

Supporting Information

Non-innocent PNN ligand Is Important for CO Oxidation by N₂O Catalyzed by (PNN)Ru–H Pincer Complex: Insights from DFT Calculations

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I. Cartesian coordinates and electronic energies for all of the calculated structures

1				H	0.458099	4.288567	-1.592787
SCF done: -1176.161559				H	-3.636422	3.212796	-0.835451
C	-0.059787	2.325176	0.024407	Ru	-0.275558	-0.475442	0.376552
C	-0.558438	3.670574	0.086501	H	-0.474459	-0.693131	-1.381418
C	-1.899230	3.922204	0.075179	P	1.925095	0.307772	-0.144784
C	-2.827370	2.861400	-0.003459	C	1.480482	1.888650	-0.840067
C	-2.324386	1.575641	-0.025392	H	2.240413	2.585441	-1.189891
N	-0.999240	1.315374	0.038224	C	0.244076	-2.286719	0.613588
H	-2.258489	4.948476	0.112131	O	0.625839	-3.366595	0.772721
H	0.163542	4.482740	0.123605	C	3.053695	0.666352	1.378216
H	-3.891911	3.060168	-0.057381	C	2.932320	-0.662608	-1.468294
Ru	-0.379870	-0.700694	-0.053217	C	3.146642	-0.556376	2.289657
H	-0.372329	-0.423931	-1.667743	H	3.804355	-0.325755	3.140079
P	1.781917	0.304544	-0.103360	H	2.171176	-0.837504	2.700743
C	1.289126	2.019357	-0.058327	H	3.562211	-1.433124	1.781354
H	2.023469	2.822323	-0.029470	C	4.457699	1.117127	0.978517
C	0.215818	-2.420367	-0.518582	H	4.431514	1.966542	0.284400
O	0.600388	-3.454868	-0.877186	H	4.989779	1.451621	1.880772
C	2.878975	-0.019263	1.451754	H	5.054938	0.315494	0.532105
C	2.848234	0.060439	-1.687710	C	3.673973	-1.850499	-0.859960
C	2.960315	-1.517733	1.744454	H	4.121559	-2.441964	-1.671330
H	3.592939	-1.681133	2.628915	H	4.489804	-1.552296	-0.191981
H	1.975821	-1.946605	1.961210	H	2.998831	-2.517641	-0.309030
H	3.399968	-2.087106	0.917135	C	1.945482	-1.192954	-2.505570
C	4.291773	0.553580	1.337705	H	2.513247	-1.635028	-3.336547
H	4.283196	1.621032	1.083108	H	1.297759	-1.972443	-2.090135
H	4.787548	0.457943	2.314767	H	1.310689	-0.397230	-2.912908
H	4.914763	0.023332	0.609612	C	2.411154	1.827983	2.136871
C	3.589179	-1.273860	-1.674138	H	2.470126	2.758233	1.562479
H	4.087072	-1.417136	-2.644003	H	1.356589	1.657574	2.371957
H	4.364753	-1.322358	-0.902276	H	2.944146	1.970874	3.087549
H	2.906146	-2.121082	-1.532061	C	3.905713	0.266807	-2.195435
C	1.912030	0.078478	-2.896302	H	4.683029	0.679378	-1.547113
H	2.522292	0.103514	-3.810597	H	4.410597	-0.304078	-2.987632
H	1.275040	-0.810231	-2.936623	H	3.374648	1.096933	-2.675245
H	1.261825	0.961633	-2.893942	N	-2.447900	-0.504938	0.414632
C	2.205505	0.697125	2.623053	C	-3.029294	0.678240	0.101141
H	2.262066	1.784789	2.508154	C	-4.417221	0.816983	0.171257
H	1.149157	0.437004	2.737112	H	-4.877893	1.770923	-0.064054
H	2.719919	0.417484	3.553508	C	-5.199113	-0.262617	0.543252
C	3.829009	1.221796	-1.868608	H	-6.279643	-0.159321	0.598965
H	4.587175	1.284418	-1.084513	C	-4.587629	-1.476515	0.840341
H	4.358102	1.090631	-2.823130	H	-5.162908	-2.351489	1.125472
H	3.296821	2.179131	-1.915988	C	-3.207842	-1.552059	0.764220
N	-2.543337	-0.809570	-0.232833	H	-2.676451	-2.476910	0.972958
C	-3.179874	0.383740	-0.151980	C	-0.249192	-0.151541	2.278930
C	-4.574502	0.439445	-0.211143	O	-0.336597	-0.040531	3.425435
H	-5.079513	1.397176	-0.136747	N	-1.639734	-2.122883	-2.292212
C	-5.307370	-0.724832	-0.359729	N	-1.312867	-1.006460	-2.465856
H	-6.392453	-0.683965	-0.406497	O	-1.550267	-3.058692	-1.521101
C	-4.638196	-1.941588	-0.447985				
H	-5.170294	-2.880139	-0.566979	2			
C	-3.256237	-1.933861	-0.376851	SCF done: -1360.732146			
H	-2.681717	-2.855198	-0.434954	C	-0.022293	2.319187	0.174436
C	-0.518354	-1.104642	1.893319	C	0.468323	3.667204	0.201180
O	-0.670220	-1.464886	2.978544	C	1.798607	3.931820	0.056879
				C	2.728266	2.881209	-0.108353
TS₁₋₂				C	2.240577	1.593975	-0.131727
SCF done: -1360.701309				N	0.915362	1.323757	-0.019451
C	0.157338	2.298126	-0.778457	H	2.150538	4.960716	0.075847
C	-0.288431	3.585958	-1.230672	H	-0.251370	4.469638	0.341368
C	-1.613660	3.908738	-1.229277	H	3.788133	3.088552	-0.204826
C	-2.579078	2.977478	-0.788511	Ru	0.291044	-0.678275	-0.240132
C	-2.126516	1.758621	-0.328394	H	0.725687	0.819663	2.106593
N	-0.808773	1.451789	-0.273754	P	-1.884643	0.307754	0.092985
H	-1.934287	4.885355	-1.585403	C	-1.357155	1.990555	0.358361

