

Supporting Information
For

**N-Insertion Reaction Mechanisms of Phenyl Azide with
Hafnium Hydride Complex: A Quantum Chemistry
Calculations**

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Cartesian coordinates and electronic energies for all of the calculated structures

1				H	1.785612	-3.283233	0.102685
SCF done:	-830.363806			H	3.496249	-2.924509	-0.157134
C	-2.401323	-0.764936	-0.687403	H	2.346031	-2.812941	-1.500566
C	-2.421311	0.660176	-0.767156	C	1.712255	1.716664	2.269038
C	-2.040866	1.180142	0.510049	H	1.183342	1.262717	3.111338
C	-1.804686	0.075698	1.384869	H	1.176713	2.632375	1.994309
C	-2.003636	-1.127654	0.638234	H	2.700540	2.024486	2.638600
C	1.853899	0.763827	1.109923	C	1.682545	-1.505783	2.422649
C	2.266414	1.136260	-0.205397	H	1.169932	-2.453471	2.225360
C	2.488543	-0.059371	-0.953164	H	1.122918	-0.981627	3.201942
C	2.239795	-1.174504	-0.096995	H	2.665536	-1.756296	2.845950
C	1.840307	-0.671249	1.177783	H	0.005499	-1.426149	-1.620848
Hf	-0.000170	-0.003703	-0.442037				
H	0.008292	1.404689	-1.637092	TS₁₂			
C	-2.878405	-1.711861	-1.755624	SCF done:	-1226.177763		
H	-2.411860	-2.695712	-1.659407	C	0.503716	2.260039	1.159562
H	-2.650231	-1.340847	-2.759089	C	0.146970	2.502296	-0.200881
H	-3.967894	-1.848610	-1.693051	C	1.290616	2.239129	-1.017441
C	-1.957916	-2.533860	1.175196	C	2.352354	1.818166	-0.165991
H	-1.354351	-2.605219	2.085328	C	1.862187	1.815524	1.185242
H	-1.539819	-3.233415	0.443017	C	1.891196	-1.945252	-0.983427
H	-2.965583	-2.893251	1.427544	C	0.551118	-2.415430	-0.795395
C	-2.902265	1.464092	-1.944707	C	0.290124	-2.457904	0.605200
H	-2.475876	2.470570	-1.946201	C	1.467493	-2.018781	1.289071
H	-3.997489	1.561210	-1.928437	C	2.465439	-1.732013	0.307915
H	-2.627910	0.993657	-2.893709	Hf	0.572545	-0.007450	-0.002200
C	-1.621379	0.164740	2.876433	C	-0.338859	2.590701	2.361284
H	-1.075260	1.063131	3.177389	H	-0.087092	1.960911	3.218849
H	-1.093640	-0.702244	3.283188	H	-1.404711	2.455616	2.157783
H	-2.600704	0.204426	3.374256	H	-0.187487	3.638260	2.660574
C	-2.027599	2.636933	0.889920	C	2.681101	1.641148	2.437598
H	-1.682120	3.265567	0.062781	H	3.584711	1.051543	2.260801
H	-1.376428	2.831032	1.748422	H	2.113663	1.149144	3.234461
H	-3.034287	2.982647	1.164553	H	3.005386	2.616207	2.828243
C	2.548268	2.539410	-0.669567	C	-1.154424	3.092377	-0.673817
H	1.881021	3.266885	-0.197018	H	-1.361326	2.831289	-1.715615
H	2.423425	2.638284	-1.750875	H	-1.124733	4.189623	-0.612876
H	3.579466	2.830329	-0.421440	H	-2.001374	2.754035	-0.070179
C	2.961077	-0.128204	-2.379295	C	3.790275	1.694181	-0.597762
H	2.613312	-1.040501	-2.873125	H	3.904231	1.134463	-1.532749
H	4.058963	-0.118213	-2.433875	H	4.407701	1.208068	0.160217
H	2.594790	0.721620	-2.963641	H	4.218124	2.691709	-0.770676
C	2.475298	-2.622314	-0.432201	C	1.408831	2.512177	-2.492178

H	0.458148	2.363593	-3.010151	H	2.445327	-1.313211	2.940301
H	2.144663	1.857070	-2.968795	H	2.615400	-3.030114	2.572946
H	1.730611	3.548917	-2.668513	C	-1.261539	2.575388	1.909275
C	-0.358269	-2.941664	-1.872541	H	-1.074039	2.007184	2.823401
H	-0.192830	-2.438019	-2.828141	H	-2.270122	2.327889	1.568985
H	-1.412260	-2.814042	-1.608337	H	-1.255945	3.642035	2.174904
H	-0.188516	-4.017038	-2.026189	C	-1.743233	2.709224	-1.254726
C	-0.952615	-3.005154	1.252203	H	-1.820712	2.183323	-2.210877
H	-1.070943	-2.627656	2.271263	H	-1.823332	3.786254	-1.459898
H	-0.911311	-4.102669	1.304237	H	-2.609253	2.421554	-0.653915
H	-1.856830	-2.736797	0.697987	C	1.077959	2.486505	-2.679908
C	1.661280	-2.028795	2.781319	H	1.968120	1.948958	-3.021121
H	2.477790	-1.370010	3.091635	H	1.234360	3.551645	-2.903372
H	1.905467	-3.038690	3.140536	H	0.233066	2.140639	-3.281588
H	0.756729	-1.703581	3.305200	C	1.847412	2.137596	2.414378
C	2.606096	-1.860079	-2.305199	H	2.801146	1.601073	2.415484
H	3.443424	-1.155721	-2.270958	H	1.225353	1.707066	3.205347
H	1.932924	-1.533224	-3.103824	H	2.062076	3.176146	2.703711
H	3.016481	-2.836870	-2.598434	C	3.299072	2.292298	-0.439662
C	3.929975	-1.532324	0.592005	H	3.649752	1.789980	-1.346524
H	4.109246	-0.954010	1.503025	H	3.896652	1.932192	0.399295
H	4.449170	-1.036539	-0.230912	H	3.526070	3.360850	-0.561399
H	4.413792	-2.508872	0.735594	H	-0.196139	-0.020742	-1.847333
H	-0.560734	-0.075656	1.437885	N	-0.749461	-0.611488	3.029025
N	-1.434014	0.138351	-2.969280	N	-1.733011	-0.746309	2.250395
N	-2.192350	0.059861	-2.091258	N	-1.589787	-0.479993	0.937310
N	-2.225559	-0.054339	-0.822762	C	-2.845002	-0.433392	0.269674
C	-3.505644	-0.055079	-0.211451	C	-4.010631	0.003193	0.931917
C	-4.708625	-0.002049	-0.936779	C	-2.945000	-0.801674	-1.082795
C	-3.549073	-0.112024	1.189685	C	-5.226570	0.066273	0.255840
C	-5.928984	-0.004619	-0.264949	H	-3.948454	0.276212	1.978926
H	-4.682109	0.040463	-2.021969	C	-4.163265	-0.711165	-1.758528
C	-4.777924	-0.114128	1.848637	H	-2.065815	-1.155499	-1.609003
H	-2.613283	-0.151053	1.737334	C	-5.312583	-0.280598	-1.095946
C	-5.974160	-0.060581	1.130387	H	-6.113383	0.400425	0.788868
H	-6.850877	0.037182	-0.839394	H	-4.212265	-0.998247	-2.806021
H	-4.796722	-0.157557	2.934633	H	-6.261973	-0.220681	-1.620744
H	-6.928713	-0.062339	1.648825	H	0.084638	-0.242309	2.512704
H	-0.001369	0.042330	-1.843651				

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SCF done: -1226.230280

C	0.922954	-2.246881	-1.161162
C	0.648558	-2.522403	0.211412
C	1.677814	-1.910871	0.998269
C	2.600368	-1.282709	0.102705
C	2.124619	-1.470890	-1.228400
C	1.167046	2.088696	1.069510
C	-0.232252	2.311814	0.844196
C	-0.444295	2.401260	-0.560260
C	0.826549	2.284405	-1.210950
C	1.821652	2.120685	-0.209522
Hf	0.351259	0.003865	-0.114842
C	0.197649	-2.832958	-2.341884
H	0.238286	-2.171564	-3.211763
H	-0.855890	-3.027066	-2.120267
H	0.648503	-3.793681	-2.628793
C	2.822299	-1.079957	-2.503253
H	3.546860	-0.276056	-2.344258
H	2.111957	-0.741279	-3.264541
H	3.372354	-1.932695	-2.925344
C	-0.423338	-3.445763	0.725550
H	-0.709353	-3.205670	1.751929
H	-0.066200	-4.485081	0.711182
H	-1.330073	-3.401067	0.115510
C	3.973934	-0.818260	0.506331
H	3.966880	-0.208605	1.415539
H	4.468101	-0.246493	-0.281099
H	4.606484	-1.692241	0.716418
C	1.948520	-2.162948	2.459953
H	1.034570	-2.366084	3.021888

