

Supporting Information For

Oxidation of Phenyl and Hydride Ligands of Bis(pentamethylcyclopentadienyl)hafnium Derivatives by Nitrous Oxide via Selective Oxygen Atom Transfer Reactions

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Table S1. The free energy barriers of different functionals for two steps (kcal/mol).

Functionals	1→TS ₂	5→TS ₆	ΔΔG [‡]
B3LYP	22.8	20.8	2.0
B2PLYP-D3	24.3	23.1	1.2
BLYP	26.2	21.4	4.8
M06	27.8	24.2	3.6
M062X	30.5	26.7	3.8
TPSS	29.2	26.9	2.3

Cartesian coordinates and electronic energies for all of the calculated structures

1				H	-2.259918	2.600003	1.416119
SCF done: -1061.411259				H	-2.472412	2.808268	-0.316319
C	-0.421862	2.451379	0.279802	H	-1.735905	4.103767	0.642334
C	0.260458	2.447296	-0.971339	C	0.247270	2.037674	2.772984
C	1.621431	2.076251	-0.735877	H	0.897373	1.334578	3.303460
C	1.778534	1.843427	0.661470	H	-0.788893	1.773652	3.008146
C	0.503780	2.032859	1.288020	H	0.430581	3.033319	3.201966
C	2.094685	-1.690538	0.116497	C	-0.321413	2.897015	-2.283673
C	1.365679	-2.150681	-1.018308	H	0.234321	2.483676	-3.129573
C	0.067455	-2.550986	-0.578012	H	-0.297006	3.992989	-2.367669
C	-0.003161	-2.353500	0.832127	H	-1.364814	2.584037	-2.391564
C	1.238722	-1.792970	1.265074	C	3.087468	1.722403	1.394345
C	-2.066020	-0.090281	0.001504	H	3.883876	1.325127	0.761106
C	-4.230731	-0.115863	1.178418	H	3.017528	1.091189	2.285083
C	-2.802271	-0.116757	-1.204857	H	3.413193	2.715751	1.734973
C	-4.923704	-0.138630	-0.034430	C	2.709363	2.066090	-1.775699
C	-4.202448	-0.138897	-1.228876	H	2.348144	1.668976	-2.729634
H	-2.275275	-0.122393	-2.158627	H	3.564884	1.457619	-1.467099
H	-4.728143	-0.158675	-2.181692	H	3.086273	3.081734	-1.961833
H	-6.010873	-0.156149	-0.047105	C	1.931457	-2.339752	-2.399231
C	-2.833314	-0.091155	1.185737	H	2.685248	-1.582720	-2.636047
H	-2.332844	-0.070644	2.154363	H	1.154508	-2.277199	-3.165412
H	-4.779952	-0.116274	2.118140	H	2.413876	-3.324026	-2.489333
Hf	0.191806	0.000501	-0.228602	C	-0.993998	-3.179337	-1.437666
H	0.243253	-0.008033	-2.067012	H	-1.997637	-2.976927	-1.054336
C	-1.795723	3.012818	0.517717	H	-0.865920	-4.270144	-1.483645

H	-0.953607	-2.801356	-2.464272	C	-3.353395	1.960389	-0.687555
C	-1.104931	-2.833510	1.734793	H	-3.906038	1.685733	0.212257
H	-1.173406	-2.241849	2.653036	H	-3.673106	1.300186	-1.497928
H	-0.919152	-3.875058	2.034307	H	-3.671388	2.976530	-0.961469
H	-2.081929	-2.794495	1.248009	C	-1.846587	2.319992	2.128516
C	3.579170	-1.434631	0.125367	H	-1.201775	1.962670	2.939558
H	3.910133	-0.953398	1.047957	H	-2.790992	1.772168	2.194876
H	3.907179	-0.812257	-0.714626	H	-2.070171	3.375343	2.342893
H	4.124037	-2.386013	0.046012	O	1.101543	-0.198788	1.654227
C	1.651299	-1.630997	2.705597	N	0.893590	-0.045668	3.026692
H	0.824325	-1.283898	3.334049	N	1.390786	-0.031236	4.045757
H	2.475225	-0.922088	2.823401				
H	1.990563	-2.589504	3.123775				

TS₂

SCF done: -1246.032309

C	-0.382261	-2.540762	0.323175
C	-0.818280	-2.376167	-1.022172
C	-2.042774	-1.637055	-1.007184
C	-2.391054	-1.388260	0.354643
C	-1.352399	-1.914479	1.174359
C	-1.863930	1.948619	-0.473176
C	-0.899407	2.063649	-1.512001
C	0.354278	2.419853	-0.918084
C	0.162304	2.511530	0.486112
C	-1.196844	2.164481	0.777931
C	2.307590	-0.290564	-0.209597
C	4.642487	0.451640	-0.028899
C	2.752089	-1.281224	-1.107645
C	5.047852	-0.512386	-0.949879
C	4.093027	-1.380634	-1.486492
H	2.042245	-1.953941	-1.570983
H	4.390284	-2.136068	-2.211374
H	6.092408	-0.595672	-1.239877
C	3.296536	0.542339	0.344853
H	3.024883	1.280147	1.090643
H	5.372426	1.125235	0.415593
Hf	-0.202548	-0.002879	-0.124245
H	0.284023	-0.201235	-1.863227
C	0.762655	-3.388236	0.811348
H	1.305157	-2.908148	1.631373
H	1.492135	-3.587701	0.023320
H	0.397562	-4.358508	1.176313
C	-1.424114	-2.046131	2.671161
H	-1.764832	-1.127619	3.163010
H	-0.457071	-2.318998	3.101665
H	-2.132359	-2.838538	2.954620
C	-0.261056	-3.037237	-2.253774
H	-0.126594	-2.327443	-3.075337
H	-0.946183	-3.824470	-2.599766
H	0.701887	-3.517769	-2.062893
C	-3.731546	-0.957112	0.885619
H	-4.358627	-0.503414	0.116517
H	-3.654218	-0.251192	1.719408
H	-4.272920	-1.834952	1.266717
C	-2.889339	-1.416152	-2.231603
H	-2.324123	-0.935580	-3.037887
H	-3.767619	-0.799741	-2.022635
H	-3.257213	-2.374509	-2.624829
C	-1.181238	2.049187	-2.989570
H	-2.059593	1.443526	-3.231551
H	-0.336325	1.643602	-3.552942
H	-1.375002	3.066621	-3.359733
C	1.587127	2.776239	-1.701386
H	2.487858	2.761736	-1.084287
H	1.490290	3.781026	-2.136903
H	1.749920	2.072008	-2.522949
C	1.124329	3.080780	1.492542
H	1.251246	2.447637	2.376621
H	0.756422	4.052412	1.850505
H	2.111594	3.251074	1.057875

3

SCF done: -1136.706094

C	-0.022855	2.521005	-0.122487
C	1.003566	2.333707	-1.091488
C	2.172069	1.859570	-0.414828
C	1.865372	1.756174	0.975159
C	0.495528	2.138078	1.153082
C	2.223863	-1.792413	0.118005
C	1.470614	-2.188255	-1.023718
C	0.145376	-2.513381	-0.588917
C	0.084073	-2.324036	0.819398
C	1.358619	-1.849645	1.262204
C	-2.929377	0.012498	-0.037582
C	-5.015685	0.095657	1.201774
C	-3.663725	-0.066719	-1.234840
C	-5.744381	0.017904	0.012726
C	-5.057183	-0.062776	-1.201940
H	-3.121882	-0.128472	-2.174010
H	-5.610695	-0.123547	-2.135965
H	-6.830404	0.019885	0.031796
C	-3.620802	0.093948	1.184578
H	-3.051541	0.150010	2.108052
H	-5.535158	0.158578	2.155060
Hf	0.370971	0.000987	-0.209830
H	0.427729	-0.010187	-2.036728
C	-1.382008	3.106471	-0.388507
H	-2.118119	2.784217	0.352176
H	-1.765524	2.817633	-1.371825
H	-1.342791	4.204474	-0.360663
C	-0.212172	2.288042	2.475085
H	0.137163	1.559012	3.214581
H	-1.294148	2.160705	2.372311
H	-0.042103	3.286341	2.903010
C	0.936704	2.737046	-2.539071
H	1.607701	2.133371	-3.156096
H	1.225380	3.791324	-2.661025
H	-0.072150	2.622286	-2.945364
C	2.854298	1.575138	2.095084
H	3.705802	0.951193	1.810860
H	2.397734	1.134148	2.985431
H	3.261051	2.551536	2.395290
C	3.523267	1.698485	-1.060200
H	3.473004	1.106953	-1.982032
H	4.239604	1.212663	-0.393023
H	3.943914	2.677070	-1.330588
C	2.019010	-2.398623	-2.408753
H	2.821982	-1.692006	-2.640590
H	1.245188	-2.273083	-3.170386
H	2.432837	-3.412012	-2.513472
C	-0.960723	-3.038277	-1.462916
H	-1.947383	-2.775044	-1.070882
H	-0.917287	-4.133895	-1.540203
H	-0.893460	-2.634556	-2.478027
C	-1.081304	-2.656060	1.710500
H	-1.069285	-2.066942	2.633560
H	-1.053388	-3.715165	2.003627
H	-2.040332	-2.476171	1.217807
C	3.719102	-1.618132	0.142908
H	4.054607	-0.993196	0.974741

H	4.098971	-1.174229	-0.781693
H	4.213749	-2.593447	0.257020
C	1.778122	-1.741700	2.705624
H	1.022538	-1.244884	3.324741
H	2.714422	-1.191111	2.821060
H	1.935359	-2.741042	3.135480
O	-1.589902	0.010538	-0.066442