H	-2.088046	2.785303	0.498259	H	4.989779	1.451621	1.880772
C	-0.352928	-2.467796	-0.353832	H	5.054938	0.315494	0.532105
O	-0.767916	-3.541884	-0.403464	C	3.673973	-1.850499	-0.859960
C	-3.009961	0.306384	-1.485890	H	4.121559	-2.441964	-1.671330
C	-2.915571	-0.263932	1.610640	H	4.489804	-1.552296	-0.191981
C	-3.035352	-1.080731	-2.127747	H	2.998831	-2.517641	-0.309030
H	-3.743379	-1.077230	-2.968657	C	1.945482	-1.192954	-2.505570
H	-2.058859	-1.369309	-2.530987	H	2.513247	-1.635028	-3.336547
H	-3.356348	-1.863614	-1.430648	H	1.297759	-1.972443	-2.090135
C	-4.443365	0.750530	-1.196744	H	1.310689	-0.397230	-2.912908
H	-4.475900	1.723098	-0.690716	C	2.411154	1.827983	2.136871
H	-4.969045	0.867366	-2.155330	H	2.470126	2.758233	1.562479
H	-5.010180	0.024225	-0.605340	H	1.356589	1.657574	2.371957
C	-3.582857	-1.607998	1.331706	H	2.944146	1.970874	3.087549
H	-4.094845	-1.948051	2.242822	C	3.905713	0.266807	-2.195435
H	-4.335458	-1.559395	0.535836	H	4.683029	0.679378	-1.547113
H	-2.847226	-2.379145	1.068472	H	4.410597	-0.304078	-2.987632
C	-1.958489	-0.425278	2.788864	H	3.374648	1.096933	-2.675245
H	-2.546828	-0.692594	3.677676	N	-2.447900	-0.504938	0.414632
H	-1.213273	-1.206942	2.619165	C	-3.029294	0.678240	0.101141
H	-1.430587	0.509556	3.011319	C	-4.417221	0.816983	0.171257
C	-2.429991	1.330839	-2.462954	H	-4.877893	1.770923	-0.064054
H	-2.587319	2.351880	-2.099952	C	-5.199113	-0.262617	0.543252
H	-1.358445	1.217641	-2.644330	H	-6.279643	-0.159321	0.598965
H	-2.942107	1.224593	-3.429755	C	-4.587629	-1.476515	0.840341
C	-3.948500	0.791107	2.012974	H	-5.162908	-2.351489	1.125472
H	-4.770809	0.903814	1.304240	C	-3.207842	-1.552059	0.764220
H	-4.388159	0.490095	2.974116	H	-2.676451	-2.476910	0.972958
H	-3.477352	1.769508	2.166096	C	-0.249192	-0.151541	2.278930
N	2.472540	-0.789710	-0.312385	O	-0.336597	-0.040531	3.425435
C	3.102386	0.403654	-0.222920	N	-1.639734	-2.122883	-2.292212
C	4.496036	0.456101	-0.167112	N	-1.312867	-2.465856	-2.465856
H	4.998132	1.414062	-0.078358	O	-1.550267	-3.058692	-1.521101
C	5.227922	-0.718485	-0.191689				
H	6.313064	-0.683880	-0.144127	3			
C	4.561184	-1.937966	-0.256395	C	-0.022293	2.319187	0.174436
H	5.096711	-2.881800	-0.256736	C	0.468323	3.667204	0.201180
C	3.178245	-1.925126	-0.308798	C	1.798607	3.931820	0.056879
H	2.601311	-2.845781	-0.340471	C	2.728266	2.881209	-0.108353
C	0.263944	-0.474841	-2.109406	C	2.240577	1.593975	-0.131727
O	0.401135	-0.436012	-3.256810	N	0.915362	1.323757	-0.019451
N	1.376352	-0.802938	2.743665	H	2.150538	4.960716	0.075847
N	1.305474	0.427806	2.875658	H	-0.251370	4.469638	0.341368
O	0.765961	-1.411988	1.741300	H	3.788133	3.088552	-0.204826
				Ru	0.291044	-0.678275	-0.240132
				H	0.725687	0.819663	2.106593
				P	-1.884643	0.307754	0.092985
				C	-1.357155	1.990555	0.358361
				H	-2.088046	2.785303	0.498259
				C	-0.352928	-2.467796	-0.353832
				O	-0.767916	-3.541884	-0.403464
				C	-3.009961	0.306384	-1.485890
				C	-2.915571	-0.263932	1.610640
				C	-3.035352	-1.080731	-2.127747
				H	-3.743379	-1.077230	-2.968657
				H	-2.058859	-1.369309	-2.530987
				H	-3.356348	-1.863614	-1.430648
				C	-4.443365	0.750530	-1.196744
				H	-4.475900	1.723098	-0.690716
				H	-4.969045	0.867366	-2.155330
				H	-5.010180	0.024225	-0.605340
				C	-3.582857	-1.607998	1.331706
				H	-4.094845	-1.948051	2.242822
				H	-4.335458	-1.559395	0.535836
				H	-2.847226	-2.379145	1.068472
				C	-1.958489	-0.425278	2.788864
				H	-2.546828	-0.692594	3.677676
				H	-1.213273	-1.206942	2.619165
				H	-1.430587	0.509556	3.011319
				C	-2.429991	1.330839	-2.462954
				H	-2.587319	2.351880	-2.099952
TS₂₋₃							
SCF done:	-1360.701309						
C	0.157338	2.298126	-0.778457				
C	-0.288431	3.585958	-1.230672				
C	-1.613660	3.908738	-1.229277				
C	-2.579078	2.977478	-0.788511				
C	-2.126516	1.758621	-0.328394				
N	-0.808773	1.451789	-0.273754				
H	-1.934287	4.885355	-1.585403				
H	0.458099	4.288567	-1.592787				
H	-3.636422	3.212796	-0.835451				
Ru	-0.275558	-0.475442	0.376552				
H	-0.474459	-0.693131	-1.381418				
P	1.925095	0.307772	-0.144784				
C	1.480482	1.888650	-0.840067				
H	2.240413	2.585441	-1.189891				
C	0.244076	-2.286719	0.613588				
O	0.625839	-3.366595	0.772721				
C	3.053695	0.666352	1.378216				
C	2.932320	-0.662608	-1.468294				
C	3.146642	-0.556376	2.289657				
H	3.804355	-0.325755	3.140079				
H	2.171176	-0.837504	2.700743				
H	3.562211	-1.433124	1.781354				
C	4.457699	1.117127	0.978517				
H	4.431514	1.966542	0.284400				

H	-1.358445	1.217641	-2.644330	H	-6.281668	-0.473351	0.454528
H	-2.942107	1.224593	-3.429755	C	-4.554511	-1.769065	0.470236
C	-3.948500	0.791107	-2.012974	H	-5.106163	-2.696575	0.585291
H	-4.770809	0.903814	1.304240	C	-3.173884	-1.791865	0.395606
H	-4.388159	0.490095	2.974116	H	-2.618362	-2.724798	0.445986
H	-3.477352	1.769508	2.166096	C	-0.270085	-0.646795	2.171161
N	2.472540	-0.789710	-0.312385	O	-0.377419	-0.760395	3.316312
C	3.102386	0.403654	-0.222920	N	-1.422639	-1.505375	-2.815842
C	4.496036	0.456101	-0.167112	O	-1.139696	-0.290510	-2.721038
H	4.998132	1.414062	-0.078358	N	-1.267168	-2.472336	-2.186838
C	5.227922	-0.718485	-0.191689				
H	6.313064	-0.683880	-0.144127	TS₁₋₄			
C	4.561184	-1.937966	-0.256395	SCF done: -1360.657459			
H	5.096711	-2.881800	-0.256736	C	-0.126438	2.349846	-0.019429
C	3.178245	-1.925126	-0.308798	C	0.360517	3.712676	0.033913
H	2.601311	-2.845781	-0.340471	C	1.694473	3.993978	-0.054178
C	0.263944	-0.474841	-2.109406	C	2.645602	2.948364	-0.191609
O	0.401135	-0.436012	-3.256810	C	2.176495	1.650491	-0.260388
N	1.376352	-0.802938	2.743665	N	0.841539	1.353065	-0.222881
N	1.305474	0.427806	2.875658	H	2.037981	5.020848	-0.005535
O	0.765961	-1.411988	1.741300	H	-0.369948	4.501799	0.159120
				H	3.701936	3.168836	-0.220664
				Ru	0.324295	-0.651882	-1.280454
TS₁₋₃				H	0.652010	-0.591155	0.444990
SCF done: -1360.680295				P	-1.937332	0.261736	0.014580
C	0.097959	2.367740	-0.319428	C	-1.458178	2.020766	0.114625
C	-0.376991	3.709188	-0.505982	C	-2.202092	2.793363	0.256561
C	-1.711310	3.992184	-0.465470	H	-0.175683	-2.472123	0.062896
C	-2.655853	2.967611	-0.241862	O	-0.522027	-3.555326	0.350237
C	-2.175278	1.691591	-0.028953	C	-3.170850	0.125899	-1.524008
N	-0.850735	1.411835	-0.017278	C	-2.902061	-0.189332	1.674283
H	-2.053795	5.012910	-0.621128	C	-3.309993	-1.345682	-1.974764
H	0.355558	4.488683	-0.700549	H	-3.939380	-1.383331	-2.873751
H	-3.718676	3.181661	-0.258834	H	-2.335014	-1.774729	-2.224496
Ru	-0.267868	-0.599632	0.243273	H	-3.776888	-1.967598	-1.206260
H	-0.468961	-0.260575	-1.577049	C	-4.565422	0.715937	-1.212699
P	1.911851	0.329731	-0.074210	H	-4.490273	1.756806	-0.880304
C	1.431300	2.008144	-0.443519	H	-5.161948	0.698535	-2.134642
H	2.176834	2.778099	-0.634288	H	-5.099724	0.137582	-0.455987
C	0.303482	-2.403493	0.114345	C	-3.706527	-1.498967	1.520419
O	0.709811	-3.487071	0.070653	H	-4.127592	-1.763043	2.499574
C	3.009497	0.397581	1.516006	H	-4.534967	-1.398049	0.814625
C	2.985057	-0.311140	-1.539571	H	-3.061780	-2.325181	1.199225
C	3.113195	-0.982238	2.163925	C	-1.844634	-0.392108	2.783837
H	3.768805	-0.922049	3.044563	H	-2.369747	-0.468101	3.746368
H	2.140695	-1.349546	2.507556	H	-1.291230	-1.320870	2.625562
H	3.534742	-1.735343	1.489547	H	-1.129681	0.430715	2.831174
C	4.411347	0.944781	1.247901	C	-2.560729	0.961450	-2.673575
H	4.380170	1.908073	0.723291	H	-2.418369	2.000646	-2.365287
H	4.910622	1.116907	2.212510	H	-1.598233	0.566564	-3.001052
H	5.043713	0.255088	0.678977	H	-3.248759	0.928553	-3.528565
C	3.741210	-1.586926	-1.177032	C	-3.823969	0.977530	2.098372
H	4.233586	-1.976539	-2.079389	H	-4.617176	1.170998	1.373672
H	4.523779	-1.423431	-0.428643	H	-4.291977	0.716642	3.056690
H	3.069122	-2.373056	-0.810762	H	-3.237430	1.890334	2.241805
C	2.045807	-0.626206	-2.701285	N	2.439129	-0.746791	-0.333031
H	2.651646	-0.898755	-3.577299	C	3.059975	0.476487	-0.342309
H	1.384838	-1.470092	-2.475802	C	4.457635	0.545504	-0.398476
H	1.428427	0.237210	-2.973198	H	4.941082	1.511397	-0.410481
C	2.334947	1.375000	2.480676	C	5.213818	-0.619611	-0.431166
H	2.397346	2.403366	2.109374	H	6.294615	-0.565818	-0.471109
H	1.277259	1.157018	2.655069	C	4.565694	-1.858810	-0.406298
H	2.847271	1.324758	3.451967	H	5.120033	-2.787313	-0.421272
C	3.952430	0.772413	-2.019592	C	3.179719	-1.882738	-0.357864
H	4.718214	1.030646	-1.284127	H	2.628796	-2.811679	-0.335659
H	4.471162	0.407634	-2.917424	C	0.246384	-0.855726	-2.225200
H	3.413309	1.685138	-2.298848	O	0.315855	-1.088837	-3.370207
N	-2.438480	-0.680292	0.249662	N	1.307815	-0.453718	2.518389
C	-3.050831	0.525945	0.164404	O	1.108194	0.812842	2.739628
C	-4.443322	0.612004	0.241983	N	1.813844	-1.454537	2.862987
H	-4.927156	1.581677	0.183970				
C	-5.198356	-0.536999	0.394551				