TS₂₃

SCF done: -1226.170199

C	1.081756	-2.175577	-1.277064
C	0.504549	-2.571801	-0.035395
C	1.354637	-2.094439	1.014260
C	2.477372	-1.444770	0.410324
C	2.302888	-1.487837	-1.006464
C	1.323721	2.063474	1.115118
C	-0.047827	2.389603	0.864936
C	-0.234664	2.492043	-0.540583
C	1.036377	2.287996	-1.169346
C	2.001631	2.061441	-0.151102
Hf	0.381818	0.011616	-0.097730
C	0.599216	-2.600437	-2.636879
H	0.877047	-1.877773	-3.408849
H	-0.488985	-2.709290	-2.664492
H	1.032878	-3.572747	-2.914280
C	3.290202	-1.070696	-2.063081
H	4.099695	-0.462661	-1.652126
H	2.815634	-0.498626	-2.868827
H	3.753049	-1.952422	-2.527843
C	-0.666555	-3.511246	0.089680
H	-0.875964	-3.760154	1.130816
H	-0.448965	-4.448226	-0.440382
H	-1.589325	-3.100029	-0.330813
C	3.738562	-1.097090	1.155064
H	3.545053	-0.574016	2.097377
H	4.418232	-0.482846	0.560463
H	4.282579	-2.017406	1.412839
C	1.277219	-2.442742	2.479178
H	0.302896	-2.852884	2.750286
H	1.461196	-1.577883	3.127951

H	2.035448	-3.197060	2.734023	C	1.929128	-1.996843	-2.769161
C	-1.054439	2.734373	1.923972	H	2.314116	-1.096213	-3.255930
H	-0.930556	2.129661	2.829801	H	0.961455	-2.224050	-3.224254
H	-2.080269	2.611391	1.569324	H	2.614719	-2.823263	-3.008335
H	-0.937388	3.783822	2.230076	C	-0.079903	-3.550808	-0.886002
C	-1.497447	2.876281	-1.260633	H	-0.811466	-3.792583	-0.109974
H	-1.604495	2.319153	-2.196594	H	0.414096	-4.490153	-1.171104
H	-1.496246	3.947270	-1.508782	H	-0.637119	-3.190739	-1.756329
H	-2.389505	2.675122	-0.662315	C	0.692974	-2.827992	2.177672
C	1.318632	2.479022	-2.634528	H	0.600123	-2.107903	2.998344
H	2.189776	1.903675	-2.962831	H	1.344165	-3.638892	2.533681
H	1.523545	3.535942	-2.858953	H	-0.294043	-3.273989	2.013790
H	0.469110	2.166271	-3.247708	C	3.921380	-0.342928	-0.984350
C	1.976538	2.072237	2.474335	H	4.412062	0.252962	-0.211892
H	2.938869	1.552893	2.471481	H	3.694995	0.320423	-1.826693
H	1.350098	1.598432	3.238529	H	4.658107	-1.074080	-1.345040
H	2.168211	3.101104	2.811941	C	3.150131	-0.898824	2.122170
C	3.492191	2.124946	-0.345553	H	2.521790	-0.566784	2.955695
H	3.808592	1.706443	-1.304807	H	3.869308	-0.104836	1.910184
H	4.042009	1.612857	0.446913	H	3.725107	-1.764006	2.481993
H	3.819927	3.174622	-0.333408	H	-1.366483	-1.752913	0.973113
H	-0.102564	0.027104	-1.855787	N	-1.489117	-0.953632	0.356863
N	-1.935535	-0.746832	3.007823	C	-2.858470	-0.759441	0.139171
N	-1.854450	-1.651447	2.275411	C	-3.324799	-0.188654	-1.062255
N	-1.559810	-0.247214	0.609356	C	-3.820003	-1.157790	1.091955
C	-2.814862	-0.168418	0.038478	C	-4.687678	0.015590	-1.276006
C	-3.897783	0.483203	0.690749	H	-2.601188	0.059425	-1.831936
C	-3.104023	-0.775180	-1.215815	C	-5.180976	-0.965254	0.865184
C	-5.176462	0.503380	0.139951	H	-3.484223	-1.609408	2.024154
H	-3.716770	0.992646	1.633090	C	-5.628148	-0.366101	-0.315726
C	-4.388069	-0.770362	-1.747654	H	-5.018020	0.457312	-2.213508
H	-2.287693	-1.243424	-1.755039	H	-5.897011	-1.279869	1.620940
C	-5.436851	-0.130846	-1.077269	H	-6.689576	-0.214588	-0.490341
H	-5.975585	1.020635	0.665722	H	0.049656	0.003679	-1.959875
H	-4.571414	-1.254306	-2.704184				
H	-6.435538	-0.114335	-1.504508				
H	-1.783963	0.159821	2.372267				

TS₂₄

SCF done:	-1226.219786		
C	0.842887	2.062629	1.419841
C	-0.175230	2.442682	0.485333
C	0.408257	2.484536	-0.810598
C	1.772396	2.069390	-0.697261
C	2.051089	1.863424	0.694587
C	1.722779	-2.022706	-1.050026
C	0.504571	-2.551586	-0.514500
C	0.538892	-2.395550	0.900790
C	1.777662	-1.774226	1.247713
C	2.518116	-1.565241	0.041480
Hf	0.435624	-0.010198	-0.060552
C	0.704396	2.078313	2.917301
H	1.396351	1.380923	3.399945
H	-0.307298	1.801949	3.227059
H	0.916567	3.079210	3.321284
C	3.420339	1.798329	1.316786
H	4.177839	1.434759	0.619948
H	3.453479	1.173042	2.213955
H	3.728370	2.807941	1.624662
C	-1.566977	2.880566	0.853643
H	-2.265470	2.766854	0.019725
H	-1.577810	3.939676	1.147779
H	-1.962621	2.301734	1.693465
C	2.762589	2.095953	-1.831132
H	2.324134	1.688266	-2.748267
H	3.663483	1.517453	-1.603780
H	3.087193	3.122840	-2.053150
C	-0.222452	3.008558	-2.068959
H	-1.308939	3.090000	-1.975966
H	-0.015177	2.353734	-2.919403
H	0.168004	4.010976	-2.294938
C	-0.547805	-3.315845	-1.275244
H	-0.579776	-3.045390	-2.336538

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SCF done:	-1116.803984		
C	-0.797000	2.100798	0.716073
C	-0.518561	2.351618	-0.653155
C	0.907202	2.397148	-0.816523
C	1.502614	2.209036	0.459472
C	0.454672	1.956100	1.404071
C	2.698832	-1.051661	-0.463145
C	1.812292	-1.817375	-1.279732
C	0.931502	-2.539912	-0.419796
C	1.254732	-2.201087	0.927788
C	2.348912	-1.279250	0.904803
Hf	0.336328	-0.045983	-0.148440
C	-2.135205	2.156182	1.399306
H	-2.233646	1.387530	2.171861
H	-2.962259	2.017024	0.700859
H	-2.267928	3.132458	1.887214
C	0.603385	1.875618	2.901883
H	1.597385	1.527670	3.197611
H	-0.133086	1.201100	3.352589
H	0.456605	2.862169	3.365076
C	-1.501019	2.722758	-1.730321
H	-1.270107	2.224514	-2.677354
H	-1.473783	3.806673	-1.912562
H	-2.525102	2.459907	-1.457085
C	2.935225	2.506285	0.809007
H	3.616710	2.321033	-0.024495
H	3.288399	1.934792	1.670772
H	3.033870	3.569502	1.071471
C	1.608638	2.782471	-2.091053
H	1.139890	2.314643	-2.962404
H	2.662747	2.488503	-2.084303
H	1.578831	3.871027	-2.244285

H	-1.548705	-3.157131	-0.863173	H	-0.303410	-4.157133	-1.820950
H	-0.343368	-4.394916	-1.235422	C	-1.072503	-3.023735	1.247131
C	-0.465927	-2.954082	1.870210	H	-1.265792	-2.571393	2.223478
H	-0.446872	-2.415129	2.821142	H	-0.995641	-4.111133	1.391001
H	-0.253538	-4.012549	2.080830	H	-1.948873	-2.834457	0.620873
H	-1.486515	-2.897721	1.479840	C	1.489861	-2.006055	2.833150
C	2.262354	-1.580029	2.659434	H	2.258280	-1.301538	3.164403
H	3.146254	-0.938640	2.705960	H	1.784904	-3.001750	3.194446
H	2.537790	-2.541723	3.114596	H	0.555873	-1.734405	3.333696
H	1.490992	-1.129916	3.293909	C	2.584101	-1.897086	-2.218116
C	2.189112	-2.119868	-2.478611	H	3.369763	-1.134624	-2.193731
H	2.880000	-1.311420	-2.737204	H	1.929988	-1.667013	-3.065747
H	1.362579	-2.076946	-3.195449	H	3.071619	-2.857145	-2.439815
H	2.714637	-3.069403	-2.654676	C	3.801961	-1.495424	0.704843
C	3.981703	-1.231511	-0.068485	H	3.951523	-0.889336	1.602852
H	4.376512	-0.796447	0.850959	H	4.346104	-1.024397	-0.116371
H	4.199470	-0.541240	-0.889590	H	4.282492	-2.466050	0.893655
H	4.554806	-2.148917	-0.263743	H	-0.474050	-0.054146	1.562895
H	-0.546924	-0.124086	1.481199	N	-0.378305	0.009834	-2.171920
N	-0.340997	0.037316	-2.221647	N	-1.659129	-0.003210	-1.967937
N	-1.668771	0.257201	-1.863781	N	-1.835415	-0.039114	-0.674401
N	-1.885187	-0.251973	-0.717129	C	-3.172726	-0.037159	-0.223308
C	-3.228605	-0.195974	-0.241571	C	-4.275246	-0.056903	-1.100684
C	-4.311376	0.019402	-1.110307	C	-3.408377	-0.011523	1.161392
C	-3.458751	-0.425721	1.121457	C	-5.571673	-0.048758	-0.593192
C	-5.608625	0.029188	-0.604341	H	-4.104817	-0.077343	-2.170638
H	-4.122934	0.167107	-2.167657	C	-4.712596	-0.003781	1.655763
C	-4.762954	-0.420995	1.614934	H	-2.554295	-0.000728	1.829945
H	-2.605350	-0.579660	1.772538	C	-5.803663	-0.021750	0.785553
C	-5.840722	-0.190134	0.757322	H	-6.411037	-0.063849	-1.284493
H	-6.444492	0.197202	-1.278239	H	-4.873284	0.016142	2.730982
H	-4.936139	-0.594645	2.673547	H	-6.818940	-0.015628	1.172483
H	-6.856158	-0.188126	1.144043	H	-0.166909	0.042546	-3.164506
H	-0.276952	-0.970245	-2.390296				