TS₄

SCF done: -1246.032761

C	-0.368879	-1.891107	1.747035
C	0.290371	-2.471519	0.625816
C	-0.632046	-2.488879	-0.468725
C	-1.888388	-1.987221	0.009295
C	-1.719709	-1.596279	1.368847
C	-1.392283	0.860566	-2.083419
C	-0.052108	1.352705	-2.169181
C	0.154320	2.274265	-1.099413
C	-1.066944	2.374074	-0.363375
C	-2.021349	1.497796	-0.962763
C	2.020163	-0.199826	-0.306140
C	4.235086	0.249295	0.671026
C	2.698855	-0.813992	-1.380038
C	4.869499	-0.364378	-0.408962
C	4.092443	-0.896218	-1.440914
H	2.130315	-1.249232	-2.201214
H	4.571919	-1.376894	-2.291518
H	5.954309	-0.426488	-0.448576
C	2.837375	0.331135	0.717216
H	2.392153	0.846211	1.566487
H	4.825097	0.675114	1.479894
Hf	-0.212280	-0.020255	0.004561
H	-0.379327	0.875474	1.800326
C	0.212083	-1.793588	3.132246
H	-0.307326	-1.049070	3.738557
H	1.272955	-1.522942	3.108731
H	0.135307	-2.762184	3.646347
C	-2.808857	-1.134340	2.300346
H	-3.650805	-0.696168	1.755874
H	-2.448222	-0.390589	3.015356
H	-3.205104	-1.983200	2.875561
C	1.628091	-3.153846	0.671211
H	2.080147	-3.241465	-0.318564
H	1.510155	-4.168285	1.078718
H	2.340055	-2.619405	1.305615
C	-3.212063	-2.160737	-0.685165
H	-3.116960	-2.168331	-1.773059
H	-3.938917	-1.392337	-0.410726
H	-3.647927	-3.128089	-0.397230
C	-0.400394	-3.178766	-1.788587
H	0.633709	-3.070892	-2.130710
H	-1.054295	-2.792782	-2.576081
H	-0.600321	-4.256392	-1.704562
C	0.883577	1.109515	-3.320017
H	0.742714	0.118594	-3.764351
H	1.930867	1.193828	-3.022715
H	0.699642	1.847654	-4.113853
C	1.382786	3.109253	-0.865027
H	1.570006	3.255479	0.202948
H	1.265247	4.100894	-1.324353
H	2.273369	2.644368	-1.294753
C	-1.379976	3.405733	0.686350
H	-2.103147	3.042176	1.421248
H	-1.813983	4.296711	0.209769
H	-0.483098	3.720298	1.223737
C	-2.080950	0.093138	-3.182192
H	-3.054538	-0.288836	-2.869612
H	-1.488110	-0.752722	-3.545645
H	-2.254927	0.752003	-4.044337
C	-3.485970	1.482596	-0.610435
H	-3.655632	1.391407	0.468045

H	-4.020640	0.668725	-1.104998
H	-3.961626	2.420662	-0.928706
N	-0.620738	1.340895	3.061937
N	0.253514	2.119912	3.298646
O	1.242907	2.582896	2.718207

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SCF done: -1246.119134

C	-0.100863	-2.593092	-0.146224
C	0.151786	-2.067733	-1.450671
C	-1.023061	-1.395942	-1.899241
C	-2.022278	-1.536720	-0.876372
C	-1.449483	-2.280983	0.198779
C	-1.780178	1.941753	-0.645642
C	-0.473635	2.294913	-1.106065
C	0.339886	2.563180	0.040363
C	-0.452734	2.341821	1.201174
C	-1.756953	1.935527	0.784794
C	2.030741	0.037290	-0.235212
C	4.286383	-0.223058	0.730208
C	2.675903	0.349633	-1.451939
C	4.882103	0.094430	-0.489979
C	4.065979	0.381672	-1.586729
H	2.079841	0.572127	-2.336102
H	4.513022	0.628770	-2.547826
H	5.964798	0.116492	-0.587038
C	2.891043	-0.247771	0.849472
C	2.471959	-0.495535	1.821575
H	4.905425	-0.452711	1.595245
Hf	-0.219757	-0.006898	0.113410
H	0.824527	-0.148858	4.087419
C	0.855734	-3.478314	0.606705
H	0.534471	-3.636321	1.636987
H	1.864624	-3.051791	0.636241
H	0.931296	-4.459146	0.116587
C	-2.231586	-2.789607	1.379662
H	-2.894845	-2.023534	1.797016
H	-1.577713	-3.127797	2.183298
H	-2.866977	-3.632974	1.073069
C	1.347857	-2.411226	-2.292329
H	1.504429	-1.696750	-3.104722
H	1.200861	-3.400157	-2.750826
H	2.268238	-2.448440	-1.705576
C	-3.501828	-1.294576	-1.019410
H	-3.737882	-0.674985	-1.885870
H	-3.943578	-0.821370	-0.135683
H	-4.020673	-2.253809	-1.156414
C	-1.243998	-0.909552	-3.308111
H	-0.355489	-0.421655	-3.721893
H	-2.073640	-0.201947	-3.378171
H	-1.484031	-1.752292	-3.971729
C	-0.108328	2.606437	-2.534089
H	-0.627328	1.958208	-3.246963
H	0.965998	2.504228	-2.711715
H	-0.378322	3.642153	-2.786488
C	1.707322	3.186694	0.041382
H	2.332962	2.797146	0.849573
H	1.623077	4.274474	0.177166
H	2.243042	3.006897	-0.892852
C	-0.028110	2.630678	2.612817
H	-0.610492	2.052225	3.334108
H	-0.170980	3.695542	2.845026
H	1.029236	2.399032	2.774963
C	-3.020677	1.969364	-1.497075
H	-3.865850	1.466972	-1.023165
H	-2.872631	1.526324	-2.485504
H	-3.320665	3.014376	-1.662057
C	-2.928015	1.698820	1.701956
H	-2.633506	1.131237	2.591214
H	-3.729779	1.142569	1.205753
H	-3.360048	2.648139	2.048174

N	0.623444	-1.167754	4.008686	O	-0.133784	-0.241209	2.036523
N	0.099049	-1.401969	2.917505				
O	-0.080798	-0.276748	2.127374				
TS₆				TS₇			
SCF done: -1246.081259				SCF done: -1246.005291			
C	-0.064658	-2.600572	-0.081906	C	-1.676172	2.094470	0.148437
C	0.111703	-2.139111	-1.422496	C	-0.541183	2.508379	-0.618455
C	-1.101588	-1.525136	-1.846345	C	0.596247	2.495194	0.244695
C	-2.041601	-1.618219	-0.764275	C	0.181827	2.000892	1.517794
C	-1.400466	-2.298660	0.314757	C	-1.233069	1.772623	1.459530
C	-1.786796	1.930660	-0.731709	C	0.595278	-2.096487	1.308886
C	-0.477918	2.268339	-1.207215	C	0.490473	-2.547511	-0.042920
C	0.338363	2.568710	-0.075826	C	-0.874251	-2.463785	-0.430309
C	-0.454178	2.388931	1.094741	C	-1.621326	-1.933181	0.672106
C	-1.765085	1.981301	0.693820	C	-0.705967	-1.728766	1.754528
C	2.039740	0.019595	-0.255410	Hf	-0.161196	0.008495	-0.135353
C	4.307913	-0.191108	0.698246	H	0.034804	0.038616	-2.041937
C	2.674175	0.283658	-1.489667	C	-3.118209	2.195032	-0.264292
C	4.891125	0.078186	-0.539933	H	-3.710312	1.324791	0.041962
C	4.063265	0.315650	-1.639756	H	-3.225084	2.314979	-1.345060
H	2.069011	0.468015	-2.376800	H	-3.584798	3.074741	0.201720
H	4.500451	0.523926	-2.614701	C	-2.145147	1.602070	2.644040
H	5.972892	0.101334	-0.648227	H	-1.629977	1.181152	3.509393
C	2.913890	-0.217295	0.829586	H	-3.013344	0.971663	2.425784
H	2.495871	-0.429268	1.810525	H	-2.536928	2.583550	2.949446
H	4.937088	-0.381537	1.565890	C	-0.573566	3.082035	-2.010262
Hf	-0.221199	-0.008017	0.098834	H	0.389101	2.961779	-2.514930
H	0.312152	0.290955	3.526267	H	-0.802352	4.157233	-1.986278
C	0.948343	-3.406794	0.683482	H	-1.328956	2.595412	-2.633140
H	0.713431	-3.447302	1.749042	C	1.000967	1.990473	2.783137
H	1.955554	-2.989316	0.582198	H	2.072741	2.008999	2.572680
H	0.982420	-4.440314	0.310584	H	0.800634	1.110718	3.405138
C	-2.093928	-2.739183	1.574004	H	0.776220	2.873788	3.397771
H	-2.709127	-1.943416	2.007365	C	1.924503	3.111694	-0.092761
H	-1.382359	-3.056272	2.338385	H	2.237521	2.877650	-1.113735
H	-2.759457	-3.589399	1.366103	H	2.720262	2.769278	0.570811
C	1.278309	-2.482781	-2.304575	H	1.856252	4.205548	-0.003236
H	1.380669	-1.790995	-3.145614	C	1.585148	-3.180399	-0.854509
H	1.142087	-3.489547	-2.726336	H	2.568277	-2.785288	-0.589611
H	2.223808	-2.474852	-1.757774	H	1.444112	-3.009127	-1.925972
C	-3.529270	-1.391539	-0.838474	H	1.601230	-4.268171	-0.692819
H	-3.813388	-0.779091	-1.696257	C	-1.436034	-3.036030	-1.705048
H	-3.930717	-0.914924	0.062839	H	-2.492936	-2.789142	-1.833148
H	-4.049299	-2.354552	-0.943516	H	-1.363789	-4.132310	-1.688366
C	-1.398248	-1.108780	-3.263195	H	-0.901313	-2.685130	-2.592775
H	-0.559918	-0.576075	-3.725379	C	-3.123107	-1.865655	0.768300
H	-2.278174	-0.464247	-3.330139	H	-3.450726	-1.196305	1.569498
H	-1.598974	-1.989391	-3.890006	H	-3.548789	-2.856328	0.982175
C	-0.114051	2.509779	-2.648449	H	-3.589188	-1.516254	-0.158439
H	-0.618147	1.812971	-3.326130	C	1.789221	-2.277834	2.205330
H	0.962624	2.417939	-2.816441	H	1.844914	-1.515109	2.989599
H	-0.403308	3.524118	-2.960154	H	2.728239	-2.250970	1.649190
C	1.709891	3.183066	-0.094489	H	1.730567	-3.252669	2.711607
H	2.332379	2.815800	0.726632	C	-1.067834	-1.511952	3.199257
H	1.635520	4.275893	0.003385	H	-2.071910	-1.102259	3.321795
H	2.245547	2.965754	-1.020893	H	-0.367732	-0.848445	3.717555
C	-0.031580	2.747621	2.489156	H	-1.043579	-2.473520	3.731832
H	-0.686472	2.290542	3.237371	N	-3.005007	-0.182580	-2.190673
H	-0.078687	3.834781	2.643274	O	-1.658838	-0.049208	-1.904271
H	0.999021	2.438790	2.698265	N	-3.815248	-0.323407	-2.969107
C	-3.021207	1.894973	-1.591452	C	2.118028	0.031719	-0.561357
H	-3.865155	1.417384	-1.089558	C	3.075367	0.103299	0.476843
H	-2.860484	1.384278	-2.544664	C	2.666519	-0.026333	-1.863631
H	-3.330422	2.922651	-1.831555	C	4.455580	0.107820	0.250492
C	-2.933489	1.782455	1.622031	H	2.745830	0.160365	1.511457
H	-2.644507	1.211582	2.511012	C	4.044752	-0.019055	-2.110356
H	-3.751495	1.241476	1.136109	H	1.999168	-0.081184	-2.720120
H	-3.340500	2.744461	1.963883	C	4.951589	0.046035	-1.052932
N	0.551907	-0.587876	4.185863	H	5.142424	0.162563	1.093546
N	0.365347	-1.478945	3.466839	H	4.407208	-0.065861	-3.135694
				H	6.022990	0.050682	-1.238913