4				Ru	-0.342653	-0.660617	0.138369
SCF done:	-1360.699354			H	-1.115693	-2.006112	-2.127822
C	0.180599	2.364177	-0.401002	P	1.837884	0.309227	0.052840
C	-0.256004	3.704066	-0.676084	C	1.383327	2.017524	0.332531
C	-1.581414	4.022230	-0.660605	H	2.139348	2.792273	0.450046
C	-2.552881	3.035962	-0.382413	C	0.068629	-2.479819	-0.360411
C	-2.109632	1.767274	-0.079991	O	0.298919	-3.631084	-0.389895
N	-0.789883	1.466235	-0.012817	C	3.109285	-0.241664	1.379553
H	-1.897462	5.038863	-0.884016	C	2.611550	0.263009	-1.710932
H	0.497469	4.447721	-0.923103	C	3.021360	-1.759387	1.547338
H	-3.609119	3.276210	-0.422113	H	3.789945	-2.088232	2.261369
Ru	-0.295899	-0.542577	0.280520	H	2.046927	-2.074046	1.936809
H	-0.820628	-2.461995	-2.277627	H	3.189131	-2.297182	0.605924
P	1.936321	0.286848	-0.130396	C	4.548035	0.143722	1.043062
C	1.504120	1.965950	-0.519748	H	4.658941	1.220797	0.865366
H	2.265589	2.703028	-0.765944	H	5.185902	-0.113571	1.900707
C	0.239980	-2.365356	0.312396	H	4.937940	-0.399494	0.175710
O	0.616739	-3.459134	0.309839	C	3.061229	-1.146592	-2.082993
C	3.064568	0.338493	1.440047	H	3.448127	-1.140808	-3.112631
C	2.939093	-0.439239	-1.602174	H	3.870414	-1.512561	-1.437692
C	3.110501	-1.021988	2.134708	H	2.230272	-1.860672	-2.049429
H	3.784980	-0.962994	3.000908	C	1.506178	0.725739	-2.665149
H	2.129850	-1.332473	2.511143	H	1.916447	0.746444	-3.684995
H	3.487083	-1.816163	1.480522	H	0.648881	0.047603	-2.661380
C	4.489380	0.793952	1.123223	H	1.171183	1.740140	-2.417648
H	4.499676	1.744942	0.576262	C	2.748618	0.448322	2.695581
H	5.021012	0.960397	2.071239	H	2.874521	1.534312	2.626816
H	5.065624	0.054682	0.557574	H	1.724371	0.251983	3.021115
C	3.644034	-1.739253	-1.223066	H	3.421410	0.072335	3.479815
H	4.098025	-2.172011	-2.125909	C	3.767442	1.254507	-1.859625
H	4.449008	-1.597145	-0.494182	H	4.692785	0.925542	-1.382666
H	2.943885	-2.484666	-0.824598	H	3.983681	1.371947	-2.931001
C	1.965206	-0.733811	-2.742042	H	3.503027	2.246253	-1.472162
H	2.550200	-0.995934	-3.635339	N	-2.518832	-0.719419	-0.034278
H	1.303399	-1.572484	-2.508450	C	-3.104382	0.497217	-0.164036
H	1.325632	0.122910	-2.976290	C	-4.483476	0.587301	-0.371475
C	2.475420	1.392407	2.381024	H	-4.946623	1.560999	-0.495832
H	2.607344	2.399819	1.972988	C	-5.251313	-0.562694	-0.429985
H	1.408098	1.264741	2.579516	H	-6.323950	-0.493066	-0.591333
H	2.999523	1.336944	3.345624	C	-4.636555	-1.802749	-0.281103
C	3.945550	0.588281	-2.125999	H	-5.201275	-2.728986	-0.315575
H	4.738367	0.834361	-1.415267	C	-3.266461	-1.830481	-0.086924
H	4.429026	0.174054	-3.021961	H	-2.730019	-2.769885	0.037248
H	3.440175	1.514024	-2.424496	C	-0.336623	-0.703528	1.958330
N	-2.456003	-0.547337	0.473154	O	-0.402490	-0.840817	3.112434
C	-3.024004	0.643401	0.180695	O	-0.236654	-1.704641	-1.860370
C	-4.413300	0.753988	0.119531				
H	-4.871252	1.704825	-0.131841	5			
C	-5.204246	-0.354970	0.366107	SCF done:	-1251.375202		
H	-6.286536	-0.273259	0.311398	C	0.021849	2.344404	0.316671
C	-4.602241	-1.567530	0.680043	C	0.540177	3.679240	0.468250
H	-5.183826	-2.462064	0.876963	C	1.875352	3.926160	0.363761
C	-3.220090	-1.616517	0.715846	C	2.793848	2.874078	0.115223
H	-2.692805	-2.542653	0.934325	C	2.288834	1.599651	0.008034
C	-0.189648	-0.447121	2.161213	N	0.958006	1.333581	0.122784
O	-0.288340	-0.458031	3.313395	H	2.246679	4.943319	0.468177
N	-1.529447	-1.700356	-2.136016	H	-0.166079	4.485331	0.651412
O	-0.807224	-0.565610	-1.745725	H	3.853964	3.079300	0.014482
N	-2.697085	-1.786713	-2.324974	Ru	0.312616	-0.648297	-0.237510
				H	0.976709	0.519633	2.010640
TS₃₋₅				P	-1.808324	0.342481	-0.031530
SCF done:	-1251.343261			C	-1.322455	2.030481	0.353963
C	0.049941	2.370286	0.198506	H	-2.054928	2.814608	0.538181
C	-0.422432	3.727544	0.220588	C	0.432654	-1.268979	1.659273
C	-1.752098	4.007980	0.098012	O	0.193088	-2.371456	2.081918
C	-2.699525	2.969385	-0.047105	C	-2.564760	0.420204	-1.795995
C	-2.221291	1.674635	-0.069295	C	-3.088530	-0.229527	1.256864
N	-0.905184	1.387285	0.027151	C	-3.259089	-0.881511	-2.181291
H	-2.090354	5.041765	0.119804	H	-3.530159	-0.845125	-3.246591
H	0.308266	4.523524	0.342664	H	-2.616518	-1.758539	-2.035152
H	-3.758976	3.192080	-0.109905	H	-4.186175	-1.039858	-1.618265