4
SCF done: -1226.270180

C	0.360218	2.293306	1.100129
C	0.078172	2.514556	-0.280728
C	1.270236	2.231335	-1.025149
C	2.277134	1.819579	-0.111639
C	1.710116	1.838521	1.207645
C	1.817219	-1.954748	-0.923435
C	0.486828	-2.466223	-0.761929
C	0.184144	-2.479314	0.628090
C	1.330277	-2.003356	1.337573
C	2.348208	-1.709910	0.381202
Hf	0.432554	-0.006494	-0.024709
C	-0.546246	2.644889	2.247658
H	-0.300338	2.069379	3.143776
H	-1.596237	2.450638	2.011788
H	-0.453254	3.711973	2.497391
C	2.448206	1.654682	2.507260
H	3.362373	1.067867	2.382834
H	1.830536	1.152386	3.258994
H	2.744848	2.625933	2.928150
C	-1.173942	3.137344	-0.836992
H	-1.421416	2.745454	-1.828070
H	-1.054434	4.225770	-0.934352
H	-2.036857	2.956861	-0.190786
C	3.736087	1.689276	-0.462115
H	3.902133	1.108428	-1.376477
H	4.313530	1.223999	0.338574
H	4.169751	2.684371	-0.635633
C	1.483392	2.507976	-2.487992
H	0.547102	2.453718	-3.050067
H	2.191086	1.806286	-2.944003
H	1.893833	3.517380	-2.634975
C	-0.377796	-3.060750	-1.839657
H	-0.074856	-2.728740	-2.835579
H	-1.433608	-2.803278	-1.711909

TS₄₅
SCF done: -1226.190835

C	0.946421	1.904790	1.451111
C	0.248236	2.523816	0.362634
C	1.085741	2.463667	-0.790494
C	2.291404	1.796999	-0.434111
C	2.220107	1.476393	0.963541
C	1.194698	-2.269524	-1.104446
C	-0.050351	-2.490129	-0.445213
C	0.147563	-2.280666	0.954055
C	1.522377	-1.953354	1.163749
C	2.170392	-1.939342	-0.114586
Hf	0.455019	-0.008244	-0.163945
C	0.526548	1.937350	2.898291
H	0.899742	1.071524	3.454930
H	-0.562490	1.950775	3.004433
H	0.913951	2.835874	3.400697
C	3.400561	1.138885	1.834708
H	4.115795	0.473211	1.345262
H	3.102773	0.677098	2.778575
H	3.946658	2.059383	2.087971
C	-1.053794	3.270077	0.465398
H	-1.606638	3.232184	-0.475669
H	-0.876086	4.324269	0.720820
H	-1.702684	2.856381	1.244398
C	3.507397	1.670430	-1.314228
H	3.244705	1.392129	-2.340992
H	4.206350	0.918960	-0.938471
H	4.054490	2.622504	-1.367597
C	0.786867	3.093903	-2.119932
H	-0.273014	2.999185	-2.375318
H	1.377869	2.643716	-2.925061
H	1.030574	4.165521	-2.105039
C	-1.307303	-2.968339	-1.116044
H	-1.449183	-2.474227	-2.081385
H	-2.194972	-2.766594	-0.510730
H	-1.264917	-4.053189	-1.290564

C	-0.849349	-2.561753	2.047459	H	0.893540	1.436077	3.034877
H	-0.688286	-1.922681	2.922251	H	1.377445	3.094132	2.676500
H	-0.767774	-3.604117	2.388933	H	2.323405	1.745948	2.040931
H	-1.879067	-2.411620	1.711405	C	-1.771015	2.507107	2.268374
C	2.183088	-1.938062	2.516573	H	-2.843266	2.557686	2.071018
H	3.217359	-1.593089	2.466071	H	-1.473799	3.482174	2.681656
H	2.200682	-2.952557	2.939470	H	-1.612479	1.770301	3.064727
H	1.654510	-1.304409	3.238577	C	-0.213103	2.539046	-2.655920
C	1.433881	-2.455930	-2.575662	H	-1.186784	2.358998	-3.123433
H	2.390526	-2.026209	-2.890141	H	0.515857	1.868558	-3.124091
H	0.638246	-1.978581	-3.158523	H	0.081371	3.569298	-2.902516
H	1.450733	-3.521979	-2.841858	C	-2.774618	2.801899	-0.798583
C	3.654337	-1.890386	-0.369002	H	-3.567779	2.533548	-0.097359
H	4.202478	-1.408192	0.443873	H	-3.035849	2.381441	-1.774535
H	3.900327	-1.362946	-1.295851	H	-2.801325	3.895830	-0.906896
H	4.055611	-2.909144	-0.465002	H	1.511561	-1.841860	0.858464
H	-1.286566	0.396904	0.704079	N	0.760379	-0.429260	-1.862007
N	-0.399147	0.076195	-2.136001	N	0.990812	-1.567470	-1.014123
N	-1.360746	0.851859	-1.472432	N	1.658715	-1.087283	0.189574
N	-1.777831	0.124286	-0.381166	C	3.076334	-0.794883	0.170976
C	-3.163386	0.134834	-0.071282	C	3.798467	-0.781576	-1.023865
C	-4.098987	0.205019	-1.113026	C	3.728520	-0.577340	1.389878
C	-3.607325	0.015811	1.253896	C	5.170704	-0.526267	-0.991977
C	-5.461618	0.147268	-0.821859	H	3.279145	-0.959464	-1.956140
H	-3.744272	0.297851	-2.132696	C	5.101715	-0.331650	1.411325
C	-4.971316	-0.056147	1.528699	H	3.160967	-0.600907	2.317340
H	-2.881952	-0.008919	2.063597	C	5.828044	-0.297664	0.218459
C	-5.908230	0.010832	0.494143	H	5.729567	-0.511630	-1.924103
H	-6.179384	0.205292	-1.636072	H	5.602104	-0.166990	2.361956
H	-5.302266	-0.150054	2.559752	H	6.896243	-0.100446	0.233966
H	-6.971215	-0.036345	0.712518	H	0.573190	-0.806114	-2.787882
H	-0.057643	0.670664	-2.891636				

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SCF done: -1226.217258

C	-1.817178	-1.525556	1.449351
C	-1.269922	-2.445266	0.504914
C	-1.850947	-2.172701	-0.771677
C	-2.769609	-1.096666	-0.614477
C	-2.777811	-0.714962	0.764089
C	-0.255373	2.326779	-1.168802
C	0.892981	2.190954	-0.337345
C	0.447220	2.085305	1.012691
C	-0.976157	2.213603	1.023030
C	-1.411736	2.361045	-0.332959
Hf	-0.398996	-0.073834	-0.171874
C	-1.610854	-1.565511	2.942494
H	-1.730933	-0.578319	3.400070
H	-0.613068	-1.929336	3.211542
H	-2.336273	-2.234989	3.427004
C	-3.879404	0.053014	1.443083
H	-4.252724	0.887263	0.844752
H	-3.574726	0.446619	2.414641
H	-4.736381	-0.613159	1.624085
C	-0.361073	-3.603791	0.806816
H	0.385769	-3.736359	0.017124
H	-0.934847	-4.538058	0.882080
H	0.158336	-3.484693	1.766065
C	-3.729020	-0.617189	-1.672575
H	-3.252355	-0.538625	-2.655978
H	-4.151057	0.361154	-1.430384
H	-4.571040	-1.315994	-1.778167
C	-1.592423	-2.958889	-2.024286
H	-0.519414	-3.128330	-2.163904
H	-1.979939	-2.446637	-2.910989
H	-2.080902	-3.942766	-1.979497
C	2.308176	2.326789	-0.824028
H	2.479434	1.732251	-1.725179
H	3.039218	2.010253	-0.076521
H	2.523461	3.377875	-1.066711
C	1.305191	2.082610	2.250400