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SCF done: -1136.698535

C	-0.351307	2.457537	0.479706
C	0.315762	2.546650	-0.775356
C	1.662755	2.107197	-0.600671
C	1.829877	1.746728	0.770098
C	0.573019	1.930137	1.432747
C	1.954391	-1.881161	-0.211180
C	0.858374	-2.412521	-0.957706
C	-0.249846	-2.559350	-0.078482
C	0.166284	-2.145740	1.228690
C	1.531094	-1.750292	1.153619
C	-2.050391	-0.013291	-0.025577
C	-4.149748	-0.032935	1.273855
C	-2.860389	-0.030520	-1.184591
C	-4.913009	-0.045703	0.104350
C	-4.259090	-0.042058	-1.127879
H	-2.385183	-0.051305	-2.162585
H	-4.837183	-0.054563	-2.050145
H	-5.999206	-0.058380	0.154275
C	-2.753589	-0.012659	1.200160
H	-2.204793	0.010058	2.140917
H	-4.642152	-0.034755	2.244731
Hf	0.217511	0.000960	-0.286899
C	-1.706700	3.037314	0.769884
H	-2.159854	2.604529	1.664022
H	-2.406404	2.874861	-0.054594
H	-1.620159	4.121935	0.930094
C	0.336918	1.827947	2.917904
H	0.915770	1.019015	3.375108
H	-0.717323	1.648366	3.148423
H	0.624462	2.757721	3.429268
C	-0.280897	3.124755	-2.030497
H	0.308722	2.872952	-2.920187
H	-0.310151	4.221836	-1.983332
H	-1.310117	2.783643	-2.192573
C	3.160326	1.564098	1.449851
H	3.858478	0.954994	0.867941
H	3.062331	1.112312	2.438579
H	3.636794	2.544967	1.590811
C	2.753750	2.151032	-1.637661
H	2.381569	1.900991	-2.636569
H	3.559250	1.446488	-1.408155
H	3.203305	3.152289	-1.697214
C	0.899136	-2.830011	-2.399412
H	1.608191	-2.227515	-2.972854
H	-0.076894	-2.717180	-2.878256
H	1.200050	-3.883710	-2.488003
C	-1.563407	-3.201443	-0.429259
H	-2.363218	-2.884988	0.244396
H	-1.483803	-4.296338	-0.369626
H	-1.879208	-2.948293	-1.445733
C	-0.610577	-2.329853	2.504192
H	-0.370063	-1.563840	3.250296
H	-0.378716	-3.303947	2.959185
H	-1.689022	-2.297858	2.132239
C	3.358575	-1.726689	-0.735747
H	3.962196	-1.062716	-0.109969
H	3.372552	-1.326019	-1.755036
H	3.874941	-2.696730	-0.765071
C	2.424804	-1.568934	2.351260
H	1.981414	-0.932216	3.124294
H	3.395624	-1.147427	2.084362
H	2.615513	-2.545294	2.819502
O	0.141287	-0.038551	-2.267833
H	0.024481	0.783950	-2.762954

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SCF done: -1321.329943

C	-0.518779	-2.101491	1.489299
C	-0.082627	-2.547754	0.214730

C	-1.141502	-2.329325	-0.724707
C	-2.273407	-1.828045	0.007714
C	-1.880031	-1.653477	1.361638
C	-1.759810	1.126597	-1.857698
C	-0.374971	1.447494	-2.050428
C	0.039175	2.289071	-0.973931
C	-1.075201	2.464192	-0.100030
C	-2.187283	1.745341	-0.642614
C	2.875937	-0.209681	-0.278249
C	5.078562	0.096879	0.674524
C	3.466143	-0.663159	-1.469494
C	5.670888	-0.357842	-0.507346
C	4.855590	-0.734777	-1.576401
H	2.827757	-0.962506	-2.295854
H	5.300339	-1.090071	-2.502850
H	6.752168	-0.415380	-0.594025
C	3.692050	0.174783	0.798418
H	3.222156	0.547746	1.702582
H	5.701719	0.399221	1.512620
Hf	-0.402591	-0.016065	0.006156
H	-0.522128	0.683155	1.874783
C	0.259488	-2.214821	2.772393
H	-0.063184	-1.473359	3.507045
H	1.332654	-2.073838	2.608572
H	0.124442	-3.209924	3.219106
C	-2.791241	-1.265568	2.495958
H	-3.608491	-0.620330	2.157072
H	-2.256350	-0.733664	3.285903
H	-3.249357	-2.159000	2.943853
C	1.226868	-3.219122	-0.086157
H	1.537329	-3.067502	-1.123723
H	1.142733	-4.302825	0.076714
H	2.034090	-2.851107	0.551759
C	-3.696106	-1.792305	-0.480641
H	-3.762739	-1.749066	-1.569518
H	-4.264416	-0.953503	-0.070733
H	-4.213235	-2.709897	-0.166089
C	-1.141676	-2.827661	-2.147872
H	-0.206309	-2.592283	-2.667950
H	-1.959983	-2.398507	-2.731618
H	-1.259907	-3.919645	-2.179178
C	0.438256	1.095781	-3.268699
H	0.144094	0.129518	-3.693301
H	1.506707	1.047856	-3.042878
H	0.302513	1.848511	-4.058078
C	1.381129	2.948109	-0.814110
H	1.706158	2.948753	0.230334
H	1.339181	3.991989	-1.154601
H	2.153573	2.441533	-1.398124
C	-1.147477	3.432559	1.049307
H	-1.845928	3.101603	1.822612
H	-1.493338	4.412338	0.689249
H	-0.171209	3.576268	1.517356
C	-2.646000	0.537144	-2.922239
H	-3.594970	0.175728	-2.521975
H	-2.169402	-0.287770	-3.460487
H	-2.883957	1.307194	-3.669668
C	-3.596234	1.852534	-0.120499
H	-3.659375	1.659940	0.956766
H	-4.275389	1.160954	-0.624873
H	-3.988264	2.865746	-0.284752
N	-0.456869	1.048720	3.201327
N	0.567969	1.640867	3.339336
O	1.527506	1.998302	2.646780
O	1.534836	-0.147181	-0.163167