C	-3.512235	1.601652	-1.983348	H	-1.014750	1.493077	-2.514036
H	-3.024853	2.547678	-1.720490	H	-0.822491	-0.267201	-2.713548
H	-3.809302	1.660283	-3.040736	H	-1.968275	0.626931	-3.736117
H	-4.428805	1.509549	-1.391988	C	-4.435003	0.290139	1.218411
C	-3.234581	-1.750238	1.196182	H	-4.964094	-0.157865	0.369328
H	-3.977291	-2.065580	1.943060	H	-5.012759	0.048642	2.122080
H	-3.582700	-2.106632	0.219897	H	-4.451825	1.382180	1.104915
H	-2.289638	-2.252838	1.434410	N	2.466178	-0.752039	-0.345347
C	-2.550314	0.159010	2.635194	C	3.099977	0.440732	-0.199990
H	-3.262256	-0.189883	3.396614	C	4.491195	0.512487	-0.144666
H	-1.583304	-0.304343	2.856505	H	4.972885	1.473890	0.009410
H	-2.441008	1.244446	2.739333	C	5.240495	-0.649641	-0.246551
C	-1.352954	0.634035	-2.711194	H	6.325397	-0.606653	-0.201728
H	-0.796201	1.539386	-2.438289	C	4.583002	-1.867682	-0.375396
H	-0.665261	-0.226949	-2.693704	H	5.127903	-2.804684	-0.433229
H	-1.691839	0.751429	-3.750959	C	3.197032	-1.873122	-0.410302
C	-4.441874	0.448787	1.059724	H	2.632182	-2.799381	-0.484420
H	-4.949550	0.121058	0.145256	C	-0.264360	-2.382298	-0.680547
H	-5.096191	0.188622	1.904002	O	-0.642728	-3.449847	-0.960046
H	-4.355669	1.543175	1.038497	O	0.945382	-0.160205	2.390062
N	2.471965	-0.769491	-0.387537				
C	3.128285	0.405923	-0.211496				
C	4.522651	0.444275	-0.220492	6			
H	5.037510	1.387845	-0.068856	SCF done: -1062.823807			
C	5.242894	-0.724935	-0.402598	C	-0.027897	2.279685	-0.337336
H	6.329381	-0.701019	-0.407208	C	-0.548166	3.619870	-0.270251
C	4.559231	-1.925495	-0.563006	C	-1.871238	3.844998	-0.060720
H	5.082239	-2.867571	-0.693462	C	-2.798160	2.763324	0.080101
C	3.174905	-1.900430	-0.544380	C	-2.370218	1.487306	-0.114529
H	2.589347	-2.810727	-0.650658	N	-1.018086	1.248503	-0.419404
C	-0.266536	-2.362614	-0.707086	H	-2.237715	4.864039	0.034986
O	-0.605346	-3.427233	-1.026859	H	0.161552	4.441577	-0.327190
O	0.890724	-0.310360	2.507320	H	-3.825109	2.961733	0.370815
				Ru	-0.385603	-0.790991	0.058879
				H	-0.892181	0.665528	-1.298786
				P	1.729684	0.157149	-0.058459
				C	1.282581	1.916349	-0.343515
				H	2.035201	2.700662	-0.427454
				C	2.647178	0.241329	1.626453
				C	2.929161	-0.277583	-1.486118
				C	3.389967	-1.068629	1.875610
				H	3.727454	-1.100000	2.921848
				H	2.749538	-1.943839	1.705712
				H	4.281869	-1.162883	1.244145
				C	3.601514	1.422417	1.774243
				H	3.077112	2.380392	1.680329
				H	4.052214	1.393500	2.777282
				H	4.421213	1.405186	1.050036
				C	3.190314	-1.783223	-1.490655
				H	3.813833	-2.035959	-2.360485
				H	3.720253	-2.125819	-0.595481
				H	2.257141	-2.352134	-1.567598
				C	2.177717	0.080550	-2.768749
				H	2.762042	-0.255984	-3.637222
				H	1.198461	-0.416064	-2.800493
				H	2.017886	1.161735	-2.863033
				C	1.534266	0.388939	2.667665
				H	0.931338	1.288437	2.486189
				H	0.860720	-0.477425	2.662719
				H	1.982933	0.479825	3.668378
				C	4.250842	0.482237	-1.448440
				H	4.883530	0.175318	-0.606904
				H	4.814737	0.271315	-2.369018
				H	4.107689	1.569635	-1.397888
				N	-2.513127	-0.910056	-0.003720
				C	-3.187735	0.274935	-0.054864
				C	-4.583166	0.317176	-0.077948
				H	-5.087741	1.275994	-0.159515
				C	-5.308201	-0.859707	-0.013836
				H	-6.394395	-0.838943	-0.028772
				C	-4.616148	-2.067595	0.054944
				H	-5.138594	-3.018358	0.102140

TS₅₋₆
SCF done: -1251.342199

C	-0.068033	2.372837	0.275308
C	0.413188	3.732667	0.180778
C	1.703830	3.978075	-0.146399
C	2.632776	2.901680	-0.364146
C	2.246637	1.633515	-0.086485
N	0.939606	1.368021	0.358397
H	2.045926	5.001340	-0.279739
H	-0.304304	4.541055	0.299032
H	3.623355	3.106646	-0.759131
Ru	0.304924	-0.692560	-0.229994
H	0.955289	0.867988	1.356576
P	-1.822076	0.247378	-0.011362
C	-1.374432	2.002181	0.279999
H	-2.138077	2.774979	0.375768
C	0.611314	-1.216830	1.773771
O	0.502152	-2.375762	2.109600
C	-2.686202	0.321361	-1.720524
C	-3.019152	-0.252130	1.386357
C	-3.351314	-1.017381	-2.029156
H	-3.716218	-1.007348	-3.066183
H	-2.655262	-1.859444	-1.934004
H	-4.214420	-1.211476	-1.382126
C	-3.694404	1.457716	-1.863333
H	-3.230849	2.436547	-1.693307
H	-4.087557	1.457849	-2.890313
H	-4.548174	1.356086	-1.188253
C	-3.036197	-1.780343	1.459114
H	-3.740270	-2.092823	2.243295
H	-3.358575	-2.245530	0.519395
H	-2.047374	-2.180641	1.712590
C	-2.437422	0.307079	2.687091
H	-3.007230	-0.107219	3.530682
H	-1.383617	0.044920	2.833755
H	-2.521562	1.399774	2.729078
C	-1.550191	0.557261	-2.721329