TS₅₆

SCF done: -1226.212903

C	-1.792851	-1.573782	1.456287
C	-1.296006	-2.446822	0.439267
C	-1.935194	-2.108317	-0.789461
C	-2.823286	-1.023138	-0.536299
C	-2.768877	-0.719643	0.862968
C	-0.254047	2.367394	-1.102016
C	0.932033	2.186298	-0.334482
C	0.548723	2.027729	1.029427
C	-0.870485	2.163941	1.114372
C	-1.369827	2.371989	-0.210413
Hf	-0.393508	-0.075782	-0.226238
C	-1.489352	-1.677226	2.929163
H	-1.604179	-0.715744	3.440320
H	-0.467388	-2.026209	3.116261
H	-2.163745	-2.388288	3.427430
C	-3.819717	0.039414	1.626726
H	-4.179135	0.926967	1.100150
H	-3.471775	0.351600	2.613632
H	-4.696293	-0.605693	1.788609
C	-0.377602	-3.621148	0.627847
H	0.354688	-3.681101	-0.184913
H	-0.945268	-4.562009	0.629406
H	0.157576	-3.581529	1.584655
C	-3.828530	-0.486072	-1.522877
H	-3.387143	-0.314489	-2.511141
H	-4.268195	0.456250	-1.186925
H	-4.654994	-1.197454	-1.660992
C	-1.761321	-2.839306	-2.089261
H	-0.702443	-3.017484	-2.299615
H	-2.178497	-2.274935	-2.928473
H	-2.272213	-3.812523	-2.059802
C	2.329975	2.355623	-0.862399
H	2.478192	1.854001	-1.823691
H	3.084315	1.966538	-0.176153
H	2.546624	3.422135	-1.020119
C	1.462581	1.974434	2.224138
H	1.073855	1.315352	3.009229

H	1.571214	2.973293	2.671664	H	2.503328	2.126416	1.241642
H	2.462572	1.623184	1.961573	C	-1.225056	1.620162	3.010888
C	-1.602286	2.402478	2.408704	H	-2.181902	1.116038	3.170617
H	-2.682424	2.460427	2.267233	H	-1.277977	2.581485	3.541517
H	-1.281917	3.358468	2.847780	H	-0.450334	1.026680	3.507810
H	-1.405832	1.631229	3.162039	C	-1.840852	2.916157	-1.937185
C	-0.305185	2.685485	-2.571219	H	-2.728345	2.325852	-2.192807
H	-1.253892	2.382162	-3.025337	H	-1.147805	2.871083	-2.783627
H	0.497310	2.186786	-3.123755	H	-2.166465	3.962636	-1.851061
H	-0.191668	3.765655	-2.742948	C	-3.390964	2.091266	0.654070
C	-2.746647	2.843078	-0.598113	H	-3.734878	1.624116	1.578289
H	-3.498343	2.609457	0.158643	H	-3.929992	1.623705	-0.178248
H	-3.083814	2.413502	-1.546366	H	-3.712801	3.142166	0.686594
H	-2.749050	3.935174	-0.725281	H	1.469289	-0.865997	1.474154
H	1.445171	-1.911426	0.720884	N	-0.695502	0.192491	-2.365097
N	0.544671	-0.409398	-2.004362	N	0.519053	0.006711	-2.308370
N	0.908779	-1.518713	-1.279357	N	1.571940	-0.473294	0.539445
N	1.616506	-1.067711	0.176581	C	2.926768	-0.364187	0.267409
C	3.027291	-0.813061	0.180870	C	3.429145	0.102972	-0.971534
C	3.759090	-0.765239	-1.012413	C	3.886983	-0.731152	1.245039
C	3.705533	-0.674383	1.401891	C	4.800846	0.195689	-1.200630
C	5.136518	-0.543749	-0.982151	H	2.734231	0.368791	-1.757061
H	3.244720	-0.934736	-1.950329	C	5.253883	-0.633901	1.003808
C	5.085399	-0.466202	1.425452	H	3.537981	-1.095664	2.211213
H	3.145918	-0.731394	2.332013	C	5.731742	-0.166100	-0.223276
C	5.807250	-0.387829	0.232525	H	5.145829	0.555776	-2.168000
H	5.690347	-0.509283	-1.916966	H	5.951794	-0.926193	1.785829
H	5.594716	-0.363741	2.380309	H	6.798531	-0.089420	-0.413122
H	6.880401	-0.219755	0.250436	H	-1.145626	0.318456	-3.297044
H	1.234411	0.010991	-2.631545				

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SCF done: -1226.275068

C	-1.070904	-1.997167	1.316392
C	-0.347405	-2.612741	0.249475
C	-1.074161	-2.415954	-0.951601
C	-2.282064	-1.710359	-0.633509
C	-2.292225	-1.477021	0.772866
C	-1.197497	2.454521	-0.658735
C	0.197513	2.527703	-0.345789
C	0.350349	2.192254	1.032503
C	-0.926455	1.835690	1.549559
C	-1.894986	2.018658	0.498249
Hf	-0.379847	0.001248	-0.214386
C	-0.748409	-2.120474	2.783367
H	-1.195003	-1.313161	3.371389
H	0.331129	-2.106366	2.973094
H	-1.125574	-3.067846	3.194303
C	-3.512471	-1.129196	1.581297
H	-4.236700	-0.542250	1.012806
H	-3.277561	-0.581862	2.498035
H	-4.020436	-2.055126	1.888506
C	0.910101	-3.425373	0.362157
H	1.613871	-3.203147	-0.444795
H	0.670736	-4.497496	0.316480
H	1.433831	-3.250848	1.305359
C	-3.428046	-1.451688	-1.575247
H	-3.088761	-1.310926	-2.606859
H	-4.000617	-0.561688	-1.294153
H	-4.130302	-2.297273	-1.585297
C	-0.685840	-2.978093	-2.292697
H	0.369295	-2.797184	-2.527399
H	-1.280079	-2.547730	-3.104666
H	-0.844522	-4.064678	-2.319376
C	1.271037	3.063568	-1.256382
H	1.148422	2.715164	-2.288513
H	2.266948	2.753384	-0.930530
H	1.253380	4.162339	-1.281844
C	1.610131	2.321715	1.837711
H	1.628112	1.628827	2.684376
H	1.692519	3.339046	2.247131

TS_{6a}

SCF done: -1226.253290

C	-1.116100	-2.020191	1.261681
C	-0.519646	-2.617113	0.109767
C	-1.310538	-2.287847	-1.022789
C	-2.439679	-1.521624	-0.572890
C	-2.327437	-1.374175	0.842516
C	-1.085498	2.481216	-0.600554
C	0.329504	2.484637	-0.365221
C	0.543809	2.138771	1.002440
C	-0.717939	1.847935	1.591408
C	-1.736534	2.088200	0.600220
Hf	-0.398958	0.006951	-0.197377
C	-0.707456	-2.255229	2.693267
H	-1.049823	-1.453526	3.354381
H	0.379227	-2.334989	2.812165
H	-1.132799	-3.193998	3.075538
C	-3.444333	-0.976767	1.768983
H	-4.178440	-0.331066	1.283715
H	-3.088976	-0.469174	2.669981
H	-3.978058	-1.878506	2.102459
C	0.673047	-3.530539	0.083417
H	1.348048	-3.298852	-0.745114
H	0.344273	-4.573184	-0.029574
H	1.257611	-3.475027	1.005313
C	-3.650616	-1.179261	-1.402805
H	-3.389986	-0.989126	-2.448564
H	-4.172631	-0.293701	-1.027208
H	-4.371491	-2.009203	-1.394678
C	-1.096229	-2.821356	-2.414160
H	-0.033074	-2.887971	-2.666376
H	-1.570920	-2.193668	-3.173527
H	-1.521785	-3.830044	-2.510117
C	1.355344	3.028621	-1.324929
H	1.182399	2.686808	-2.350840
H	2.368621	2.730321	-1.047156
H	1.322319	4.127133	-1.339680
C	1.845833	2.192728	1.746563
H	1.929932	1.386614	2.481278
H	1.930692	3.145798	2.288375
H	2.704970	2.107990	1.079071

C	-0.934305	1.615836	3.064561	H	-2.571133	2.023057	-2.649139
H	-1.923660	1.203220	3.279686	H	-1.882616	1.494117	-4.183465
H	-0.853869	2.560084	3.621532	H	-0.877739	2.366273	-3.023415
H	-0.188776	0.934264	3.488101	C	-1.814097	-3.350429	-1.703926
C	-1.760338	3.008059	-1.838318	H	-2.900206	-3.408286	-1.588330
H	-2.790060	2.647710	-1.928104	H	-1.359877	-3.793461	-0.810329
H	-1.228054	2.725526	-2.752674	H	-1.545526	-3.991733	-2.554935
H	-1.798409	4.106417	-1.815022	C	-3.573873	-0.827812	-2.737844
C	-3.214341	2.236530	0.847480	H	-4.120583	0.064898	-2.417889
H	-3.516466	1.809991	1.805358	H	-4.113157	-1.702734	-2.370181
H	-3.826843	1.774108	0.065596	H	-3.627771	-0.853576	-3.835847
H	-3.482311	3.302154	0.871029	N	2.498300	-2.480386	2.936747
H	1.423515	-1.205001	1.302265	N	2.916683	-1.690313	2.228646
N	-0.549694	0.247965	-2.753242	N	3.264810	-0.736675	1.519691
N	0.511160	-0.012147	-2.269465	C	4.359576	-0.923155	0.628112
N	1.540071	-0.641942	0.463869	C	5.082051	-2.120029	0.525899
C	2.902156	-0.512370	0.227460	C	4.700554	0.176878	-0.169644
C	3.426000	0.091995	-0.939614	C	6.142081	-2.207999	-0.375854
C	3.841941	-1.004151	1.167884	H	4.820398	-2.974087	1.144731
C	4.801794	0.205889	-1.133416	C	5.762771	0.073591	-1.065926
H	2.745480	0.439887	-1.705173	H	4.131110	1.096292	-0.078571
C	5.213159	-0.886983	0.962931	C	6.488114	-1.115675	-1.174200
H	3.474110	-1.478158	2.077861	H	6.699043	-3.137913	-0.451645
C	5.713086	-0.274486	-0.189525	H	6.022712	0.929545	-1.682363
H	5.165136	0.672708	-2.046732	H	7.314983	-1.191053	-1.874271
H	5.896953	-1.276306	1.714349	N	0.467815	1.177639	0.440461
H	6.783245	-0.181418	-0.350598	H	1.149306	0.648998	0.994577
H	-1.453970	0.384648	-1.922052	C	0.877243	2.488890	0.293375