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SCF done: -1321.408642

C	0.728339	2.382370	1.063368
C	0.160838	2.573357	-0.221581
C	1.100174	2.113792	-1.198073

C	2.286955	1.700367	-0.502192	C	1.581575	2.170984	0.918338
C	2.041308	1.828640	0.894166	C	1.805293	-1.541923	-1.521802
C	1.394443	-1.520179	-1.764529	C	0.496995	-2.102455	-1.456789
C	0.038642	-1.925771	-1.592747	C	0.276444	-2.569912	-0.124289
C	-0.097782	-2.496052	-0.289067	C	1.460365	-2.314870	0.629956
C	1.181241	-2.451339	0.340916	C	2.395912	-1.653483	-0.218255
C	2.103431	-1.835401	-0.555099	C	-2.848789	-0.092066	-0.483704
C	-2.887158	0.214631	-0.265308	C	-4.924464	-0.023200	0.781240
C	-5.017992	-0.127608	0.837562	C	-3.603674	-0.110699	-1.672609
C	-3.569194	0.556689	-1.445554	C	-5.669155	-0.039349	-0.400784
C	-5.698301	0.214758	-0.334624	C	-4.996452	-0.083861	-1.625022
C	-4.964021	0.554640	-1.472976	H	-3.077855	-0.143234	-2.622589
H	-2.994902	0.821218	-2.328637	H	-5.560525	-0.097494	-2.554801
H	-5.478132	0.822333	-2.392993	H	-6.754736	-0.019513	-0.368754
H	-6.784251	0.215664	-0.360283	C	-3.530291	-0.048373	0.747784
C	-3.624473	-0.131688	0.880759	H	-2.950626	-0.043382	1.665381
H	-3.087745	-0.407324	1.783092	H	-5.432261	0.008495	1.742543
H	-5.576127	-0.397097	1.730914	Hf	0.388985	-0.001786	0.064239
Hf	0.382605	0.003176	0.078237	H	-0.560161	0.487028	3.334976
H	0.228637	-0.338460	4.300426	C	-0.732402	2.935142	1.872900
C	0.115703	2.790928	2.372176	H	-0.363032	2.619970	2.853837
H	0.417236	2.118191	3.178837	H	-1.742510	2.530929	1.744678
H	-0.977850	2.785971	2.327926	H	-0.819326	4.030018	1.904377
H	0.429453	3.807578	2.647491	C	2.349661	2.213079	2.209961
C	3.021174	1.579634	2.008822	H	3.325644	1.726820	2.118066
H	3.869228	0.971480	1.678157	H	1.806197	1.707617	3.014693
H	2.544303	1.059492	2.845915	H	2.531151	3.249009	2.528102
H	3.429511	2.523931	2.394688	C	-1.434865	2.876222	-1.225902
C	-1.158559	3.227196	-0.515672	H	-1.666751	2.298385	-2.124910
H	-1.576606	2.891083	-1.468041	H	-1.405613	3.937037	-1.512989
H	-1.040416	4.318318	-0.572997	H	-2.270653	2.744781	-0.534242
H	-1.902446	3.015407	0.257007	C	3.576778	1.867171	-0.720743
C	3.644428	1.523450	-1.126203	H	3.771410	1.305079	-1.637564
H	3.600741	1.091217	-2.128270	H	4.174344	1.421229	0.077957
H	4.307999	0.904371	-0.518800	H	3.962889	2.883864	-0.882717
H	4.126927	2.506283	-1.227003	C	1.184317	2.139542	-2.828494
C	0.961501	2.316859	-2.685205	H	0.297374	1.748045	-3.339305
H	-0.035546	2.043473	-3.049086	H	2.049408	1.575263	-3.184430
H	1.691102	1.730068	-3.248626	H	1.314382	3.177444	-3.167856
H	1.119692	3.371524	-2.951099	C	-0.447387	-2.284413	-2.612438
C	-1.026670	-1.888300	-2.654024	H	-0.311625	-1.514282	-3.379512
H	-0.875807	-1.061593	-3.356322	H	-1.490005	-2.244611	-2.286824
H	-2.025618	-1.776997	-2.225644	H	-0.287907	-3.257459	-3.098737
H	-1.020245	-2.817207	-3.241717	C	-0.948038	-3.310410	0.341425
C	-1.334534	-3.156526	0.258172	H	-1.025827	-3.317510	1.431697
H	-1.404057	-3.046741	1.342806	H	-0.927503	-4.355778	0.002965
H	-1.333223	-4.230414	0.024131	H	-1.864904	-2.857964	-0.048757
H	-2.244884	-2.728368	-0.170114	C	1.766654	-2.765835	2.029566
C	1.554802	-3.073175	1.657037	H	2.062654	-1.930240	2.672605
H	2.286635	-2.468503	2.203002	H	2.591692	-3.491610	2.023359
H	2.004495	-4.062919	1.493811	H	0.905458	-3.248614	2.495329
H	0.686714	-3.207392	2.305221	C	2.519553	-1.185768	-2.797576
C	2.003866	-1.153546	-3.091717	H	3.347995	-0.490704	-2.637510
H	2.975550	-0.667015	-2.986199	H	1.847797	-0.741957	-3.538381
H	1.360119	-0.494494	-3.682142	H	2.947052	-2.089559	-3.255154
H	2.164199	-2.061325	-3.690513	C	3.838193	-1.424242	0.150340
C	3.596295	-1.831861	-0.350166	H	3.947139	-0.902448	1.108424
H	3.890816	-1.400835	0.613758	H	4.371100	-0.846345	-0.607609
H	4.118135	-1.281474	-1.135649	H	4.363248	-2.384899	0.252268
H	3.981432	-2.860959	-0.366316	N	-1.015001	-0.348757	3.949849
N	-0.550253	-0.968298	4.011387	N	-0.736659	-1.264907	3.293489
N	-0.604770	-1.007134	2.777601	O	0.152976	-0.105272	2.013872
O	0.335150	-0.225404	2.141425	O	-1.512153	-0.121802	-0.537369
O	-1.543172	0.224861	-0.225442				

TS₁₀

SCF done: -1321.329943

C	0.191882	2.498441	0.772044
C	-0.127774	2.464661	-0.611590
C	1.044629	2.086118	-1.329837
C	2.112205	1.927402	-0.378586

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SCF done: -1136.698535

C	-0.250924	-2.592482	-0.095098
C	-1.244961	-2.291466	-1.065966
C	-2.340957	-1.654260	-0.407090
C	-2.035872	-1.602789	0.992141
C	-0.733831	-2.154246	1.178285

C	-2.013135	1.951842	0.293218	C	-0.772621	-2.517669	-0.847284
C	-1.265076	2.347083	-0.850391	C	-1.980443	-1.769501	-0.975944
C	0.098234	2.522414	-0.453733	C	2.318568	-0.245261	-0.132559
C	0.189239	2.251362	0.940956	C	4.130097	-1.407308	-1.304142
C	-1.104517	1.867283	1.405428	C	3.290609	0.637909	0.370568
C	2.855440	-0.248047	0.213853	C	5.066547	-0.485673	-0.828610
C	5.119027	-0.445708	1.076933	C	4.640025	0.539764	0.014544
C	3.386570	0.061301	-1.052635	H	3.001278	1.417466	1.065274
C	5.644658	-0.139382	-0.181141	H	5.357131	1.254750	0.412525
C	4.767939	0.111596	-1.239937	H	6.114960	-0.575870	-1.101865
H	2.700952	0.259519	-1.870878	C	2.783268	-1.298335	-0.946456
H	5.161711	0.351678	-2.225060	H	2.087747	-2.016659	-1.361350
H	6.719409	-0.097389	-0.333667	H	4.446463	-2.215914	-1.960134
C	3.740520	-0.501555	1.278338	Hf	-0.195040	-0.009264	-0.209152
H	3.327767	-0.737773	2.255277	C	1.522270	3.019147	-1.492418
H	5.787190	-0.643811	1.911874	H	1.600644	2.565929	-2.487409
Hf	-0.343635	-0.000572	-0.207054	H	2.447136	2.784250	-0.960551
C	1.041004	-3.324333	-0.329761	H	1.486348	4.106919	-1.645623
H	1.841390	-2.940350	0.307882	C	-1.270707	2.309106	-2.831084
H	1.382000	-3.235867	-1.366550	H	-2.065048	1.611958	-3.112432
H	0.928036	-4.396203	-0.115575	H	-0.403685	2.078612	-3.456636
C	-0.035919	-2.372999	2.493256	H	-1.605474	3.321032	-3.101300
H	-0.397393	-1.687351	3.266998	C	1.066075	3.043563	1.692999
H	1.043841	-2.224859	2.398837	H	1.268265	2.343917	2.509275
H	-0.199531	-3.394750	2.863933	H	0.641861	3.948325	2.150428
C	-1.224518	-2.677085	-2.518826	H	2.023682	3.329092	1.251175
H	-1.691694	-1.915596	-3.153000	C	-3.385417	1.965057	-0.561733
H	-1.775887	-3.613325	-2.680687	H	-3.942831	1.682266	0.331747
H	-0.206348	-2.850575	-2.887027	H	-3.693749	1.303299	-1.376793
C	-3.020744	-1.336423	2.098396	H	-3.710210	2.978740	-0.836297
H	-3.793369	-0.619750	1.811454	C	-1.867460	2.146657	2.289404
H	-2.539491	-0.967877	3.007817	H	-1.221781	1.714061	3.062052
H	-3.535228	-2.270718	2.365209	H	-2.816352	1.603726	2.313617
C	-3.666096	-1.350221	-1.056732	H	-2.081327	3.180522	2.598286
H	-3.550446	-0.820498	-2.009760	C	-1.596417	-1.834427	2.752931
H	-4.304995	-0.738913	-0.415018	H	-1.872613	-0.852137	3.153302
H	-4.216398	-2.277394	-1.271341	H	-0.698573	-2.169214	3.277748
C	-1.799380	2.633022	-2.225364	H	-2.402930	-2.527575	3.034099
H	-2.820854	2.260182	-2.351651	C	0.723794	-3.332802	1.132375
H	-1.174034	2.163831	-2.991028	H	1.598900	-3.377109	0.478987
H	-1.820126	3.714244	-2.419761	H	0.405391	-4.365827	1.331448
C	1.193693	3.022887	-1.354221	H	1.058344	-2.904777	2.080979
H	2.186297	2.802522	-0.952062	C	-0.113346	-3.243819	-1.984088
H	1.123028	4.111763	-1.486695	H	0.194469	-2.543334	-2.767531
H	1.127394	2.561167	-2.343924	H	-0.812387	-3.963837	-2.430778
C	1.398357	2.434575	1.814075	H	0.762545	-3.809559	-1.652573
H	1.434655	1.695185	2.620260	C	-3.787971	-0.978490	0.742902
H	1.386838	3.429965	2.280502	H	-4.362927	-0.557657	-0.083376
H	2.329731	2.343661	1.250594	H	-3.803630	-0.262217	1.570235
C	-3.516396	1.943947	0.374947	H	-4.331345	-1.869746	1.090050
H	-3.888370	1.333719	1.200953	C	-2.737289	-1.606802	-2.265345
H	-3.983422	1.581969	-0.545353	H	-2.071794	-1.274336	-3.068928
H	-3.887734	2.965087	0.542121	H	-3.551157	-0.880158	-2.175581
C	-1.472362	1.716898	2.859673	H	-3.188545	-2.558423	-2.580855
H	-0.791171	1.049259	3.400759	O	1.078956	-0.179224	1.652811
H	-2.486152	1.331335	2.988283	N	0.891559	-0.102586	3.038982
H	-1.430213	2.690395	3.368247	N	1.408436	-0.158394	4.046892
O	1.530089	-0.323027	0.418325	O	0.204431	-0.271658	-2.153858
O	0.010385	0.131678	-2.165691	H	0.856134	0.335084	-2.534298
H	0.170618	-0.679792	-2.666810				

TS₁₂

SCF done: -1321.279218

C	0.299269	2.539335	-0.757048
C	0.115108	2.505249	0.659375
C	-1.226436	2.113476	0.926871
C	-1.896696	1.966438	-0.336035
C	-0.951390	2.231583	-1.365024
C	-2.397479	-1.384036	0.335122
C	-1.410408	-1.831581	1.259208
C	-0.401406	-2.537360	0.526354

TS₁₃

SCF done: -1246.007211

C	0.145363	0.015738	-2.558764
C	0.002707	-1.362512	-2.228419
C	1.211843	-1.794319	-1.593669
C	2.129096	-0.688022	-1.604160
C	1.461897	0.431598	-2.178886
C	1.803638	-0.727997	1.938985
C	0.490236	-1.160174	2.308654
C	-0.317455	0.002820	2.511859
C	0.483236	1.148154	2.223084