C	-3.233372	-2.047090	0.051012	H	-1.875429	4.787256	-1.563679
H	-2.652315	-2.964323	0.091099	H	0.511815	4.279825	-1.189210
C	0.166530	-2.533780	0.176221	H	-3.605298	3.031744	-1.125229
O	0.544562	-3.644368	0.232064	Ru	-0.360616	-0.564511	0.481165

TS₅₋₇

SCF done: -1251.318684

C	0.094599	2.361227	-0.122284
C	-0.391559	3.711822	-0.145558
C	-1.722274	3.974712	-0.005236
C	-2.650269	2.922737	0.173096
C	-2.164874	1.634229	0.162845
N	-0.848498	1.356889	-0.012939
H	-2.074812	5.003748	-0.016591
H	0.330834	4.515934	-0.261471
H	-3.703904	3.133385	0.319976
Ru	-0.284791	-0.665688	-0.047506
H	0.679364	-0.560113	-1.479343
P	1.880954	0.315848	-0.002901
C	-0.950934	-0.940968	-2.070785
O	0.096741	-0.728704	-2.745911
C	2.440297	0.046095	1.825364
C	3.298838	-0.093135	-1.218171
C	3.021941	-1.343401	2.059228
H	3.217830	-1.472819	3.133640
H	2.335009	-2.141445	1.753392
H	3.974454	-1.493884	1.538571
C	3.427250	1.124523	2.268625
H	3.038680	2.127923	2.057126
H	3.572692	1.044322	3.355657
H	4.410648	1.025124	1.802436
C	3.028831	0.666137	-2.520128
H	3.766660	0.338692	-3.266488
H	2.032676	0.474852	-2.928404
H	3.139659	1.747519	-2.386206
C	4.667741	0.339817	-0.696698
H	5.406015	0.194105	-1.497769
H	4.690484	1.402418	-0.422988
H	5.003655	-0.251594	0.162379
C	1.169760	0.211796	2.664921
H	0.701495	1.189076	2.497359
H	0.427301	-0.573600	2.457876
H	1.431921	0.142677	3.730761
C	3.301218	-1.597460	-1.494352
H	2.389517	-1.916858	-2.012307
H	4.153858	-1.839919	-2.143982
H	3.401404	-2.194279	-0.579992
C	-3.016619	0.450010	0.368847
C	-5.133757	-0.656704	0.629624
H	-6.219038	-0.619990	0.675633
C	-4.460539	-1.866998	0.754585
H	-4.990136	-2.803044	0.899931
C	-3.079236	-1.858210	0.670860
H	-2.503537	-2.778120	0.735571
O	-2.101390	-1.205495	-2.289539
C	0.218048	-2.468165	0.048499
O	0.538886	-3.580538	0.161031
C	1.439749	2.031521	-0.184096
H	2.194141	2.806559	-0.298764
N	-2.372187	-0.735243	0.495830
C	-4.408136	0.506334	0.432656
H	-4.917469	1.456831	0.309390

TS₅₋₇

SCF done: -1251.272783

C	0.170576	2.240069	-0.540713
C	-0.252754	3.529193	-1.005213
C	-1.573467	3.804062	-1.209862
C	-2.553631	2.819287	-0.967499
C	-2.130083	1.583768	-0.523573
N	-0.816339	1.300722	-0.322955

H	-1.875429	4.787256	-1.563679
H	0.511815	4.279825	-1.189210
H	-3.605298	3.031744	-1.125229
Ru	-0.360616	-0.564511	0.481165
H	0.729807	-1.730593	0.963767
P	1.872879	0.198357	0.040986
C	1.492532	1.905592	-0.305201
H	2.276348	2.628380	-0.519101
C	-0.327952	-2.145366	-0.789604
O	-0.526450	-2.686987	-1.841855
C	3.162737	0.212771	1.464290
C	2.670329	-0.533753	-1.557531
C	3.903889	-1.115722	1.578664
H	4.485033	-1.121740	2.511660
H	3.218867	-1.973759	1.616226
H	4.610108	-1.274722	0.757023
C	4.159814	1.359261	1.278950
H	3.655340	2.330815	1.323849
H	4.889455	1.325135	2.100179
H	4.719154	1.304382	0.341262
C	2.908678	-2.040591	-1.476751
H	3.196622	-2.403074	-2.473602
H	3.718655	-2.304946	-0.790320
H	2.016018	-2.602732	-1.185647
C	1.683449	-0.237125	-2.690649
H	2.122950	-0.594136	-3.632695
H	0.725815	-0.750379	-2.561682
H	1.497454	0.838477	-2.787933
C	2.422286	0.467728	2.774747
H	1.770523	1.347294	2.711091
H	1.823624	-0.396073	3.082735
H	3.161050	0.654308	3.566891
C	3.986503	0.170228	-1.888500
H	4.795870	-0.085913	-1.194960
H	4.312150	-0.147032	-2.889435
H	3.874580	1.261700	-1.914758
N	-2.490250	-0.649489	0.248302
C	-3.054799	0.481037	-0.232321
C	-4.437147	0.540432	-0.419016
H	-4.893206	1.444913	-0.808937
C	-5.217823	-0.561167	-0.110926
H	-6.294345	-0.521026	-0.254797
C	-4.613384	-1.717278	0.375752
H	-5.191415	-2.602656	0.620255
C	-3.239163	-1.719365	0.537608
H	-2.693568	-2.592271	0.894498
C	-0.594762	0.162750	2.327195
O	-0.871185	0.349051	3.431193
O	-0.134965	-2.717752	0.422399

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SCF done: -1062.820635

C	-0.001200	2.250579	-0.364735
C	-0.509982	3.592216	-0.469837
C	-1.843018	3.847603	-0.391249
C	-2.785112	2.793117	-0.212530
C	-2.330231	1.505476	-0.176319
N	-0.978626	1.231539	-0.305550
H	-2.201800	4.872421	-0.449100
H	0.211457	4.398708	-0.575971
H	-3.838916	3.016467	-0.082200
Ru	-0.370276	-0.771260	0.130111
H	-0.735941	0.356830	-1.145694
P	1.760616	0.163127	-0.002143
C	1.320219	1.898161	-0.338502
H	2.071623	2.672703	-0.488081
C	2.635042	0.241040	1.704465
C	2.969552	-0.324997	-1.400710
C	3.325738	-1.082212	2.019333
H	3.600976	-1.103364	3.083956
H	2.671719	-1.942593	1.825256

H	4.250242	-1.212768	1.444565
C	3.619109	1.397906	1.844207
H	3.127960	2.364506	1.682765
H	4.028533	1.401030	2.865345
H	4.465405	1.322706	1.154453
C	3.306976	-1.812942	-1.322668
H	3.913244	-2.086550	-2.198413
H	3.888777	-2.068558	-0.431057
H	2.407596	-2.438524	-1.331434
C	2.200583	-0.075564	-2.699529
H	2.811861	-0.411183	-3.549633
H	1.256304	-0.634964	-2.711761
H	1.970375	0.987326	-2.840865
C	1.495360	0.454857	2.705743
H	0.919118	1.359794	2.473117
H	0.805120	-0.399573	2.718968
H	1.915272	0.572425	3.716041
C	4.253820	0.498376	-1.410614
H	4.913697	0.247185	-0.571893
H	4.812208	0.284698	-2.333826
H	4.060304	1.578640	-1.389410
N	-2.514269	-0.872330	0.131234
C	-3.169420	0.311291	-0.019768
C	-4.563962	0.364076	-0.049392
H	-5.062624	1.317966	-0.194114
C	-5.301045	-0.798722	0.093292
H	-6.386988	-0.766252	0.073429
C	-4.625410	-2.005996	0.249805
H	-5.157734	-2.946199	0.357132
C	-3.241905	-1.996101	0.257925
H	-2.670923	-2.914773	0.363330
C	0.131358	-2.542529	-0.023806
O	0.438181	-3.663320	-0.178226