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SCF done: -1512.633475

C	-2.229646	0.977660	1.929081
C	-1.721788	-0.232804	2.471387
C	-2.442775	-1.322722	1.882524
C	-3.397014	-0.781923	0.979847
C	-3.234557	0.645858	0.963397
C	-1.344538	-1.937712	-1.927317
C	0.030740	-1.532349	-1.929459
C	0.088649	-0.162161	-2.315013
C	-1.250965	0.297437	-2.506411
C	-2.133010	-0.815697	-2.304266
Hf	-1.035477	-0.225829	-0.005149
C	-1.866118	2.365080	2.378253
H	-1.951509	3.100236	1.573584
H	-0.839879	2.416002	2.750271
H	-2.532072	2.687570	3.191472
C	-4.147867	1.641808	0.294851
H	-4.609806	1.236511	-0.610155
H	-3.618198	2.558448	0.012907
H	-4.964919	1.939636	0.967463
C	-0.670968	-0.345659	3.541084
H	-0.153177	-1.308243	3.495198
H	-1.113138	-0.255179	4.543226
H	0.083228	0.443301	3.448578
C	-4.544704	-1.554511	0.387329
H	-4.233563	-2.507941	-0.051342
H	-5.071434	-0.986895	-0.382414
H	-5.278317	-1.790239	1.171381
C	-2.333157	-2.769686	2.279381
H	-1.314859	-3.028712	2.581977
H	-2.612571	-3.438268	1.458804
H	-3.000608	-2.994983	3.123794
C	1.209245	-2.449645	-1.747169
H	0.964317	-3.289689	-1.091291
H	2.067022	-1.930803	-1.310192
H	1.533040	-2.861982	-2.713930
C	1.344916	0.614840	-2.593114
H	1.217190	1.684602	-2.409828
H	1.649014	0.487165	-3.641943
H	2.175478	0.276037	-1.967611
C	-1.665352	1.614147	-3.112151

TS_{7b}

SCF done: -1512.613387

C	-1.595296	1.128820	2.134224
C	-1.201593	-0.166161	2.571607
C	-2.168977	-1.112264	2.100121
C	-3.155857	-0.398958	1.365013
C	-2.776015	0.988267	1.338957
C	-1.867661	-1.994339	-1.663842
C	-0.459646	-1.877979	-1.909176
C	-0.203658	-0.572076	-2.417408
C	-1.444192	0.134584	-2.460840
C	-2.478596	-0.759201	-2.032171
Hf	-0.953005	-0.213907	0.014261
C	-0.961553	2.408067	2.601660
H	-1.258030	3.268012	1.998629
H	0.130346	2.357614	2.577511
H	-1.261802	2.608822	3.639872
C	-3.634803	2.119656	0.832548
H	-4.171136	1.856705	-0.084966
H	-3.044397	3.016614	0.623871
H	-4.392536	2.397858	1.578566
C	-0.060119	-0.449389	3.509132
H	0.276093	-1.486065	3.439454
H	-0.364042	-0.262236	4.549003
H	0.801258	0.193793	3.302088
C	-4.512190	-0.935707	0.997806
H	-4.474732	-1.956308	0.607096
H	-5.021179	-0.309738	0.263087
H	-5.149104	-0.961671	1.893616
C	-2.214674	-2.571581	2.466989
H	-1.214444	-3.012818	2.504351

H	-2.809339	-3.151475	1.754886	H	1.259372	3.942102	-2.314272
H	-2.672326	-2.707053	3.457227	C	-0.112714	-1.321189	-3.367847
C	0.520533	-3.019117	-1.869925	H	0.317710	-2.294847	-3.124662
H	0.299836	-3.722225	-1.062654	H	0.048755	-1.144740	-4.441274
H	1.546257	-2.667725	-1.733483	H	-1.191619	-1.374112	-3.206178
H	0.484681	-3.577702	-2.816253	C	3.468283	1.886597	-1.699616
C	1.115504	-0.062243	-2.925130	H	4.252299	1.228389	-1.316196
H	1.199479	1.021901	-2.808765	H	3.467892	2.801501	-1.104897
H	1.232613	-0.293598	-3.993121	H	3.764498	2.167301	-2.721304
H	1.956827	-0.519448	-2.395741	C	2.993144	-1.021123	-2.718265
C	-1.663801	1.494627	-3.069505	H	2.643952	-2.049887	-2.823014
H	-2.561133	1.980949	-2.671685	H	3.847290	-1.033191	-2.034210
H	-1.797808	1.414609	-4.157900	H	3.370494	-0.688033	-3.696277
H	-0.817834	2.164209	-2.891863	C	1.614948	-2.727380	2.386742
C	-2.562397	-3.284375	-1.315047	H	2.242509	-3.287807	1.691654
H	-3.588029	-3.122150	-0.972789	H	0.601419	-3.128311	2.296147
H	-2.034214	-3.838615	-0.531914	H	1.968736	-2.939974	3.405387
H	-2.616683	-3.944887	-2.192116	C	-0.381963	-0.572820	3.621649
C	-3.946437	-0.511348	-2.256992	H	-1.306301	-0.038970	3.364661
H	-4.272704	0.475107	-1.911054	H	-0.110539	-0.241251	4.633348
H	-4.572718	-1.261529	-1.771507	H	-0.608481	-1.640266	3.685960
H	-4.163911	-0.555564	-3.333418	C	0.659106	2.295030	2.898110
N	1.197497	-2.528636	1.274039	H	0.967012	3.161399	2.303712
N	2.273103	-2.130275	0.963345	H	1.005577	2.471495	3.926987
N	2.793848	-1.185240	0.279544	H	-0.434025	2.277472	2.915388
C	4.206395	-1.156642	0.226288	C	4.015959	-1.125173	1.012028
C	5.050266	-2.050327	0.908469	H	4.499022	-0.518658	0.240217
C	4.779524	-0.150568	-0.568147	H	3.895243	-2.135460	0.610455
C	6.433338	-1.932608	0.791583	H	4.723010	-1.195556	1.851031
H	4.614356	-2.830266	1.525709	C	3.457762	1.985728	1.509781
C	6.164704	-0.040370	-0.676316	H	3.021462	2.917749	1.137054
H	4.127517	0.538641	-1.096877	H	4.291577	1.719999	0.859522
C	7.001685	-0.929302	0.001466	H	3.880985	2.207991	2.499760
H	7.072715	-2.631488	1.325293	N	1.674466	-3.095067	-0.842452
H	6.589887	0.745092	-1.295790	N	0.425969	-3.165855	-0.688384
H	8.081135	-0.842617	-0.083601	N	-0.260306	-2.106539	-0.211312
H	0.193601	-1.651285	0.688526	C	-1.649109	-2.459588	-0.105164
N	0.575026	1.187228	-0.064353	C	-2.326135	-3.069854	-1.175569
H	1.416248	0.593310	-0.103906	C	-2.354071	-2.260653	1.089923
C	0.919955	2.531221	-0.121084	C	-3.669633	-3.424009	-1.062084
C	-0.039097	3.519344	-0.436623	H	-1.783258	-3.281434	-2.088313
C	2.245335	2.965721	0.111965	C	-3.702897	-2.606355	1.200010
C	0.306268	4.867969	-0.498183	H	-1.833022	-1.869129	1.954506
H	-1.060081	3.210438	-0.643736	C	-4.373048	-3.183292	0.120853
C	2.582358	4.314960	0.040364	H	-4.169586	-3.891826	-1.906596
H	3.005453	2.229390	0.362559	H	-4.221537	-2.441512	2.141331
C	1.619126	5.282245	-0.261306	H	-5.421212	-3.456496	0.204910
H	-0.459057	5.601019	-0.743896	H	2.025457	-2.154768	-0.550528
H	3.611417	4.613223	0.227515	N	-1.260457	0.777087	0.576882
H	1.886980	6.333373	-0.315614	H	-1.569860	0.101451	1.277893