C	1.794047	0.698237	1.867688	C	-4.223313	-0.779627	-0.152190
C	-1.969521	-0.643772	0.015273	C	-1.949383	-2.305425	-0.583939
C	-4.255094	0.240822	-0.216667	C	-4.362192	-2.124891	-0.494086
C	-2.556717	-1.900019	0.274628	C	-3.213223	-2.888262	-0.713801
C	-4.798820	-1.016274	0.049356	H	-1.083827	-2.937780	-0.777828
C	-3.941003	-2.091537	0.293913	H	-3.301903	-3.937574	-0.989651
H	-1.922164	-2.765885	0.462589	H	-5.348787	-2.571434	-0.592588
H	-4.350997	-3.078798	0.498386	C	-2.950123	-0.211105	-0.025392
H	-5.876758	-1.158344	0.063971	H	-2.880170	0.842954	0.232735
C	-2.866202	0.420887	-0.233302	H	-5.107654	-0.167407	0.015557
H	-2.480941	1.417874	-0.443205	Hf	0.239792	0.110965	0.031232
H	-4.911433	1.086441	-0.412897	H	-0.831791	1.986730	1.508491
Hf	0.221480	-0.090427	0.003480	C	-1.294532	2.198669	-2.441065
H	0.105622	1.811025	-0.270345	H	-1.364521	2.944666	-1.644483
C	-0.859397	0.862515	-3.290872	H	-2.227897	1.627768	-2.441723
H	-0.860582	1.888464	-2.913353	H	-1.229717	2.731275	-3.400357
H	-1.873118	0.467705	-3.178271	C	1.538124	3.137421	-1.384071
H	-0.631173	0.890189	-4.365825	H	2.471527	3.179959	-0.813181
C	2.076622	1.771028	-2.484572	H	0.754705	3.605089	-0.780328
H	2.934287	1.980186	-1.836963	H	1.680674	3.750804	-2.284914
H	1.352836	2.578347	-2.349279	C	-1.045651	-0.852207	-3.343468
H	2.437144	1.802752	-3.522679	H	-0.970291	-1.928661	-3.170726
C	-1.125304	-2.258343	-2.655919	H	-0.909903	-0.679623	-4.421073
H	-1.243584	-3.118700	-1.991775	H	-2.063803	-0.553691	-3.082631
H	-0.928152	-2.647138	-3.665332	C	3.541866	0.684734	-1.629040
H	-2.082401	-1.732905	-2.679579	H	4.006185	-0.298869	-1.539221
C	3.610571	-0.767052	-1.348721	H	3.859975	1.285708	-0.770703
H	3.878012	-1.617232	-0.718150	H	3.966998	1.160856	-2.523881
H	4.009333	0.138955	-0.882425	C	1.864690	-1.873952	-2.632659
H	4.143034	-0.894216	-2.301827	H	1.134352	-2.678098	-2.491848
C	1.545091	-3.228442	-1.267238	H	2.753816	-2.130441	-2.049370
H	0.695479	-3.760245	-0.825145	H	2.160307	-1.894943	-3.691480
H	2.384233	-3.308568	-0.570811	C	1.034908	-3.402298	1.025711
H	1.828221	-3.779043	-2.175514	H	1.498399	-3.553409	0.044302
C	0.109455	-2.576131	2.651117	H	0.021948	-3.809064	0.981686
H	0.593867	-3.304874	1.991838	H	1.599947	-4.015216	1.742961
H	-0.970235	-2.732422	2.584918	C	-1.214927	-1.920466	2.779135
H	0.412718	-2.821895	3.678909	H	-2.016516	-1.184034	2.890450
C	-1.695149	0.041559	3.112543	H	-1.030176	-2.363268	3.768412
H	-2.298248	0.853250	2.695773	H	-1.596283	-2.706392	2.124031
H	-1.628117	0.198642	4.198539	C	-0.111206	0.950046	3.538409
H	-2.244037	-0.886748	2.939941	H	0.236441	1.977140	3.379686
C	0.075327	2.578361	2.452966	H	0.118189	0.700561	4.583450
H	0.672520	3.270019	1.854511	H	-1.203757	0.939122	3.447139
H	0.207493	2.846096	3.511049	C	3.536239	-1.524235	0.900354
H	-0.973532	2.748677	2.196411	H	4.203221	-0.680817	0.713159
C	3.019605	-1.614948	1.949035	H	3.512945	-2.145163	-0.000213
H	3.878667	-1.149432	1.462282	H	3.999608	-2.132432	1.690829
H	2.841920	-2.583208	1.471158	C	2.786520	1.284397	2.280356
H	3.312725	-1.824335	2.987654	H	2.259873	2.244847	2.274700
C	2.973486	1.602610	1.625670	H	3.576764	1.342105	1.525831
H	2.718254	2.438697	0.965317	H	3.279965	1.189715	3.258081
H	3.814760	1.068268	1.175690	N	-3.139454	4.542053	1.113899
H	3.332670	2.035219	2.569686	O	-0.558219	1.835913	0.593626
N	-0.965529	4.396306	-0.703267	N	-2.590575	3.874124	1.801919
O	-0.581317	2.956775	-0.724190				
N	-0.871570	5.402407	-0.202986				

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SCF done: -1246.222570

C	-0.102661	1.306843	-2.235707
C	-0.014896	-0.077771	-2.571987
C	1.302759	-0.526989	-2.256967
C	2.044324	0.598634	-1.763571
C	1.168510	1.726040	-1.748856
C	2.166870	-1.086693	1.345013
C	1.040746	-1.956111	1.446647
C	0.046347	-1.302520	2.242164
C	0.550062	-0.020885	2.599135
C	1.853089	0.128712	2.029500
C	-1.762601	-0.950565	-0.230241

TS₁₅

SCF done: -1246.024921

C	-0.677585	-1.873158	1.777877
C	0.317889	-2.365554	0.887420
C	-0.261771	-2.449289	-0.416718
C	-1.631289	-2.051161	-0.316421
C	-1.889778	-1.680773	1.033615
C	-0.606603	1.064188	-2.150173
C	0.412315	1.894114	-1.596984
C	-0.145131	2.604270	-0.488714
C	-1.537002	2.287225	-0.420807
C	-1.823452	1.322915	-1.423548
C	2.057376	-0.109454	-0.124798
C	4.413936	0.135197	0.584161
C	2.571690	-0.712823	-1.296433

C	4.872501	-0.477085	-0.581282	H	-2.568929	-0.074834	1.927703
C	3.937173	-0.901289	-1.527625	H	-4.993438	-0.200074	1.672129
H	1.889099	-1.049183	-2.073631	H	-6.026882	-0.230885	-0.596586
H	4.270892	-1.375158	-2.449244	C	-2.728062	-0.065414	-1.455940
H	5.936953	-0.618169	-0.752557	H	-2.115639	-0.029504	-2.353934
C	3.040853	0.309402	0.800075	H	-4.554475	-0.134712	-2.603982
H	2.735747	0.786340	1.729517	Hf	0.180575	0.014448	-0.098416
H	5.123721	0.478801	1.334277	H	0.411378	-0.156235	-4.040165
Hf	-0.229121	0.110862	0.209790	C	0.778247	-3.128903	-1.819178
H	0.723927	0.918993	1.711590	H	1.694781	-2.895897	-2.365310
C	-0.541011	-1.793686	3.275896	H	-0.070652	-2.818762	-2.438319
H	-1.272459	-1.110363	3.714960	H	0.722075	-4.221568	-1.718386
H	0.456037	-1.461952	3.582677	C	3.282047	-1.826022	-0.298500
H	-0.706347	-2.781656	3.728497	H	3.886270	-1.110291	0.267684
C	-3.234956	-1.345256	1.619414	H	3.315687	-1.525382	-1.349724
H	-3.922285	-0.949528	0.864555	H	3.778763	-2.802946	-0.211924
H	-3.157296	-0.602292	2.417858	C	-1.661103	-3.188887	0.141735
H	-3.706895	-2.240955	2.047413	H	-2.469305	-2.817597	0.775056
C	1.662164	-2.892905	1.303525	H	-1.559855	-4.269343	0.319466
H	2.377372	-2.890335	0.478744	H	-1.979375	-3.052031	-0.896126
H	1.563688	-3.926527	1.665635	C	2.343157	-1.317962	2.724475
H	2.100541	-2.299901	2.111241	H	1.895024	-0.650652	3.465885
C	-2.664582	-2.321327	-1.375593	H	3.305506	-0.898503	2.426488
H	-2.309343	-2.083550	-2.382704	H	2.552655	-2.266375	3.240530
H	-3.593357	-1.773484	-1.205196	C	-0.717989	-1.939504	2.955115
H	-2.915981	-3.391914	-1.374483	H	-1.793965	-2.011470	2.779871
C	0.330489	-3.155891	-1.607743	H	-0.536643	-1.047627	3.564758
H	1.416951	-3.233104	-1.535566	H	-0.430383	-2.807787	3.565820
H	0.093540	-2.660671	-2.556049	C	-1.934937	2.914308	1.025218
H	-0.067817	-4.178808	-1.674320	H	-2.349965	2.424047	1.909099
C	1.750023	2.197568	-2.208476	H	-2.639936	2.756640	0.205397
H	2.095590	1.400515	-2.869143	H	-1.897445	3.993460	1.234329
H	2.523926	2.351359	-1.452381	C	-0.578922	3.085160	-1.826376
H	1.673844	3.117997	-2.806119	H	-0.071267	2.723797	-2.725378
C	0.575637	3.674834	0.288688	H	-0.563617	4.183601	-1.856974
H	0.080976	3.898034	1.238280	H	-1.624796	2.767788	-1.888477
H	0.616606	4.611999	-0.284325	C	2.538384	2.392018	-1.456502
H	1.606524	3.383886	0.513756	H	2.130449	2.406885	-2.470176
C	-2.569841	2.964691	0.435532	H	3.277986	1.586496	-1.413926
H	-2.130881	3.437898	1.317130	H	3.076390	3.339346	-1.307269
H	-3.338857	2.269670	0.785649	C	0.203721	1.877499	3.114614
H	-3.075697	3.751971	-0.141836	H	0.954835	1.255876	3.609017
C	-0.502663	0.307337	-3.449488	H	-0.781198	1.471980	3.369726
H	-1.225255	-0.511543	-3.512186	H	0.264408	2.875960	3.571022
H	0.493980	-0.118562	-3.599257	C	3.036031	1.743514	1.562622
H	-0.699372	0.972810	-4.302166	H	3.715948	1.105230	0.988192
C	-3.217221	0.942813	-1.848925	H	2.993178	1.358426	2.582648
H	-3.861033	0.680456	-1.002467	H	3.501943	2.738063	1.612639
H	-3.222716	0.105193	-2.548251	N	1.156413	-0.265541	-3.332893
H	-3.694172	1.791567	-2.359670	N	2.296145	-0.495568	-3.457655
N	-0.348028	1.412242	2.736986	O	0.377687	-0.020190	-2.078851
N	0.018163	1.960269	3.677360				
O	-1.357389	0.975825	2.093169				