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SCF done: -1062.871535

C	-0.099975	2.271412	-0.027553
C	-0.629728	3.609196	-0.023204
C	-1.974037	3.828036	-0.013626
C	-2.882556	2.741786	-0.008259
C	-2.354123	1.469397	-0.009171
N	-1.019280	1.233878	-0.008275
H	-2.357576	4.846278	-0.012384
H	0.073049	4.438924	-0.031753
H	-3.952458	2.918590	-0.004077
Ru	-0.362809	-0.758873	-0.012375
H	-0.285024	-0.872122	-1.559047
P	1.738083	0.261315	-0.036604
C	1.252965	1.988495	-0.042457
H	1.976716	2.800796	-0.075462
C	2.657726	-0.016641	1.621582
C	2.891261	-0.018839	-1.530796
C	3.379065	-1.359418	1.659363
H	3.724764	-1.557802	2.684676
H	2.725055	-2.189851	1.363524
H	4.266491	-1.372026	1.014141
C	3.624686	1.116448	1.954697
H	3.114329	2.086635	1.948783
H	4.033809	0.958184	2.963545
H	4.472619	1.169395	1.263580
C	3.090612	-1.512148	-1.782111
H	3.720357	-1.645425	-2.673768
H	3.588184	-2.022563	-0.950200
H	2.136151	-2.018742	-1.965324
C	2.180031	0.591780	-2.738907
H	2.770591	0.385802	-3.643205
H	1.181097	0.160295	-2.881839
H	2.065584	1.676301	-2.636044
C	1.538805	-0.013875	2.667977
H	0.942722	0.906261	2.610225
H	0.869305	-0.878596	2.549891

H	1.974370	-0.070664	3.676353
C	4.241850	0.668994	-1.355075
H	4.848137	0.198649	-0.571806
H	4.810001	0.597482	-2.293982
H	4.132918	1.735365	-1.118471
N	-2.519622	-0.931867	-0.001243
C	-3.186497	0.251235	-0.012959
C	-4.581548	0.275884	-0.032816
H	-5.104858	1.226816	-0.043584
C	-5.294169	-0.911531	-0.042781
H	-6.380793	-0.896335	-0.059668
C	-4.600466	-2.117322	-0.033633
H	-5.116122	-3.072590	-0.043433
C	-3.216800	-2.077680	-0.013186
H	-2.624240	-2.989403	-0.008938
C	0.254523	-2.508621	0.013795
O	0.663718	-3.602822	0.019144

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SCF done: -1251.326184

C	-0.084286	2.125740	-0.659210
C	-0.578583	3.399869	-1.120288
C	-1.905498	3.681972	-1.128145
C	-2.816852	2.702040	-0.670386
C	-2.320012	1.457616	-0.337718
N	-1.006380	1.109220	-0.387965
H	-2.266835	4.648660	-1.471032
H	0.155105	4.136182	-1.439318
H	-3.884487	2.894514	-0.648081
Ru	-0.050436	-0.867210	0.040862
H	-2.371356	-1.218661	-0.965295
P	1.866659	0.384200	0.150204
C	1.269240	1.942607	-0.473680
H	1.952836	2.754857	-0.716094
C	-0.250047	-1.708608	-1.754627
O	0.502783	-1.923347	-2.668792
C	2.360787	0.666837	1.984193
C	3.372979	-0.112979	-0.913460
C	3.157632	-0.503457	2.551270
H	3.303882	-0.351789	3.630909
H	2.642111	-1.462364	2.420642
H	4.152974	-0.588585	2.099001
C	3.119410	1.977046	2.185492
H	2.570015	2.823316	1.756055
H	3.235221	2.162593	3.263450
H	4.122211	1.958604	1.748623
C	3.651742	-1.607875	-0.776491
H	4.547689	-1.856513	-1.363155
H	3.835591	-1.921798	0.257602
H	2.818487	-2.195506	-1.177840
C	3.010349	0.184050	-2.368580
H	3.835841	-0.164132	-3.006144
H	2.103566	-0.347276	-2.675759
H	2.871341	1.255895	-2.545728
C	1.024193	0.775204	2.723693
H	0.409180	1.589774	2.321218
H	0.447368	-0.160577	2.666992
H	1.210050	0.986423	3.787043
C	4.609713	0.700497	-0.538786
H	4.993431	0.455569	0.458404
H	5.408430	0.475906	-1.260013
H	4.423081	1.781489	-0.586703
N	-3.232440	-0.811212	-0.310408
C	-3.322388	0.466988	0.096419
C	-4.388699	0.819274	0.931221
H	-4.451550	1.838576	1.297719
C	-5.318866	-0.134417	1.307512
H	-6.141663	0.142800	1.961560
C	-5.188762	-1.451355	0.864658
H	-5.894661	-2.223365	1.150988
C	-4.116084	-1.752045	0.052908

H	-3.916640	-2.746600	-0.338521	Ru	0.532731	-0.694086	0.481515
C	0.806772	-2.389848	0.624637	H	1.707320	-0.379650	1.747159
O	1.338495	-3.331583	1.061119	P	-1.609669	0.251710	0.161881
O	-1.497921	-2.003496	-1.572774	C	-1.235051	2.005661	0.255502

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SCF done: -1062.812093

C	-0.105372	2.421500	-0.142048
C	0.392673	3.754148	0.067904
C	1.731157	3.977896	0.256286
C	2.683826	2.924727	0.218127
C	2.173830	1.693388	-0.117948
N	0.865732	1.468001	-0.356127
H	2.072638	4.992148	0.455871
H	-0.321001	4.570987	0.145788
H	3.743557	3.091174	0.386391
Ru	0.655728	-0.619284	-0.203383
H	3.936052	0.550218	1.476515
P	-1.634787	0.203092	0.004964
C	-1.415406	1.985832	-0.097184
H	-2.234921	2.685659	0.051104
C	-2.680384	-0.298328	-1.519798
C	-2.565640	-0.120643	1.649243
C	-3.177873	-1.736674	-1.429322
H	-3.582449	-2.043751	-2.404907
H	-2.371630	-2.434415	-1.167012
H	-3.985920	-1.848939	-0.696366
C	-3.851797	0.654833	-1.742454
H	-3.510926	1.694458	-1.813286
H	-4.348918	0.399524	-2.689921
H	-4.606204	0.591724	-0.951098
C	-2.674333	-1.612255	1.952292
H	-3.124958	-1.741613	2.947291
H	-3.308661	-2.146129	1.237722
H	-1.694709	-2.101577	1.968189
C	-1.694546	0.530563	2.725238
H	-2.124242	0.317537	3.714653
H	-0.670751	0.132925	2.702545
H	-1.636191	1.616787	2.597190
C	-1.720168	-0.169295	-2.704421
H	-1.299636	0.842746	-2.766620
H	-0.887068	-0.880681	-2.619756
H	-2.263250	-0.373790	-3.638930
C	-3.952530	0.513940	1.671966
H	-4.658391	-0.016526	1.022010
H	-4.356541	0.466196	2.694031
H	-3.930499	1.570360	1.376210
N	3.735456	-0.063002	0.696399
C	2.792833	0.363940	-0.205132
C	2.439669	-0.469152	-1.314555
H	2.152531	-0.045483	-2.275230
C	2.565197	-1.854328	-1.073830
H	2.253807	-2.557962	-1.839993
C	3.451929	-2.297836	-0.030495
H	3.663750	-3.354976	0.089787
C	4.048569	-1.397701	0.792269
H	4.752511	-1.669138	1.570680
C	0.414701	-2.346234	0.494306
O	0.333184	-3.381284	1.027122

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SCF done: -1062.796433

C	0.097221	2.371507	0.272802
C	0.578185	3.724721	0.189625
C	1.914635	3.999881	0.109847
C	2.873358	2.957798	0.107251
C	2.375998	1.680598	0.230519
N	1.060464	1.379821	0.357184
H	2.245877	5.034156	0.040019
H	-0.155563	4.527183	0.169488
H	3.940042	3.145244	0.034264