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SCF done: -1512.646823

C	-0.126191	1.027445	-2.258802
C	0.512026	-0.208934	-2.574325
C	1.900724	-0.090356	-2.257614
C	2.119578	1.223130	-1.750909
C	0.867453	1.913103	-1.729329
C	2.709813	-0.530153	1.474886
C	1.660736	-1.245921	2.128179
C	0.745733	-0.293493	2.665802
C	1.230103	1.011639	2.363050
C	2.449651	0.874804	1.642013
Hf	0.582984	0.027844	0.024505
C	-1.533794	1.371732	-2.662244
H	-1.883941	2.295528	-2.200647
H	-2.244823	0.585495	-2.392578
H	-1.583454	1.501703	-3.752476
C	0.733077	3.399959	-1.516138
H	1.164273	3.736684	-0.566090
H	-0.309849	3.718690	-1.536775

H	1.259372	3.942102	-2.314272
C	-0.112714	-1.321189	-3.367847
H	0.317710	-2.294847	-3.124662
H	0.048755	-1.144740	-4.441274
H	-1.191619	-1.374112	-3.206178
C	3.468283	1.886597	-1.699616
H	4.252299	1.228389	-1.316196
H	3.467892	2.801501	-1.104897
H	3.764498	2.167301	-2.721304
C	2.993144	-1.021123	-2.718265
H	2.643952	-2.049887	-2.823014
H	3.847290	-1.033191	-2.034210
H	3.370494	-0.688033	-3.696277
C	1.614948	-2.727380	2.386742
H	2.242509	-3.287807	1.691654
H	0.601419	-3.128311	2.296147
H	1.968736	-2.939974	3.405387
C	-0.381963	-0.572820	3.621649
H	-1.306301	-0.038970	3.364661
H	-0.110539	-0.241251	4.633348
H	-0.608481	-1.640266	3.685960
C	0.659106	2.295030	2.898110
H	0.967012	3.161399	2.303712
H	1.005577	2.471495	3.926987
H	-0.434025	2.277472	2.915388
C	4.015959	-1.125173	1.012028
H	4.499022	-0.518658	0.240217
H	3.895243	-2.135460	0.610455
H	4.723010	-1.195556	1.851031
C	3.457762	1.985728	1.509781
H	3.021462	2.917749	1.137054
H	4.291577	1.719999	0.859522
H	3.880985	2.207991	2.499760
N	1.674466	-3.095067	-0.842452
N	0.425969	-3.165855	-0.688384
N	-0.260306	-2.106539	-0.211312
C	-1.649109	-2.459588	-0.105164
C	-2.326135	-3.069854	-1.175569
C	-2.354071	-2.260653	1.089923
C	-3.669633	-3.424009	-1.062084
H	-1.783258	-3.281434	-2.088313
C	-3.702897	-2.606355	1.200010
H	-1.833022	-1.869129	1.954506
C	-4.373048	-3.183292	0.120853
H	-4.169586	-3.891826	-1.906596
H	-4.221537	-2.441512	2.141331
H	-5.421212	-3.456496	0.204910
H	2.025457	-2.154768	-0.550528
N	-1.260457	0.777087	0.576882
H	-1.569860	0.101451	1.277893
C	-2.309136	1.709915	0.418755
C	-2.062806	3.093206	0.441427
C	-3.643952	1.276906	0.286664
C	-3.105430	4.010742	0.294739
H	-1.049126	3.440500	0.603258
C	-4.681678	2.197468	0.155977
H	-3.853477	0.210859	0.275141
C	-4.421570	3.571175	0.147843
H	-2.885634	5.075648	0.315823
H	-5.702086	1.836917	0.050499
H	-5.233041	4.285505	0.041011

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SCF done: -1512.624943

C	-0.712290	0.529441	2.482142
C	-0.431648	-0.866795	2.523021
C	-1.612881	-1.561685	2.103461
C	-2.574207	-0.604670	1.702557
C	-2.007814	0.706341	1.913126
C	-1.944954	-1.016060	-2.172449
C	-0.614952	-0.668612	-2.597136

C	-0.459031	0.737303	-2.438884	H	2.430788	6.230043	0.437071
C	-1.656200	1.253432	-1.857287				
C	-2.583016	0.162931	-1.723549				
Hf	-0.579788	-0.284970	-0.024872	TS₈₉			
C	0.147516	1.582616	3.116486	SCF done:	-1512.591623		
H	-0.089526	2.587919	2.765303	C	-0.290049	-1.212653	-2.377814
H	1.210048	1.415529	2.923201	C	-0.805277	0.096739	-2.605470
H	0.000938	1.564369	4.206290	C	-2.125073	0.155003	-2.050036
C	-2.789846	1.994847	1.903083	C	-2.419790	-1.115567	-1.486013
H	-3.507668	2.043247	1.078533	C	-1.273504	-1.960668	-1.662987
H	-2.137419	2.868561	1.826264	C	-2.265485	0.182352	1.964351
H	-3.365490	2.103479	2.833670	C	-1.078965	0.826410	2.445797
C	0.790180	-1.493535	3.139928	C	-0.066436	-0.156225	2.608648
H	0.973526	-2.498606	2.747852	C	-0.631371	-1.424075	2.272030
H	0.682883	-1.582329	4.230561	C	-1.999451	-1.219351	1.917492
H	1.689699	-0.900412	2.948592	Hf	-0.509755	-0.054269	0.000132
C	-4.029913	-0.924917	1.484394	C	0.992891	-1.727710	-2.968108
H	-4.187030	-1.737145	0.765505	H	1.270565	-2.704226	-2.568831
H	-4.596499	-0.059768	1.137070	H	1.833379	-1.056577	-2.769801
H	-4.487487	-1.247492	2.430824	H	0.892335	-1.826318	-4.057778
C	-1.880927	-3.028754	2.287098	C	-1.255534	-3.448199	-1.414912
H	-0.967881	-3.627644	2.232325	H	-1.473307	-3.718565	-0.375734
H	-2.590900	-3.418352	1.548924	H	-0.286832	-3.884324	-1.669118
H	-2.326942	-3.204770	3.276849	C	-2.008670	-3.949645	-2.038136
C	0.333164	-1.590910	-3.314342	H	-0.181596	1.107558	-3.529596
H	0.354533	-2.588588	-2.866404	H	-0.279934	2.130422	-3.166606
H	1.356720	-1.208136	-3.306403	H	-0.657868	1.056517	-4.519592
H	0.032755	-1.707586	-4.365253	H	0.882076	0.902658	-3.679887
C	0.694366	1.551390	-2.950842	C	-3.817797	-1.579422	-1.179179
H	0.856175	2.454940	-2.360603	H	-4.372666	-0.883078	-0.543309
H	0.507870	1.855063	-3.991070	H	-3.836833	-2.562146	-0.705700
H	1.627687	0.981903	-2.943148	C	-3.154634	1.229469	-2.286494
C	-2.071928	2.702503	-1.832094	H	-2.718427	2.106632	-2.767084
H	-2.623022	2.974912	-0.926010	H	-3.647122	1.565498	-1.366150
H	-2.737610	2.910307	-2.682850	H	-3.946799	0.848825	-2.947205
H	-1.215389	3.373628	-1.913150	C	-1.041273	2.227073	2.976057
C	-2.610980	-2.350016	-2.374445	H	-1.507277	2.953248	2.299909
H	-3.277216	-2.616360	-1.545359	H	-0.021773	2.559288	3.181081
H	-1.878390	-3.153108	-2.488448	H	-1.600213	2.280252	3.921243
H	-3.224938	-2.340252	-3.286119	C	1.311415	0.071648	3.165100
C	-4.064166	0.339231	-1.533327	H	2.031037	-0.639957	2.752041
H	-4.309694	1.090694	-0.778028	H	1.318767	-0.043398	4.258224
H	-4.565590	-0.591907	-1.260968	H	1.679766	1.077286	2.937509
H	-4.512638	0.683320	-2.477215	C	-0.011348	-2.764374	2.563976
N	-0.480056	-2.562591	-0.229454	H	-0.385494	-3.551356	1.901056
N	0.784852	-2.822067	-0.245932	H	-0.250047	-3.074261	3.592519
N	1.411207	-1.676337	-0.243206	H	1.075992	-2.746245	2.468879
C	2.821379	-1.766340	-0.201967	C	-3.605297	0.861287	1.846099
C	3.479437	-2.792266	0.501578	H	-4.334716	0.246550	1.312034
C	3.592413	-0.799691	-0.869637	H	-3.539107	1.821400	1.320483
C	4.870682	-2.848323	0.523709	H	-4.029299	1.073963	2.838417
H	2.888862	-3.538526	1.021530	C	-3.023305	-2.320483	1.879814
C	4.986603	-0.856638	-0.829180	H	-2.732714	-3.163682	1.246323
H	3.093065	-0.019886	-1.434634	H	-4.000636	-1.969236	1.545603
C	5.633889	-1.879384	-0.134716	H	-3.153993	-2.721779	2.895038
H	5.363140	-3.649032	1.069853	N	-1.569917	3.915151	-0.425567
H	5.565772	-0.102535	-1.355746	N	-1.154161	3.396922	-1.383130
H	6.718989	-1.922855	-0.105938	N	-0.039722	1.990499	-0.141362
H	-1.034319	-3.412093	-0.228602	C	1.183318	2.642434	-0.104536
N	1.052092	1.093266	0.180210	C	1.466527	3.640102	0.866637
H	1.894950	0.539358	0.294976	C	2.201033	2.394154	-1.068815
C	1.393564	2.432444	0.251595	C	2.677590	4.329816	0.876278
C	0.429375	3.466328	0.276570	H	0.724264	3.855934	1.626720
C	2.753544	2.833585	0.311166	C	3.396538	3.106326	-1.065552
C	0.800970	4.808967	0.338046	H	2.015369	1.654139	-1.838364
H	-0.620052	3.200365	0.263868	C	3.652473	4.074740	-0.089208
C	3.114838	4.175082	0.377297	H	2.854925	5.078913	1.644425
H	3.526287	2.067058	0.305174	H	4.138430	2.900220	-1.833553
C	2.145276	5.183396	0.386725	H	4.593077	4.617803	-0.082858
H	0.024299	5.571027	0.357177	H	-1.154535	3.349056	0.437061
H	4.170154	4.436184	0.421248	N	1.541269	-0.554619	-0.007333