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SCF done: -830.363807

C	-2.401323	-0.764936	-0.687403
C	-2.421311	0.660176	-0.767156
C	-2.040866	1.180142	0.510049
C	-1.804686	0.075698	1.384869
C	-2.003636	-1.127654	0.638234
C	1.853899	0.763827	1.109923
C	2.266414	1.136260	-0.205397
C	2.488543	-0.059371	-0.953164
C	2.239795	-1.174504	-0.096995
C	1.840307	-0.671249	1.177783
Hf	-0.000170	-0.003703	-0.442037
H	0.008292	1.404689	-1.637092
C	-2.878405	-1.711861	-1.755624
H	-2.411860	-2.695712	-1.659407
H	-2.650231	-1.340847	-2.759089
H	-3.967894	-1.848610	-1.693051
C	-1.957916	-2.533860	1.175196

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SCF done: -1246.090155

C	0.757801	-2.480909	-0.462488
C	-0.357527	-2.494339	0.421070
C	0.059342	-1.923391	1.665358
C	1.440023	-1.583350	1.550841
C	1.868450	-1.895874	0.221061
C	0.417134	1.957018	1.625114
C	-0.556996	2.418538	0.690407
C	0.079988	2.567962	-0.578258
C	1.455839	2.234513	-0.423677
C	1.671756	1.856501	0.935588
C	-2.098814	-0.051219	-0.189752
C	-4.118952	-0.127003	-1.606351
C	-2.974722	-0.098616	0.917479
C	-4.946457	-0.180496	-0.485004
C	-4.364155	-0.164491	0.784633

H	-1.354351	-2.605219	2.085328	C	-2.033964	-2.304554	-1.868240
H	-1.539819	-3.233415	0.443017	H	-1.434114	-3.178664	-1.598441
H	-2.965583	-2.893251	1.427544	H	-1.632377	-1.902501	-2.803961
C	-2.902265	1.464092	-1.944707	H	-3.053285	-2.661450	-2.072879
H	-2.475876	2.470570	-1.946201	C	-2.869313	0.748734	-2.220559
H	-3.997489	1.561210	-1.928437	H	-2.549740	1.793287	-2.280841
H	-2.627910	0.993657	-2.893709	H	-3.965847	0.730855	-2.299517
C	-1.621379	0.164740	2.876433	H	-2.460334	0.233109	-3.093027
H	-1.075260	1.063131	3.177389	C	-2.911157	2.099440	0.659939
H	-1.093640	-0.702244	3.283188	H	-2.430834	2.515375	1.549288
H	-2.600704	0.204426	3.374256	H	-3.994864	2.082826	0.843991
C	-2.027599	2.636933	0.889920	H	-2.736258	2.791068	-0.169852
H	-1.682120	3.265567	0.062781	C	-1.695881	-2.860489	1.256360
H	-1.376428	2.831032	1.748422	H	-1.259946	-2.810125	2.256836
H	-3.034287	2.982647	1.164553	H	-1.097283	-3.556425	0.661697
C	2.548268	2.539410	-0.669567	H	-2.692914	-3.310726	1.363596
H	1.881021	3.266885	-0.197018	C	-2.006903	-0.069928	2.801692
H	2.423425	2.638284	-1.750875	H	-1.621019	0.919322	3.068001
H	3.579466	2.830329	-0.421440	H	-1.384848	-0.814360	3.309053
C	2.961077	-0.128204	-2.379295	H	-3.018803	-0.153818	3.222877
H	2.613312	-1.040501	-2.873125	N	0.246507	3.502430	0.967638
H	4.058963	-0.118213	-2.433875	N	0.149087	3.425981	-0.183959
H	2.594790	0.721620	-2.963641	O	0.008479	2.597399	-1.090448
C	2.475298	-2.622314	-0.432201	H	-0.002399	0.240094	-2.006040
H	1.785612	-3.283233	0.102685				
H	3.496249	-2.924509	-0.157134				
H	2.346031	-2.812941	-1.500566				
C	1.712255	1.716664	2.269038				
H	1.183342	1.262717	3.111338				
H	1.176713	2.632375	1.994309				
H	2.700540	2.024486	2.638600				
C	1.682545	-1.505783	2.422649				
H	1.169932	-2.453471	2.225360				
H	1.122918	-0.981627	3.201942				
H	2.665536	-1.756296	2.845950				
H	0.005499	-1.426149	-1.620848				

TS₁₇
SCF done: -1014.991965

C	2.519672	0.504439	-0.225786
C	2.249407	-0.579154	-1.115684
C	1.751196	-1.670997	-0.339609
C	1.742785	-1.264935	1.039050
C	2.220187	0.076097	1.105172
C	-1.820868	-1.504148	0.615537
C	-2.035715	-1.267677	-0.777660
C	-2.417695	0.101160	-0.940174
C	-2.412647	0.714535	0.346846
C	-2.022174	-0.271955	1.309956
Hf	-0.000500	0.145346	-0.176266
H	0.094004	1.691712	1.068647
C	3.149844	1.813954	-0.617891
H	2.965807	2.591521	0.129079
H	2.770705	2.177414	-1.578078
H	4.239442	1.707577	-0.714337
C	2.508286	0.831404	2.374003
H	1.794279	0.583134	3.165346
H	2.463544	1.912819	2.224123
H	3.512238	0.584614	2.748749
C	2.603020	-0.623804	-2.577041
H	1.965724	-1.321731	-3.126580
H	3.645934	-0.947370	-2.709963
H	2.494903	0.356425	-3.048968
C	1.547683	-2.156334	2.237514
H	1.030229	-3.082980	1.981169
H	0.981597	-1.666768	3.037621
H	2.521577	-2.437320	2.662400
C	1.533238	-3.064379	-0.868389
H	1.029568	-3.061906	-1.840663
H	0.936550	-3.675382	-0.185852
H	2.493782	-3.581021	-1.004677

18
SCF done: -1015.078233

C	2.559385	0.024199	-0.270940
C	2.101910	-1.066073	-1.069383
C	1.430116	-1.990206	-0.213915
C	1.474714	-1.469822	1.120652
C	2.167726	-0.218771	1.082165
C	-2.103635	-1.286869	0.254192
C	-2.325595	-0.628769	-0.988055
C	-2.407162	0.779659	-0.733431
C	-2.246087	0.986042	0.665145
C	-2.017374	-0.283942	1.279713
Hf	0.009693	0.139574	-0.223779
H	0.514936	4.105489	-0.988267
C	3.431905	1.143389	-0.772605
H	3.517160	1.950202	-0.042947
H	3.048968	1.579410	-1.702013
H	4.444052	0.770785	-0.982550
C	2.542952	0.616083	2.278964
H	1.853755	0.457270	3.115034
H	2.537945	1.683396	2.044920
H	3.548228	0.351327	2.635904
C	2.441711	-1.293487	-2.516855
H	1.678986	-1.891019	-3.023663
H	3.399630	-1.826262	-2.607904
H	2.533454	-0.349908	-3.061489
C	1.119226	-2.219460	2.377220
H	0.324609	-2.952194	2.213731
H	0.797123	-1.553020	3.182450
H	1.993973	-2.772586	2.747543
C	0.990439	-3.368416	-0.633900
H	0.424415	-3.357367	-1.572453
H	0.371071	-3.852947	0.123800
H	1.865173	-4.013317	-0.797398
C	-2.594018	-1.300049	-2.307524
H	-2.052680	-2.246975	-2.400888
H	-2.292598	-0.668492	-3.147177
H	-3.664523	-1.523604	-2.421449
C	-2.698964	1.842304	-1.756649
H	-2.264866	2.804406	-1.468670
H	-3.781450	1.990439	-1.876191
H	-2.289898	1.577470	-2.736405
C	-2.368588	2.298675	1.386478
H	-1.818567	2.297094	2.332891
H	-3.420642	2.514271	1.619835
H	-1.984004	3.127314	0.786394

C	-2.235652	-2.768755	0.483014
H	-1.668266	-3.113127	1.352102
H	-1.910027	-3.352382	-0.382221
H	-3.288055	-3.027822	0.667462
C	-2.000536	-0.532247	2.766104
H	-1.413953	0.218217	3.307584
H	-1.589311	-1.513839	3.012910
H	-3.020250	-0.496775	3.174745
N	1.216902	4.129203	-0.219114
N	1.210220	3.051480	0.381699
O	0.291612	2.138940	-0.082905
H	0.010135	0.078014	-2.050698

TS₁₉

SCF done: -1015.038892			
C	2.507233	0.046766	-0.706339
C	1.991356	-1.244566	-1.051370
C	1.584427	-1.892214	0.149436
C	1.801419	-0.983680	1.237790
C	2.415397	0.194803	0.706617
C	-1.940506	-1.037545	1.039021
C	-2.039086	-1.437440	-0.335039
C	-2.363653	-0.285273	-1.109513
C	-2.484609	0.822351	-0.218394
C	-2.221584	0.361952	1.107631
Hf	0.000820	0.154912	-0.170337
H	-0.506639	3.503412	0.015361
C	3.137997	1.009242	-1.675614
H	3.165695	2.026261	-1.276539
H	2.584871	1.042338	-2.619501
H	4.171719	0.714385	-1.905702
C	2.967608	1.314962	1.544260
H	2.226914	1.709934	2.247701
H	3.307489	2.149696	0.928431
H	3.827711	0.962806	2.130847
C	2.025187	-1.859741	-2.424146
H	1.234231	-2.605142	-2.558929
H	2.983449	-2.367983	-2.605121
H	1.896480	-1.102914	-3.202782
C	1.699002	-1.302853	2.706736
H	1.000233	-2.120524	2.901592
H	1.370661	-0.437695	3.293808
H	2.675570	-1.609703	3.108593
C	1.238416	-3.351064	0.276971
H	0.747318	-3.742365	-0.618291
H	0.589884	-3.556996	1.133462
H	2.153789	-3.942548	0.423315
C	-2.032021	-2.846454	-0.866388
H	-1.599377	-3.553171	-0.154502
H	-1.474400	-2.935183	-1.806103
H	-3.057491	-3.184187	-1.073038
C	-2.712072	-0.279253	-2.572858
H	-2.492672	0.687274	-3.034685
H	-3.782572	-0.486490	-2.718818
H	-2.150228	-1.037429	-3.125710
C	-2.918550	2.205855	-0.609603
H	-2.719116	2.928875	0.187384
H	-3.998653	2.239143	-0.808112
H	-2.411406	2.551179	-1.517940
C	-1.847147	-1.959534	2.226449
H	-1.344600	-1.489899	3.077211
H	-1.309602	-2.882968	1.994164
H	-2.851422	-2.250292	2.566131
C	-2.326637	1.186799	2.361956
H	-1.906821	2.187555	2.221600
H	-1.791071	0.723701	3.196822
H	-3.374299	1.302622	2.673079
N	0.318283	4.247739	-0.205300
N	1.247500	3.561431	-0.100082
O	0.112918	2.047581	0.324844
H	0.018441	0.399168	-1.996150