H	0.532731	-0.694086	0.481515
H	1.707320	-0.379650	1.747159
P	-1.609669	0.251710	0.161881
C	-1.235051	2.005661	0.255502
H	-2.003768	2.769206	0.154063
C	-2.318963	-0.092611	-1.586960
C	-2.924796	-0.065001	1.516340
C	-2.392937	-1.595218	-1.851594
H	-2.754560	-1.764603	-2.876795
H	-1.405061	-2.061726	-1.756398
H	-3.075886	-2.114873	-1.171738
C	-3.682633	0.552388	-1.813936
H	-3.675995	1.622188	-1.567776
H	-3.955083	0.461744	-2.875848
H	-4.477887	0.066483	-1.235216
C	-3.612972	-1.416685	1.352081
H	-4.231294	-1.613823	2.240181
H	-4.282447	-1.439446	0.483407
H	-2.895580	-2.241695	1.262257
C	-2.148980	-0.052334	2.835072
H	-2.857148	-0.112422	3.674587
H	-1.458023	-0.901123	2.905289
C	-1.566799	0.872099	2.943053
H	-1.309844	0.520011	-2.558407
H	-1.261413	1.610109	-2.459384
H	-0.301551	0.117985	-2.387629
H	-1.606395	0.275411	-3.588743
C	-3.967333	1.050890	1.563846
H	-4.566282	1.113754	0.649339
H	-4.659525	0.858966	2.396644
H	-3.499534	2.026365	1.738909
N	2.641556	-0.580993	0.957055
C	3.147346	0.443019	0.130017
C	4.056646	0.119952	-0.840870
H	4.429810	0.921363	-1.473351
C	4.371173	-1.225693	-1.107369
H	5.076745	-1.473357	-1.894450
C	3.703422	-2.225214	-0.424526
C	3.862545	-3.273243	-0.657373
C	2.839668	-1.905456	0.624174
H	2.493043	-2.633046	1.348543
C	-0.149313	-2.381549	0.820388
O	-0.597319	-3.425077	1.109838

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SCF done: -1364.654956

C	0.045720	2.346954	-0.303051
C	-0.441675	3.689196	-0.482987
C	-1.776898	3.959218	-0.456230
C	-2.724713	2.923814	-0.264977
C	-2.246825	1.640849	-0.128996
N	-0.916489	1.358338	-0.173692
H	-2.123572	4.982694	-0.580606
H	0.287430	4.483480	-0.622540
H	-3.785692	3.144850	-0.229251
Ru	-0.318675	-0.613816	0.306676
H	-1.022837	0.572347	-2.120112
P	1.882563	0.309975	-0.030037
C	1.388295	2.019988	-0.261330
H	2.129473	2.797958	-0.437265
C	-0.597931	-1.225194	-1.702433
O	-0.532577	-2.368989	-2.091228
C	3.095185	0.300991	1.475198
C	2.869591	-0.248785	-1.599980
C	3.828012	-1.032997	1.587866
H	4.408881	-1.046458	2.521211
H	3.127891	-1.877576	1.625874
H	4.529804	-1.210028	0.767487
C	4.080943	1.469280	1.396785
H	3.549472	2.428194	1.391913
H	4.719881	1.450482	2.290940

H	4.739972	1.436603	0.528311	H	1.843254	0.135235	3.038706
C	2.897408	-1.776096	-1.678498	H	3.249004	1.152274	3.377317
H	3.469405	-2.073375	-2.569429	C	4.241890	-0.177938	-1.789244
H	3.386177	-2.237136	-0.812306	H	4.920501	-0.528256	-1.005352
H	1.892768	-2.201672	-1.780413	H	4.594147	-0.616228	-2.734234
C	2.151406	0.307580	-2.829521	H	4.342069	0.910727	-1.885710
H	2.688876	-0.033056	-3.725568	N	-2.461492	-0.564571	0.280310
H	1.120855	-0.037542	-2.925126	C	-3.043087	0.587249	-0.160070
H	2.147221	1.403554	-2.832619	C	-4.429130	0.684379	-0.305108
C	2.288679	0.502235	2.754791	H	-4.859766	1.599700	-0.701652
H	1.625345	1.373827	2.690606	C	-5.231438	-0.391685	0.028716
H	1.698304	-0.383641	3.008197	H	-6.310288	-0.328822	-0.083519
H	2.985080	0.675302	3.587169	C	-4.629043	-1.561683	0.489743
C	4.296792	0.298608	-1.652447	H	-5.215420	-2.437786	0.748549
H	4.958439	-0.113215	-0.883558	C	-3.251181	-1.608063	0.590645
H	4.730200	0.023124	-2.624313	H	-2.733372	-2.509421	0.908643
H	4.319711	1.394083	-1.590521	C	0.167738	-2.214522	0.972807
N	-2.494484	-0.728245	0.220143	O	0.483893	-3.292699	1.281331
C	-3.116530	0.459996	0.027560	O	-1.225032	-0.837182	-2.481905
C	-4.508607	0.516583	-0.046669	C	-0.501542	0.340188	2.298728
H	-5.002662	1.469828	-0.205692	O	-0.738734	0.373720	3.434479
C	-5.250983	-0.647515	0.061883				
H	-6.335417	-0.608854	0.002632				
C	-4.594050	-1.861858	0.229391				
H	-5.135858	-2.799607	0.298220				
C	-3.211201	-1.855304	0.299588				
H	-2.641161	-2.774448	0.412042				
C	0.266028	-2.381095	0.648277				
O	0.635084	-3.458285	0.842073				
O	-1.098818	-0.287645	-2.562530				
C	-0.567342	-0.132006	2.225313				
O	-0.983157	0.122577	3.267834				

TS₉₋₁₁

SCF done: -1364.605061

C	0.241118	2.320871	-0.729031
C	-0.194765	3.678161	-0.922485
C	-1.501650	4.010049	-0.772351
C	-2.490308	3.020488	-0.452115
C	-2.152812	1.707716	-0.452934
N	-0.804934	1.331532	-0.700664
H	-1.809527	5.049057	-0.856006
H	0.562211	4.435669	-1.110047
H	-3.498239	3.325887	-0.187371
Ru	-0.307761	-0.484223	0.506883
H	-0.778808	0.724497	-1.538827
P	1.912146	0.193696	-0.044390
C	1.524618	1.912900	-0.568500
H	2.318397	2.637989	-0.751161
C	-1.037257	-1.775815	-1.743767
O	-1.098093	-2.946806	-1.548176
C	3.216209	0.419099	1.361202
C	2.793497	-0.605606	-1.573168
C	3.840784	-0.941534	1.670099
H	4.452121	-0.856897	2.579603
H	3.072863	-1.703569	1.859928
H	4.495913	-1.304155	0.870447
C	4.294608	1.454935	1.037536
H	3.863755	2.455512	0.910787
H	4.984299	1.512047	1.891513
H	4.894640	1.220525	0.156266
C	2.714163	-2.125200	-1.434581
H	3.165181	-2.590614	-2.322445
H	3.252288	-2.499776	-0.556193
H	1.676790	-2.471773	-1.365977
C	2.011386	-0.179369	-2.815097
H	2.423993	-0.706259	-3.686896
H	0.949933	-0.433290	-2.756551
H	2.100286	0.897429	-3.004187
C	2.495599	0.903813	2.616533
H	1.896956	1.803887	2.430550

