292	H	5.49733	-1.83114	2.02284
C	-2.5049	-13.01816	-3.33344	H	7.49722	1.32233	1.31009
H	-2.36812	-13.93431	-3.89895	H	8.31575	3.56554	0.68067
C	-3.67527	-12.83679	-2.58915	H	7.53081	4.64148	-1.41762
C	-3.80934	-11.64324	-1.87102	H	5.92976	3.4337	-2.88603
H	-4.69809	-11.47848	-1.27019	H	5.13554	1.17829	-2.2699
C	-2.81749	-10.66878	-1.89076	H	4.77041	-2.53636	-0.8416
H	-2.93695	-9.76054	-1.31217	H	2.38609	-3.12668	-1.00463
C	-1.27272	-0.14571	-3.0382	H	3.75299	1.42914	0.47249
H	-2.06299	0.3571	-3.58733	H	-0.2599	-3.23675	-1.00933
C	-0.40062	0.70974	-2.41512	H	-2.67447	-2.8592	-0.86341
C	0.72418	0.31932	-1.63169	H	-2.00952	1.19525	0.43488
C	-0.6014	2.11885	-2.53767	H	-4.18346	0.47818	0.22616
C	4.80607	-11.59013	-1.81263	H	-4.7711	-2.39469	-0.69168
H	5.34479	-10.85893	-1.19979	H	-10.19916	-0.86367	-0.14205
H	4.8489	-12.54834	-1.29026	H	-6.29987	0.94247	0.43744
H	5.35258	-11.69116	-2.75322	H	-10.24719	-3.19562	-0.92892
C	-4.76558	-13.88038	-2.57927	H	-8.85556	-4.1184	-0.31915
H	-5.31198	-13.87659	-1.63326	H	-8.86811	-3.55496	-1.99148
H	-5.49378	-13.69709	-3.3772	H	0.82054	2.90689	-2.65173
H	-4.3594	-14.88265	-2.73272	H	1.75591	1.43151	-2.39786
				H	-0.01015	1.37018	-2.39971
				H	-0.05321	2.82016	-0.33078
				H	1.69678	2.88076	-0.33098

	H	0.88736	0.82637	3.87769
	H	0.06045	-0.29692	2.79627
	H	1.82573	-0.21239	2.80237
	H	1.70988	2.16177	1.95345
	H	-0.03903	2.08368	1.95138

5				6			
N	-8.76718	-2.9781	-1.45438	S	-0.05758	0.41353	0.03025
C	-4.2988	-0.62107	-1.77426	O	-4.94568	-1.90919	-0.77501
C	-4.01145	0.74346	-1.15145	N	-4.78299	-11.38297	-4.51985
C	-2.85336	1.48788	-1.1917	C	-3.9802	-12.06212	-5.47794
H	-1.97972	1.12895	-1.72608	C	-3.8016	-13.44999	-5.39765
C	-2.77704	2.72813	-0.50719	H	-4.27278	-14.0023	-4.5938
C	-3.93168	3.20927	0.15318	C	-3.02683	-14.11428	-6.34341
H	-3.91199	4.1821	0.62624	H	-2.89903	-15.1883	-6.2661
C	-5.10821	2.48226	0.16482	C	-2.40492	-13.40882	-7.37251
H	-5.98567	2.88283	0.65902	H	-1.79698	-13.92853	-8.10373
C	-5.14945	1.23475	-0.47336	C	-2.57476	-12.02718	-7.45097
C	-6.22511	0.26803	-0.61006	H	-2.10394	-11.46626	-8.25069
C	-7.54287	0.27699	-0.14117	C	-3.36149	-11.35697	-6.51951
H	-7.91956	1.10397	0.45032	H	-3.50029	-10.28538	-6.59417
C	-8.37242	-0.79762	-0.41997	C	-6.02457	-11.95143	-4.11719
H	-9.38739	-0.8043	-0.04482	C	-6.90359	-12.48466	-5.06912
C	-7.91119	-1.89574	-1.17839	H	-6.63464	-12.45541	-6.11802
C	-6.58283	-1.89635	-1.65082	C	-8.11157	-13.04897	-4.67045
H	-6.22675	-2.73232	-2.24008	H	-8.78085	-13.45709	-5.41963
C	-5.75493	-0.82727	-1.36202	C	-8.47022	-13.07675	-3.32359
C	-3.37183	-1.72752	-1.19134	H	-9.4146	-13.51112	-3.01723
H	-3.64918	-2.67535	-1.66533	C	-7.60034	-12.54113	-2.37459
H	-2.34863	-1.51169	-1.51753	H	-7.86249	-12.56407	-1.32268
C	-3.39796	-1.8905	0.33048	C	-6.38306	-11.99032	-2.76299
H	-4.39706	-2.14909	0.68993	H	-5.7039	-11.58899	-2.02065
H	-3.08173	-0.97804	0.84131	C	-4.35736	-10.14668	-3.97511
H	-2.71855	-2.69144	0.63349	C	-5.28621	-9.11667	-3.7391
C	-4.12683	-0.60345	-3.32036	H	-6.32942	-9.27447	-3.98613
H	-3.06683	-0.43222	-3.53704	C	-4.8545	-7.91716	-3.19854
H	-4.35332	-1.60869	-3.69187	C	-5.68121	-6.67577	-2.86694