20

SCF done: -905.656825			
C	2.518453	-0.681744	-0.494591
C	2.257147	-0.661657	0.905498
C	1.823333	0.654792	1.258484
C	1.838048	1.453274	0.066862
C	2.262520	0.625439	-1.013855
C	-1.771685	1.346834	0.615234
C	-1.954259	0.105764	1.311299
C	-2.434744	-0.853004	0.363370
C	-2.473931	-0.234933	-0.915984
C	-2.060928	1.129146	-0.760017
Hf	0.004471	-0.344502	-0.253218
H	-0.004423	-0.165687	-2.080579
C	3.030233	-1.864058	-1.269241
H	2.804187	-1.770975	-2.335821
H	2.572193	-2.792643	-0.916867
H	4.120414	-1.961636	-1.168445
C	2.561108	1.101851	-2.409399
H	1.893508	1.914263	-2.711964
H	2.449411	0.299146	-3.142819
C	3.592269	1.478353	-2.478178
H	2.475281	-1.814377	1.846859
H	1.955563	-1.666125	2.799191
H	3.543275	-1.936982	2.075318
C	2.114190	-2.751425	1.412813
C	1.678140	2.948947	-0.018725
H	1.205605	3.364357	0.874402
H	1.083225	3.258909	-0.885904
H	2.659251	3.434294	-0.118903
C	1.659020	1.159426	2.668525
H	1.193215	0.416889	3.324730
H	1.053026	2.068348	2.715275
H	2.637049	1.404679	3.106350
C	-1.922149	-0.089607	2.805160
H	-1.224842	0.596936	3.294106
H	-1.627380	-1.108810	3.078084
H	-2.913305	0.088043	3.246927
C	-2.897014	-2.244959	0.696645
H	-2.914096	-2.893992	-0.186840
H	-3.921835	-2.233456	1.091973
H	-2.264502	-2.720593	1.454581
C	-2.966077	-0.856025	-2.195105
H	-2.454655	-0.433107	-3.063847
H	-4.045218	-0.691424	-2.324629
H	-2.797931	-1.937852	-2.217922
C	-1.570846	2.688338	1.267573
H	-1.130209	3.419390	0.585011
H	-0.936593	2.633382	2.156611
H	-2.539675	3.094509	1.591876
C	-2.075684	2.170416	-1.846353
H	-1.774617	1.746749	-2.808921
H	-1.396033	3.000144	-1.626686
H	-3.080501	2.599220	-1.969587
O	0.085173	-2.323253	-0.193351
H	-0.709693	-2.865891	-0.284238

TS₂₁

SCF done: -1090.282650			
C	2.216544	1.350230	-0.201135
C	2.392736	0.245905	-1.079256
C	2.330784	-0.956031	-0.303081
C	2.159916	-0.579890	1.071902
C	2.071826	0.841569	1.132236
C	-0.999469	-2.230928	0.351534
C	-1.509943	-1.800516	-0.915894
C	-2.375038	-0.683952	-0.684550
C	-2.356282	-0.391667	0.709763
C	-1.492998	-1.339703	1.350498
Hf	0.005097	0.092183	-0.196873

22			
SCF done: -1090.360923			
C	2.542862	-0.012210	-0.557576
C	2.049670	-1.317418	-0.870037
C	1.529581	-1.896485	0.323490
C	1.693665	-0.939499	1.382847
C	2.340761	0.209615	0.836636
C	-1.888963	-1.020316	1.131009
C	-2.065581	-1.397028	-0.241520
C	-2.468714	-0.229754	-0.963853
C	-2.490607	0.866973	-0.063549
C	-2.115527	0.382673	1.232403
Hf	0.001361	0.128063	-0.246624
H	-0.001932	4.235393	0.789163
C	3.249404	0.893319	-1.528094
H	3.187299	1.939723	-1.222478
H	2.803502	0.818407	-2.524010
H	4.310800	0.620090	-1.611387
C	2.849823	1.366893	1.650146
H	2.125616	1.692005	2.405073
H	3.084128	2.230745	1.025568
C	3.768106	1.079030	2.181620
C	2.155455	-1.975678	-2.216999
H	1.536666	-2.876659	-2.279103

23		
SCF done:	-1090.318296	
C	2.540024	0.049480
C	2.027765	-1.238049
C	1.592781	-1.887620
C	1.807421	-0.987026
C	2.426231	0.189995
C	-1.885305	-1.093778
C	-2.010368	-1.499224
C	-2.424351	-0.363735
C	-2.520352	0.744740
C	-2.203702	0.293228
Hf	-0.003237	0.164199
H	-0.574633	3.351088
C	3.221846	1.012095
H	3.079168	2.053231
H	2.859130	0.909430
H	4.303990	0.825302
C	2.965038	1.304702
H	2.197934	1.713900
H	3.344729	2.129315
C	3.793524	0.941292
C	2.055156	-1.835572
H	1.364296	-2.679776
H	3.057855	-2.205932
H	1.769758	-1.106164
C	1.683906	-1.300678
H	1.049210	-2.170654
H	1.270741	-0.459331
C	2.670037	-1.522498
C	1.267506	-3.352185
H	0.779398	-3.748031
H	0.625198	-3.572218
H	2.193356	-3.928225
C	-1.996407	-2.914223

H	-1.535630	-3.605705	-0.071620
H	-1.461789	-3.008611	-1.732369
H	-3.022153	-3.268252	-0.954221
C	-2.770863	-0.332698	-2.477703
H	-2.150981	0.397248	-3.008452
H	-3.825796	-0.062118	-2.619755
H	-2.614556	-1.308136	-2.948292
C	-2.982152	2.118998	-0.524872
H	-2.784257	2.853174	0.262657
H	-4.065692	2.134326	-0.707976
H	-2.490975	2.458704	-1.443566
C	-1.765194	-2.015934	2.296483
H	-1.278432	-1.535564	3.149783
H	-1.204682	-2.925175	2.064429
H	-2.762576	-2.333735	2.632814
C	-2.324360	1.106440	2.448969
H	-1.934726	2.119745	2.314770
H	-1.770439	0.654931	3.277932
H	-3.374222	1.188284	2.763345
N	0.198005	4.133196	0.097860
N	1.138655	3.450554	0.109370
O	0.100266	1.948531	0.674143
O	-0.053341	0.769945	-2.091213
H	0.766534	1.060033	-2.514120

TS₂₄

SCF done: -980.937851

C	2.420544	-0.577637	0.814656
C	1.897848	0.672963	1.267268
C	1.747471	1.523223	0.122094
C	2.123455	0.774046	-1.030930
C	2.551451	-0.521014	-0.600182
C	-1.884421	1.313011	-0.597976
C	-1.768411	1.269420	0.831922
C	-2.153832	-0.032606	1.262089
C	-2.548192	-0.783978	0.110467
C	-2.394966	0.051554	-1.030732
Hf	0.001635	-0.400374	-0.123652
H	-0.654417	-1.619575	-2.323783
C	2.850183	-1.701746	1.716094
H	2.948145	-2.649361	1.173963
H	2.148059	-1.856166	2.543141
H	3.832867	-1.492980	2.160586
C	3.101491	-1.583283	-1.509455
H	2.430852	-1.747756	-2.358106
H	3.223309	-2.540226	-0.991634
H	4.087420	-1.294284	-1.898305
C	1.772048	1.071150	2.715359
H	1.211696	2.002090	2.835202
H	2.762107	1.231687	3.165566
H	1.269803	0.303161	3.315331
C	2.188922	1.270135	-2.449819
H	1.604213	2.185623	-2.589330
H	1.805757	0.517272	-3.146332
H	3.223712	1.499171	-2.741493
C	1.548938	3.015606	0.148477
H	1.043369	3.352392	1.055845
H	0.980609	3.382143	-0.711386
H	2.525959	3.518761	0.120955
C	-1.585382	2.453146	1.743988
H	-1.082651	3.286723	1.249658
H	-1.019230	2.205374	2.646695
H	-2.566356	2.822476	2.075206
C	-2.250741	-0.524439	2.680155
H	-1.837827	-1.534067	2.771997
H	-3.296389	-0.555771	3.017323
H	-1.706451	0.124819	3.373778
C	-3.091022	-2.185000	0.151936
H	-3.165562	-2.625093	-0.848074
H	-4.097628	-2.204101	0.591694
H	-2.442236	-2.830538	0.751550

C	-1.755114	2.525555	-1.483216
H	-1.226707	2.304486	-2.417908
H	-1.220569	3.339770	-0.987415
H	-2.745606	2.913360	-1.761206
C	-2.790267	-0.270407	-2.444929
H	-2.915550	-1.347884	-2.601096
H	-2.053232	0.091870	-3.169969
H	-3.752823	0.195173	-2.697216
O	0.122074	-1.169045	-1.964286
O	-0.117754	-2.086066	0.941864
H	0.653063	-2.668924	0.973472