H	2.015772	0.343797	0.090316	H	3.966717	-2.129276	-1.338312
C	2.494708	-1.561268	0.016271	C	4.626096	1.284422	0.350733
C	3.875509	-1.245932	0.063659	H	2.493411	1.439199	0.565777
C	2.154222	-2.932132	-0.006352	C	5.706167	0.528451	-0.107899
C	4.847123	-2.241798	0.080230	H	6.273616	-1.309153	-1.089381
H	4.173337	-0.199036	0.080201	H	4.800749	2.248311	0.823557
C	3.134591	-3.922828	0.008877	H	6.724077	0.890310	0.003969
H	1.107630	-3.212960	-0.028426	H	1.782315	-1.671586	-1.230762
C	4.491257	-3.593631	0.051622	N	0.123411	1.591886	-0.501984
H	5.896179	-1.956269	0.115855	H	1.004559	1.579020	-1.015744
H	2.829961	-4.967254	-0.008635	C	-0.348362	2.895009	-0.430877
H	5.251337	-4.369251	0.065772	C	0.492897	3.993501	-0.731521

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SCF done:	-1403.230903		
C	0.110947	0.431444	2.432831
C	0.732344	-0.843321	2.348617
C	-0.294290	-1.827167	2.151594
C	-1.551460	-1.156234	2.169186
C	-1.302840	0.244209	2.287595
C	-1.937395	-2.167728	-1.113783
C	-0.697497	-2.335465	-1.793284
C	-0.446569	-1.145125	-2.553260
C	-1.508723	-0.235864	-2.312067
C	-2.420267	-0.848484	-1.395027
Hf	-0.245663	-0.433229	-0.030188
C	0.766785	1.733890	2.800882
H	0.456734	2.552986	2.145768
H	1.856400	1.663751	2.756039
H	0.501246	2.015278	3.829397
C	-2.359365	1.267042	2.618192
H	-3.269160	1.139866	2.020914
H	-2.003220	2.287645	2.465149
H	-2.657329	1.173881	3.673496
C	2.162587	-1.191619	2.653709
H	2.570293	-1.917225	1.943753
H	2.229908	-1.636693	3.656770
H	2.817481	-0.319322	2.632038
C	-2.898468	-1.783796	2.401533
H	-2.908864	-2.851116	2.175529
H	-3.700734	-1.305799	1.831610
H	-3.163977	-1.677541	3.463432
C	-0.048404	-3.312620	2.191741
H	0.780812	-3.609322	1.539340
H	-0.930140	-3.885252	1.892092
H	0.216879	-3.636393	3.208295
C	0.064532	-3.632206	-1.883258
H	-0.004127	-4.212442	-0.957471
H	1.128934	-3.484083	-2.098171
H	-0.329478	-4.263526	-2.692552
C	0.655141	-0.932077	-3.555696
H	1.074627	0.077582	-3.498945
H	0.277143	-1.073243	-4.577725
H	1.481625	-1.636872	-3.424074
C	-1.712373	1.070189	-3.025671
H	-2.316955	1.770131	-2.444369
H	-2.224100	0.903844	-3.984584
H	-0.762673	1.567975	-3.240046
C	-2.739045	-3.301971	-0.534831
H	-3.606006	-2.951610	0.026591
H	-2.153200	-3.954541	0.119183
H	-3.118578	-3.932695	-1.351723
C	-3.780827	-0.299405	-1.049052
H	-3.755203	0.779503	-0.863702
H	-4.207148	-0.777748	-0.163554
H	-4.487483	-0.463062	-1.875020
N	1.740248	-0.887201	-0.589158
C	3.040583	-0.415505	-0.399179
C	4.146441	-1.165903	-0.862745
C	3.314804	0.829605	0.208742
C	5.450203	-0.702171	-0.720151

H	3.966717	-2.129276	-1.338312
C	4.626096	1.284422	0.350733
H	2.493411	1.439199	0.565777
C	5.706167	0.528451	-0.107899
H	6.273616	-1.309153	-1.089381
H	4.800749	2.248311	0.823557
H	6.724077	0.890310	0.003969
H	1.782315	-1.671586	-1.230762
N	0.123411	1.591886	-0.501984
H	1.004559	1.579020	-1.015744
C	-0.348362	2.895009	-0.430877
C	0.492897	3.993501	-0.731521
C	-1.683345	3.188005	-0.076475
C	0.025253	5.302551	-0.664690
H	1.526304	3.800868	-1.014860
C	-2.141451	4.502731	-0.003417
H	-2.363540	2.367006	0.123607
C	-1.295367	5.574960	-0.294285
H	0.702765	6.119635	-0.902204
H	-3.177684	4.687695	0.271432
H	-1.657265	6.597612	-0.242143

TS_{12b}

SCF done:	-1226.159923		
C	-1.572738	2.439113	-0.504867
C	-0.146541	2.511480	-0.508039
C	0.321674	2.113710	0.784270
C	-0.812969	1.769610	1.578173
C	-1.988729	1.971015	0.778085
C	-0.586255	-2.152592	1.016854
C	-0.506703	-2.514599	-0.369995
C	-1.750121	-2.199293	-0.984038
C	-2.614487	-1.656681	0.016009
C	-1.903217	-1.649068	1.255115
Hf	-0.716472	0.036692	-0.302156
C	-2.478294	2.951146	-1.590950
H	-3.449185	2.448766	-1.578840
H	-2.044788	2.798997	-2.582722
H	-2.657880	4.028926	-1.464018
C	-3.415075	1.973144	1.262030
H	-3.550732	1.364293	2.159667
H	-4.110486	1.606475	0.500714
H	-3.729668	2.994726	1.518488
C	0.690655	3.070938	-1.628150
H	1.710887	2.677328	-1.616665
H	0.758828	4.165219	-1.552521
H	0.262073	2.834505	-2.606595
C	-0.762968	1.533861	3.064818
H	0.017828	0.820470	3.351350
H	-1.713868	1.164735	3.454668
H	-0.541959	2.474348	3.589427
C	1.725491	2.248346	1.309650
H	2.468815	2.229058	0.510067
H	1.983193	1.450249	2.012272
H	1.838911	3.204465	1.841253
C	0.600898	-3.281462	-1.043245
H	1.456028	-3.428416	-0.378333
H	0.958738	-2.794584	-1.956923
H	0.246264	-4.280296	-1.330458
C	-2.116648	-2.503075	-2.409806
H	-2.960531	-1.893420	-2.742513
H	-2.398044	-3.560360	-2.522157
H	-1.282372	-2.306623	-3.089927
C	-4.070256	-1.336316	-0.189692
H	-4.480461	-0.747110	0.634768
H	-4.665467	-2.257657	-0.256540
H	-4.230336	-0.773403	-1.115230
C	0.423687	-2.482457	2.084472
H	0.334739	-1.814848	2.947296
H	1.450987	-2.399861	1.721046
H	0.283741	-3.508404	2.454153

C	-2.513175	-1.447276	2.616244	H	-3.339224	-0.731587	2.603764
H	-3.339224	-0.731587	2.603764	H	-1.782976	-1.106066	3.353799
H	-1.782976	-1.106066	3.353799	H	-2.921411	-2.399229	2.984624
H	-2.921411	-2.399229	2.984624	H	-1.821588	0.281329	-1.727205
H	-1.821588	0.281329	-1.727205	N	0.564250	-0.113161	-2.280710
N	0.564250	-0.113161	-2.280710	N	1.551733	-0.064905	-1.608988
N	1.551733	-0.064905	-1.608988	N	2.800701	0.176346	-1.726820
N	2.800701	0.176346	-1.726820	C	3.705859	-0.093300	-0.699344
C	3.705859	-0.093300	-0.699344	C	3.636251	-1.205129	0.158331
C	3.636251	-1.205129	0.158331	C	4.801767	0.785101	-0.589577
C	4.801767	0.785101	-0.589577	C	4.616872	-1.399897	1.133433
C	4.616872	-1.399897	1.133433	H	2.842820	-1.928712	0.030489
H	2.842820	-1.928712	0.030489	C	5.779174	0.574439	0.376648
C	5.779174	0.574439	0.376648	H	4.860893	1.626864	-1.272835
H	4.860893	1.626864	-1.272835	C	5.687358	-0.513739	1.252217
C	5.687358	-0.513739	1.252217	H	4.550767	-2.265015	1.788452
H	4.550767	-2.265015	1.788452	H	6.615925	1.263912	0.451248
H	6.615925	1.263912	0.451248	H	6.451950	-0.675784	2.006660
H	6.451950	-0.675784	2.006660	H	1.247710	-0.235220	-0.061707
H	1.247710	-0.235220	-0.061707				