C	-4.9748	0.42206	-4.07692	C	-6.38413	-6.09049	-4.12538
H	-4.74957	1.44362	-3.76053	H	-7.1374	-6.81465	-4.45543
H	-6.04326	0.25074	-3.92489	H	-6.93666	-5.19762	-3.81307
H	-4.77696	0.35619	-5.14995	C	-5.46831	-5.73696	-5.29983
C	-8.24819	-4.30277	-1.57066	H	-4.9322	-6.61443	-5.66968
C	-7.38288	-4.81497	-0.59576	H	-4.72798	-4.98407	-5.01903
H	-7.10816	-4.19853	0.25165	H	-6.05591	-5.33218	-6.12818
C	-6.88275	-6.10832	-0.71419	C	-6.77018	-6.97496	-1.79678
H	-6.21474	-6.49308	0.04811	H	-7.31112	-6.04259	-1.60155
C	-7.25065	-6.91235	-1.79283	H	-7.49769	-7.66209	-2.24322
H	-6.86501	-7.92145	-1.87851	C	-6.26604	-7.55658	-0.4737
C	-8.12114	-6.40784	-2.75801	H	-5.57129	-6.87678	0.02514
H	-8.41158	-7.02226	-3.60271	H	-5.75425	-8.51043	-0.62332
C	-8.61325	-5.10966	-2.65489	H	-7.10471	-7.73144	0.2055
H	-9.28183	-4.71685	-3.41137	C	-4.60007	-5.7378	-2.33249
C	-10.16807	-2.77562	-1.63066	C	-4.72919	-4.44516	-1.86583
C	-10.64167	-1.74585	-2.45388	H	-5.68722	-3.94051	-1.82731
H	-9.9358	-1.0978	-2.95905	C	-3.59497	-3.73934	-1.41881
C	-12.01026	-1.55839	-2.62309	C	-2.34201	-4.37427	-1.44626
H	-12.3629	-0.75803	-3.26384	H	-1.45887	-3.86035	-1.0902
C	-12.92328	-2.40219	-1.99119	C	-2.20494	-5.67978	-1.90919
H	-13.9882	-2.2578	-2.13059	H	-1.22851	-6.15124	-1.91596
C	-12.45342	-3.43468	-1.18044	C	-3.33544	-6.36319	-2.35787
H	-13.15311	-4.09482	-0.68039	C	-3.49532	-7.71199	-2.89685
C	-11.08653	-3.61902	-0.99332	C	-2.56818	-8.72842	-3.1345
H	-10.72524	-4.41586	-0.35461	H	-1.51812	-8.59232	-2.89964
C	-1.5439	3.46794	-0.61598	C	-3.0011	-9.93806	-3.6625
C	-1.02096	4.50028	0.12083	H	-2.2911	-10.73679	-3.83612
C	-0.00918	5.43728	-0.40705	C	-3.80608	-2.34458	-0.91886
C	-1.44823	5.05362	1.41518	C	-2.62833	-1.49915	-0.61783
C	-0.20736	6.70355	0.3152	H	-1.6353	-1.88363	-0.81214
C	-1.08687	6.47634	1.40272	C	-2.79503	-0.25483	-0.12712
C	0.30231	7.98115	0.08246	H	-3.81864	0.07314	0.03755
C	-1.45507	7.52113	2.24822	C	-1.77911	0.70681	0.21015
C	-0.08048	9.02145	0.92746	C	-1.99319	1.97402	0.71222
H	0.97097	8.18286	-0.74065	H	-2.98761	2.35833	0.89966
C	-0.95017	8.79555	1.99571	C	-0.80073	2.70333	0.95099
H	-2.13206	7.36617	3.07542	H	-0.77396	3.71115	1.3427
H	0.30002	10.01925	0.74617	C	0.32227	1.99155	0.63084
H	-1.24185	9.61965	2.6353	H	1.3544	2.29703	0.71067
H	-0.9742	3.19311	-1.49584				
C	-1.86846	4.3324	2.50852				
C	-1.91335	2.90837	2.52996				
N	-1.92419	1.75537	2.61078				
C	-2.19282	4.93698	3.75772				
N	-2.47334	5.39454	4.78208				
C	0.96718	5.18009	-1.34402				
C	1.9002	6.16108	-1.78879				
N	2.67634	6.92477	-2.17873				
C	1.18947	3.89613	-1.92173				