TS₂₅

SCF done: -1014.982179

C	-2.020277	-0.864559	-1.194059
C	-2.530606	0.210549	-0.398731
C	-2.353307	-0.127316	0.972680
C	-1.723371	-1.412403	1.032811
C	-1.546740	-1.878526	-0.308871
C	2.177316	-0.366250	1.219277
C	2.417798	0.801471	0.430054
C	2.344968	0.433061	-0.944168
C	2.036573	-0.963429	-1.012266
C	1.962758	-1.460383	0.329822
Hf	-0.009754	0.167842	0.001278
H	-0.124590	0.991589	-1.733869
C	-2.146398	-0.993960	-2.688149
H	-1.334070	-1.590159	-3.116189
H	-2.129004	-0.016903	-3.179125
H	-3.090675	-1.487603	-2.960597
C	-1.196921	-3.280926	-0.730000
H	-0.670421	-3.830422	0.053358
H	-0.579873	-3.308113	-1.633607
H	-2.114761	-3.842478	-0.955144
C	-3.234334	1.428343	-0.931556
H	-3.225377	2.249957	-0.208663
H	-4.287133	1.205661	-1.154596
H	-2.770183	1.793524	-1.852784
C	-1.497582	-2.193340	2.300610
H	-1.062972	-1.570757	3.090431
H	-0.829722	-3.045284	2.144441
H	-2.444290	-2.594601	2.689174
C	-2.883257	0.639904	2.153610
H	-2.881566	1.719243	1.974974
H	-2.285497	0.458825	3.050449
H	-3.919801	0.344728	2.372866
C	2.781373	2.159144	0.964037
H	2.249256	2.380097	1.895004
H	2.542576	2.950595	0.246804
H	3.858335	2.226382	1.173392
C	2.676664	1.323506	-2.111110
H	2.244249	0.945968	-3.041697
H	3.765301	1.387996	-2.250500
H	2.300231	2.340337	-1.966405
C	2.023664	-1.781668	-2.276817
H	1.535558	-2.750025	-2.133367
H	3.046556	-1.986033	-2.623645
H	1.503261	-1.266352	-3.091451
C	2.301917	-0.456946	2.715388
H	1.674010	-1.252275	3.129580
H	2.005753	0.478698	3.197343
H	3.338873	-0.674298	3.010231
C	1.958466	-2.909132	0.741139
H	1.547720	-3.559993	-0.033800
H	1.394953	-3.083871	1.662958
H	2.987653	-3.246342	0.929855
N	-0.455801	3.485510	0.163787
H	-0.106522	1.007114	1.637278
O	-0.221238	2.307552	-0.588231
N	-0.823890	4.548333	0.223204

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SCF done: -1015.180507

C	0.779948	2.076436	-1.074046
C	2.001012	1.411655	-0.732388
C	2.082698	1.328940	0.684493
C	0.928891	1.980232	1.231555
C	0.145500	2.470404	0.149615
C	-1.879173	-1.278145	1.195480
C	-1.537798	-2.086977	0.065818
C	-1.865032	-1.360697	-1.114368
C	-2.390541	-0.089227	-0.722870
C	-2.413222	-0.049085	0.711363
Hf	0.079883	-0.121662	-0.012941
H	1.989662	-1.232056	-1.433987
C	0.374641	2.501183	-2.462032
H	-0.705032	2.660003	-2.541794
H	0.653693	1.755632	-3.214620
H	0.862556	3.444725	-2.746107
C	-0.984872	3.457257	0.262205
H	-1.513912	3.376099	1.214752
H	-1.718813	3.353858	-0.541689
H	-0.589420	4.481347	0.201082
C	3.052490	0.966503	-1.711076
H	3.690575	0.177300	-1.297047
H	3.718044	1.798970	-1.976974
H	2.615198	0.595846	-2.645012
C	0.679023	2.219524	2.696452
H	1.020685	1.375094	3.302593
H	-0.384166	2.368142	2.911698
H	1.208620	3.116447	3.048136
C	3.228970	0.766451	1.480228
H	3.725560	-0.057625	0.957930
H	2.890095	0.378627	2.444512
H	3.989436	1.536509	1.673715
C	-0.986407	-3.485008	0.107840
H	-0.459096	-3.678353	1.047067
H	-0.277419	-3.653165	-0.707844
H	-1.788885	-4.230892	0.018728
C	-1.737665	-1.878049	-2.520494
H	-1.738021	-1.065022	-3.254005
H	-2.575901	-2.543374	-2.770778
H	-0.808401	-2.439945	-2.650465
C	-3.062609	0.887952	-1.652658
H	-3.133334	1.889898	-1.220714
H	-4.088917	0.562975	-1.875225
H	-2.542647	0.976316	-2.612446
C	-1.853366	-1.710084	2.636525
H	-1.679895	-0.865971	3.310951
H	-1.063977	-2.442727	2.823157
H	-2.811559	-2.168362	2.922212
C	-3.100107	0.979315	1.571276
H	-3.290136	1.909396	1.030312
H	-2.524935	1.227163	2.470751
H	-4.073973	0.601913	1.914060
N	3.535452	-2.984563	-0.050358
H	0.688605	-0.797248	1.582778
O	1.061379	-1.366656	-1.200404
N	3.278669	-3.782590	0.669176

TS₂₇

SCF done: -1014.992995

C	2.528103	0.364362	-0.400935
C	2.183384	-0.854067	-1.060759
C	1.677087	-1.760008	-0.079066
C	1.719192	-1.100858	1.195875
C	2.253792	0.208716	0.993217
C	-1.866784	-1.427765	0.633625
C	-2.106903	-1.202216	-0.755412
C	-2.439387	0.180174	-0.927217
C	-2.386169	0.807369	0.348834
C	-2.001111	-0.177748	1.317417

Hf	-0.002344	0.145119	-0.215141
H	0.123265	1.783350	0.982546
C	3.183164	1.548142	-1.060414
H	3.136734	2.442327	-0.432249
H	2.709848	1.794421	-2.015964
H	4.244321	1.343444	-1.257548
C	2.621520	1.173662	2.089675
H	1.943466	1.095834	2.945222
H	2.603004	2.212973	1.750738
H	3.636581	0.966582	2.457482
C	2.484976	-1.190243	-2.495329
H	1.786390	-1.931366	-2.893069
H	3.499851	-1.604489	-2.587260
H	2.424118	-0.306789	-3.136098
C	1.514847	-1.737588	2.545661
H	0.931120	-2.658589	2.480456
H	1.008474	-1.070730	3.251892
H	2.483095	-2.001542	2.993923
C	1.411503	-3.221400	-0.331515
H	0.810704	-3.386108	-1.232570
H	0.896315	-3.697179	0.506238
H	2.357214	-3.762106	-0.475935
C	-2.166499	-2.253618	-1.830095
H	-1.554557	-3.126135	-1.581149
H	-1.810728	-1.864894	-2.788640
H	-3.195986	-2.610668	-1.973932
C	-2.853221	0.843823	-2.211557
H	-2.428240	1.848645	-2.301029
H	-3.946829	0.938484	-2.268737
H	-2.519408	0.270846	-3.080243
C	-2.809789	2.220686	0.644771
H	-2.311980	2.625135	1.530846
H	-3.892274	2.263708	0.829072
H	-2.597527	2.891757	-0.193069
C	-1.785175	-2.776555	1.296477
H	-1.229432	-2.750198	2.237211
H	-1.328829	-3.533008	0.652990
H	-2.797935	-3.131011	1.535805
C	-1.980159	0.027451	2.809184
H	-1.624035	1.027995	3.075871
H	-1.333650	-0.697602	3.312770
H	-2.986588	-0.085091	3.236704
N	0.472550	3.956158	0.504852
N	0.269845	2.905440	0.069402
O	0.106526	2.278437	-1.048922
H	-0.010909	-0.029179	-2.035133

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SCF done: -1015.042629

C	2.398556	-0.484973	-0.801057
C	1.596879	-1.663358	-0.966874
C	1.156577	-2.083849	0.319183
C	1.628092	-1.132400	1.282070
C	2.438378	-0.176851	0.585978
C	-2.116619	-0.578050	1.071918
C	-2.229853	-1.101048	-0.258741
C	-2.350173	0.000265	-1.156153
C	-2.332939	1.203315	-0.385221
C	-2.195007	0.847622	0.987010
Hf	0.013091	0.205500	-0.141952
H	1.057659	3.878693	0.908474
C	3.158054	0.212807	-1.896645
H	3.232743	1.287752	-1.716063
H	2.663751	0.081435	-2.863206
H	4.175962	-0.193614	-1.983743
C	3.299827	0.856362	1.258800
H	2.750003	1.432985	2.011572
H	3.720606	1.562218	0.539980
H	4.138838	0.369894	1.775858
C	1.402027	-2.405317	-2.261680
H	0.493980	-3.016598	-2.250764

H	2.245282	-3.082415	-2.459311
H	1.324390	-1.717165	-3.108186
C	1.548408	-1.267623	2.780837
H	0.669617	-1.838032	3.095323
H	1.504605	-0.291953	3.277604
H	2.431989	-1.789113	3.176778
C	0.561777	-3.426224	0.645911
H	-0.007443	-3.843575	-0.187668
H	-0.092183	-3.398990	1.521868
H	1.366989	-4.139535	0.873646
C	-2.469518	-2.536711	-0.645275
H	-2.221010	-3.228410	0.162356
H	-1.897822	-2.836675	-1.530861
H	-3.530653	-2.692103	-0.886491
C	-2.639046	-0.107116	-2.628693
H	-2.296677	0.777295	-3.172062
H	-3.719463	-0.213480	-2.805213
H	-2.145434	-0.974891	-3.076152
C	-2.495420	2.597781	-0.920877
H	-1.936663	3.319870	-0.318605
H	-3.550958	2.904141	-0.917627
H	-2.131474	2.677157	-1.950024
C	-2.196577	-1.364603	2.354107
H	-1.607395	-0.909773	3.156957
H	-1.848686	-2.393291	2.231545
H	-3.235563	-1.417791	2.709235
C	-2.219186	1.804210	2.147541
H	-1.666859	2.720452	1.918333
H	-1.774299	1.365185	3.046814
H	-3.249793	2.089332	2.401168
N	2.232135	3.366422	-0.627490
N	1.386064	3.240697	0.164818
O	0.387347	2.108854	0.345019
H	0.101777	0.428919	-1.955271

N₂

SCF done: -109.524129

N	0.000000	0.000000	0.552965
N	0.000000	0.000000	-0.552965

N₂O

SCF done: -184.660274

N	0.000000	0.000000	-0.072670
N	0.000000	0.000000	-1.207149
O	0.000000	0.000000	1.119842