2b

SCF done: -1226.227920

C	-1.572738	2.439113	-0.504867
C	-0.146541	2.511480	-0.508039
C	0.321674	2.113710	0.784270
C	-0.812969	1.769610	1.578173
C	-1.988729	1.971015	0.778085
C	-0.586255	-2.152592	1.016854
C	-0.506703	-2.514599	-0.369995
C	-1.750121	-2.199293	-0.984038
C	-2.614487	-1.656681	0.016009
C	-1.903217	-1.649068	1.255115
Hf	-0.716472	0.036692	-0.302156
C	-2.478294	2.951146	-1.590950
H	-3.449185	2.448766	-1.578840
H	-2.044788	2.798997	-2.582722
H	-2.657880	4.028926	-1.464018
C	-3.415075	1.973144	1.262030
H	-3.550732	1.364293	2.159667
H	-4.110486	1.606475	0.500714
H	-3.729668	2.994726	1.518488
C	0.690655	3.070938	-1.628150
H	1.710887	2.677328	-1.616665
H	0.758828	4.165219	-1.552521
H	0.262073	2.834505	-2.606595
C	-0.762968	1.533861	3.064818
H	0.017828	0.820470	3.351350
H	-1.713868	1.164735	3.454668
H	-0.541959	2.474348	3.589427
C	1.725491	2.248346	1.309650
H	2.468815	2.229058	0.510067
H	1.983193	1.450249	2.012272
H	1.838911	3.204465	1.841253
C	0.600898	-3.281462	-1.043245
H	1.456028	-3.428416	-0.378333
H	0.958738	-2.794584	-1.956923
H	0.246264	-4.280296	-1.330458
C	-2.116648	-2.503075	-2.409806
H	-2.960531	-1.893420	-2.742513
H	-2.398044	-3.560360	-2.522157
H	-1.282372	-2.306623	-3.089927
C	-4.070256	-1.336316	-0.189692
H	-4.480461	-0.747110	0.634768
H	-4.665467	-2.257657	-0.256540
H	-4.230336	-0.773403	-1.115230
C	0.423687	-2.482457	2.084472
H	0.334739	-1.814848	2.947296
H	1.450987	-2.399861	1.721046
H	0.283741	-3.508404	2.454153
C	-2.513175	-1.447276	2.616244

TS_{12c}

SCF done: -1226.167465

C	2.053399	-2.142664	-0.794911
C	0.696050	-2.483801	-0.494743
C	0.443448	-2.135790	0.880684
C	1.661302	-1.613603	1.432581
C	2.649596	-1.595173	0.395350
C	0.037510	1.824451	1.236931
C	-0.421104	2.226015	-0.069684
C	0.729968	2.527182	-0.869359
C	1.897687	2.347633	-0.059859
C	1.471863	1.924268	1.243468
Hf	0.865491	0.043825	-0.369172
C	2.759793	-2.426784	-2.096602
H	3.623629	-1.769671	-2.223550
H	2.092048	-2.265563	-2.948051
H	3.106164	-3.469168	-2.122375
C	4.096476	-1.195131	0.542140
H	4.225161	-0.442181	1.326092
H	4.481020	-0.776008	-0.392791
H	4.713726	-2.064432	0.807007
C	-0.243709	-3.241107	-1.398298
H	-1.282297	-2.970002	-1.197496
H	-0.125701	-4.321263	-1.237646
H	-0.035271	-3.027442	-2.450118
C	1.900552	-1.396428	2.906094
H	1.075823	-0.856037	3.381665
H	2.823581	-0.842215	3.087032
H	1.990295	-2.370559	3.406382
C	-0.762949	-2.551713	1.684669
H	-1.657079	-2.572981	1.058440
H	-0.943975	-1.864852	2.518814
H	-0.607417	-3.554966	2.105061
C	-1.843082	2.519226	-0.473241
H	-2.562610	2.045966	0.196424
H	-2.053713	2.173589	-1.489561
H	-2.010264	3.604346	-0.444377
C	0.702322	3.001137	-2.299604
H	1.628355	2.729633	-2.814675
H	0.586152	4.092557	-2.345505
H	-0.126261	2.539543	-2.843665
C	3.313420	2.697552	-0.441077
H	4.032144	2.015457	0.023381
H	3.552804	3.718993	-0.113405
H	3.450305	2.641454	-1.523756
C	-0.838690	1.604513	2.447753
H	-0.391475	0.885778	3.142127
H	-1.825175	1.230545	2.159630
H	-0.982502	2.548487	2.991341
C	2.365277	1.890488	2.459179
H	3.306908	1.366785	2.265059

H	1.872831	1.408432	3.306066
H	2.613612	2.918523	2.757272
H	2.223457	0.301347	-1.565890
N	-0.553389	-0.178064	-1.901769
N	-1.768060	-0.413163	-1.917848
N	-2.214480	-0.655236	-0.551200
C	-3.544108	-0.418016	-0.163387
C	-4.541327	-0.080608	-1.101873
C	-3.905439	-0.534163	1.193150
C	-5.853812	0.123466	-0.686973
H	-4.269273	0.004308	-2.144469
C	-5.220406	-0.309159	1.595390
H	-3.152435	-0.807736	1.920901
C	-6.206210	0.017571	0.661739
H	-6.606720	0.374907	-1.425648
H	-5.475315	-0.399140	2.645438
H	-7.228531	0.184861	0.977735
H	-1.012783	-0.317588	0.006122

2c

SCF done:	-1226.256716		
C	1.623684	-2.365465	-1.010771
C	0.437281	-2.508073	-0.233234
C	0.739195	-2.120616	1.113621
C	2.120301	-1.761647	1.167260
C	2.663146	-1.896979	-0.151604
C	1.563284	1.875920	1.330419
C	0.359976	2.300972	0.690436
C	0.638808	2.502675	-0.696174
C	2.026741	2.234556	-0.910833
C	2.600751	1.852180	0.337206
Hf	0.929037	0.000055	-0.284561
C	1.789593	-2.790823	-2.443648
H	2.592016	-2.235974	-2.936861
H	0.876515	-2.624959	-3.022173
H	2.033770	-3.861608	-2.504339
C	4.110083	-1.763031	-0.546367
H	4.680017	-1.169091	0.173253
H	4.222008	-1.292776	-1.529685
H	4.591974	-2.749335	-0.604172
C	-0.852057	-3.112457	-0.718173
H	-1.705223	-2.805420	-0.107272
H	-0.801044	-4.209746	-0.683854
H	-1.071853	-2.824537	-1.750530
C	2.910658	-1.556201	2.432008
H	2.314862	-1.095073	3.224957
H	3.797638	-0.935686	2.275748
H	3.263050	-2.523998	2.816959
C	-0.181071	-2.241673	2.299813
H	-1.231359	-2.185417	1.999232
H	-0.005311	-1.452538	3.039673
H	-0.040970	-3.202944	2.814777
C	-0.928506	2.630160	1.394220
H	-1.100638	1.977786	2.257234
H	-1.791822	2.541900	0.729551
H	-0.909501	3.663297	1.770143
C	-0.325123	3.011430	-1.732421
H	-0.074587	2.631432	-2.727311
H	-0.310738	4.109439	-1.781399
H	-1.352498	2.702724	-1.518250
C	2.785470	2.476165	-2.187233
H	3.640752	1.800785	-2.285148
H	3.171347	3.505482	-2.221559
H	2.152058	2.325181	-3.064839
C	1.746509	1.762069	2.821445
H	2.664097	1.229947	3.082987
H	0.912086	1.240428	3.304618
H	1.808987	2.758706	3.281289
C	4.076011	1.691711	0.592583
H	4.587722	1.203476	-0.242483
H	4.281086	1.109811	1.495798

H	4.550682	2.673732	0.730365
H	1.345883	-0.000832	-2.068934
N	-1.079731	-0.022685	-0.512793
N	-2.280694	-0.037231	-0.783275
N	-3.133595	-0.072713	0.287792
C	-4.522430	-0.042057	0.138974
C	-5.130647	-0.034686	-1.127291
C	-5.322980	-0.024545	1.292347
C	-6.520190	-0.009571	-1.220808
H	-4.510915	-0.048145	-2.015740
C	-6.711606	-0.000313	1.179569
H	-4.854868	-0.030376	2.274284
C	-7.321825	0.007576	-0.076037
H	-6.980602	-0.003613	-2.205444
H	-7.316994	0.013052	2.082117
H	-8.404243	0.026696	-0.161862
H	-2.706265	-0.041045	1.213330

N2

SCF done:	-109.524128		
N	0.000000	0.000000	0.552965
N	0.000000	0.000000	-0.552965

PhN3

SCF done:	-395.838293		
N	-3.377243	0.531678	-0.000076
N	-2.417420	-0.086885	-0.000008
N	-1.471032	-0.884099	0.000230
C	-0.148793	-0.362371	-0.000256
C	0.153522	1.006127	0.000014
C	0.882586	-1.309242	-0.000028
C	1.485785	1.415904	0.000064
H	-0.644598	1.743705	0.000171
C	2.209249	-0.886440	0.000038
H	0.626274	-2.363859	-0.000003
C	2.518406	0.476110	-0.000076
H	1.714683	2.478163	0.000217
H	3.004880	-1.626311	0.000074
H	3.554090	0.802922	-0.000014