N	1.40746	2.87022	-2.40949
	7		
S	-2.51374	2.3163	1.01793
N	-4.70938	-11.38838	-4.51437
C	-3.94687	-12.04524	-5.52003
C	-3.73396	-13.42912	-5.45792
H	-4.14731	-13.99532	-4.63222
C	-2.99906	-14.07171	-6.44942
H	-2.84369	-15.14299	-6.38581
C	-2.45136	-13.34781	-7.50746
C	-2.65541	-11.96992	-7.56828
H	-2.2425	-11.3951	-8.38981
C	-3.40313	-11.32165	-6.59033
H	-3.56926	-10.25304	-6.6507
C	-5.91544	-11.98451	-4.04882
C	-6.83392	-12.53013	-4.95544
H	-6.62289	-12.48935	-6.01712
C	-8.00692	-13.12127	-4.49586
H	-8.70748	-13.53872	-5.21051
C	-8.29136	-13.16417	-3.13178
C	-7.38211	-12.61655	-2.22758
H	-7.58615	-12.65132	-1.16318
C	-6.19901	-12.03874	-2.67747
H	-5.48856	-11.62837	-1.97017
C	-4.27884	-10.14754	-3.98461
C	-5.2138	-9.13834	-3.68823
H	-6.26582	-9.31673	-3.87699
C	-4.77658	-7.93411	-3.16376
C	-5.60761	-6.71195	-2.77527
C	-6.39416	-6.13403	-3.98678
H	-7.14857	-6.87304	-4.27891
H	-6.94921	-5.25634	-3.63733
C	-5.55506	-5.7522	-5.20868
H	-5.0213	-6.61504	-5.61432
H	-4.81683	-4.98434	-4.96527
H	-6.19792	-5.35646	-5.99945
C	-6.62571	-7.04161	-1.64589
H	-7.17557	-6.12319	-1.41201
H	-7.36312	-7.74113	-2.05494
C	-6.03319	-7.62148	-0.35919
H	-5.32407	-6.93125	0.10393
H	-5.51149	-8.56307	-0.54666
H	-6.82683	-7.81905	0.36628
C	-4.51582	-5.756	-2.29704
C	-4.64105	-4.46633	-1.81359
H	-5.61587	-3.99555	-1.73142
C	-3.49892	-3.7383	-1.4167
C	-2.23527	-4.35532	-1.52648
H	-1.34671	-3.81248	-1.22695
C	-2.10164	-5.64742	-2.01165

H	-1.11825	-6.09833	-2.08693
C	-3.24532	-6.35417	-2.3994
C	-3.40676	-7.70201	-2.93811
C	-2.47414	-8.69747	-3.2356
H	-1.41544	-8.54136	-3.05939
C	-2.91179	-9.91247	-3.74751
H	-2.19648	-10.69494	-3.96724
C	-3.68238	-2.38476	-0.91309
C	-2.74475	-1.51744	-0.48341
H	-1.69409	-1.77811	-0.47749
C	-3.13528	-0.17565	-0.00535
C	-2.06078	0.72714	0.44975
C	-0.69523	0.55403	0.51857
H	-0.19165	-0.35429	0.2179
C	-0.01212	1.68866	1.02438
H	1.06069	1.74361	1.15225
C	-0.8661	2.71411	1.33526
H	-0.61714	3.68566	1.735
H	-4.7086	-2.02657	-0.87902
O	-4.30473	0.20159	0.02332
H	-9.20876	-13.61959	-2.77776
H	-1.87413	-13.85052	-8.27456