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SCF done: -1176.109274

C	0.021992	2.362542	-0.144313
C	-0.469166	3.694737	0.016083
C	-1.808490	3.942352	0.135505
C	-2.766382	2.894187	0.089369
C	-2.343491	1.620769	-0.179808
N	-0.980769	1.382544	-0.367516
H	-2.151158	4.959959	0.305765
H	0.259192	4.496669	0.107149
H	-3.811156	3.094012	0.305348
Ru	-0.377327	-0.759431	0.153660
H	-0.782529	0.803236	-1.218325
P	1.793245	0.185859	-0.083635
C	1.327100	1.952285	-0.103171
H	2.097418	2.722775	-0.088621
C	3.130179	0.076054	1.297172
C	2.638954	-0.109548	-1.804147
C	3.919268	-1.223111	1.152015
H	4.503706	-1.392616	2.067396
H	3.254886	-2.088170	1.019155
H	4.627556	-1.194198	0.316160
C	4.076169	1.277493	1.306693
H	3.543191	2.202574	1.554873
H	4.832642	1.120324	2.088934
H	4.609206	1.428168	0.364452
C	2.941598	-1.587432	-2.040490
H	3.254973	-1.723102	-3.085732
H	3.751795	-1.964059	-1.409351
C	2.061720	-2.219216	-1.878840
C	1.614033	0.335134	-2.848502
H	2.035469	0.182515	-3.852138
H	0.691270	-0.256942	-2.779889
H	1.361561	1.398547	-2.746254
C	2.407152	0.049660	2.640678
H	1.693003	0.875936	2.743767
H	1.870673	-0.890664	2.794468
H	3.152917	0.144450	3.442867
C	3.908072	0.715406	-1.997676
H	4.734327	0.365024	-1.368655
H	4.240340	0.625002	-3.042256
H	3.743815	1.782913	-1.801200
N	-2.515078	-0.780583	-0.168802
C	-3.162111	0.421437	-0.249802
C	-4.554157	0.482072	-0.397453
H	-5.032009	1.452423	-0.501524
C	-5.297240	-0.679272	-0.427992
H	-6.377255	-0.640160	-0.539982
C	-4.630836	-1.904074	-0.329851

H	-5.169121	-2.846479	-0.356608	C	-2.265384	1.580333	-0.397197
C	-3.256950	-1.907123	-0.212387	N	-0.960956	1.193543	-0.443449
H	-2.698233	-2.837264	-0.150214	H	-2.084824	4.821582	-1.364358
C	0.040702	-2.490677	-0.411459	H	0.317999	4.227562	-1.299175
O	0.244829	-3.624703	-0.616970	H	-3.775314	3.078078	-0.664020
C	-0.523608	-0.790026	2.079666	Ru	-0.086163	-0.851017	-0.026540
O	-0.669866	-1.123483	3.183991	H	-2.386824	-1.031427	-1.187696

TS₁₁₋₁

SCF done: -1176.108942

C	-0.015285	2.370449	0.013942
C	-0.511364	3.701232	0.127234
C	-1.856296	3.962451	0.157205
C	-2.800705	2.918555	0.078205
C	-2.344389	1.623292	-0.035030
N	-0.989171	1.359095	-0.099585
H	-2.203205	4.988606	0.251093
H	0.215943	4.504579	0.214613
H	-3.863501	3.130861	0.127152
Ru	-0.371913	-0.713748	0.039999
H	-0.701236	0.658302	-1.075590
P	1.790275	0.265208	-0.063419
C	1.311426	2.001302	-0.036581
H	2.066105	2.786545	-0.054240
C	2.934845	-0.015310	1.460423
C	2.812585	0.038461	-1.682790
C	3.102131	-1.511637	1.722999
H	3.722785	-1.653142	2.619400
H	2.141898	-2.005409	1.906215
H	3.596360	-2.032696	0.895847
C	4.308579	0.636338	1.309672
H	4.235522	1.702840	1.060916
H	4.840448	0.562314	2.269302
H	4.934620	0.142786	0.558070
C	3.574715	-1.283418	-1.691735
H	4.016396	-1.438176	-2.686636
H	4.397309	-1.298028	-0.967977
H	2.919355	-2.140265	-1.490145
C	1.807766	0.033046	-2.835873
H	2.360488	-0.013548	-3.785386
H	1.127324	-0.823301	-2.792830
H	1.198870	0.946300	-2.843516
C	2.246237	0.637238	2.659420
H	2.192689	1.725904	2.547135
H	1.227489	0.268035	2.814731
H	2.824629	0.409446	3.565984
C	3.766332	1.208256	-1.925760
H	4.565219	1.281974	-1.184006
H	4.243224	1.077424	-2.907598
H	3.225578	2.161749	-1.949604
N	-2.526492	-0.763661	-0.193070
C	-3.174917	0.433143	-0.134788
C	-4.574453	0.487801	-0.199793
H	-5.072497	1.452060	-0.163213
C	-5.306848	-0.675093	-0.308952
H	-6.391795	-0.637671	-0.356735
C	-4.631544	-1.896975	-0.362751
H	-5.164435	-2.838294	-0.453872
C	-3.254095	-1.891855	-0.303949
H	-2.682635	-2.815691	-0.345708
C	0.137194	-2.306369	-0.822387
O	0.444303	-3.302232	-1.341933
C	-0.360855	-1.379827	1.878133
O	-0.372222	-1.934036	2.896074

TS₉₋₁₀

SCF done: -1364.607793

C	-0.003690	2.189456	-0.633536
C	-0.447091	3.499850	-1.040284
C	-1.763561	3.826751	-1.065230
C	-2.713379	2.855323	-0.677886

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SCF done: -1176.118934

C	0.049555	2.217895	0.389784
C	-0.409029	3.561191	0.653655
C	-1.731596	3.871504	0.675895
C	-2.681543	2.859520	0.406157
C	-2.213345	1.573816	0.212589
N	-0.909740	1.210001	0.291814
H	-2.057742	4.892403	0.860467
H	0.346910	4.325909	0.817563
H	-3.730812	3.101379	0.275852
Ru	-0.134736	-0.894284	0.469702
H	-1.675386	-0.614693	-0.987758
P	1.929201	0.290254	-0.135408
C	1.395167	1.961261	0.237690
H	2.087351	2.800566	0.287346
C	3.364618	-0.039138	1.083079

C	2.524244	0.272246	-1.957324	H	-1.485688	1.109865	3.766556
C	4.096285	-1.337107	0.751116	H	-0.267009	0.650655	2.557317
H	4.761540	-1.598629	1.586707	H	-1.190387	2.151867	2.352476
H	3.406392	-2.177704	0.603722	C	-2.708450	-0.573041	-2.385726
H	4.725724	-1.243321	-0.142187	H	-2.074508	0.225737	-2.788911
C	4.359832	1.116571	1.149885	H	-2.128508	-1.501956	-2.360681
H	3.875067	2.047126	1.466659	H	-3.546814	-0.722498	-3.080916
H	5.134067	0.881188	1.894972	C	-3.663664	1.081831	2.141309
H	4.866990	1.299224	0.196899	H	-4.521491	0.532742	1.736997
C	2.769133	-1.164936	-2.412266	H	-3.847041	1.219169	3.217254
H	2.984822	-1.174722	-3.490961	H	-3.637135	2.079974	1.685140
H	3.619640	-1.631504	-1.904200	N	2.437233	-0.804216	0.470887
H	1.888017	-1.795345	-2.238926	C	3.131416	0.375196	0.199651
C	1.346641	0.836641	-2.754410	C	4.525811	0.380066	0.251147
H	1.583368	0.802032	-3.827767	H	5.042331	1.308799	0.026265
H	0.434458	0.246634	-2.588728	C	5.239823	-0.764629	0.536141
H	1.131966	1.875642	-2.478427	H	6.324587	-0.750376	0.562920
C	2.696948	-0.181923	2.452865	C	4.527548	-1.952437	0.784078
H	2.113672	0.711514	2.708557	H	5.043458	-2.884671	0.994266
H	2.021358	-1.045854	2.483778	C	3.164089	-1.947368	0.755708
H	3.472086	-0.318176	3.221428	H	2.562763	-2.829155	0.957209
C	3.755382	1.131024	-2.220469	C	-0.289368	-2.508040	0.083493
H	4.664542	0.696843	-1.787905	O	-0.696599	-3.574579	0.297242
H	3.921721	1.212591	-3.305134	C	0.423658	-1.008127	-2.121874
H	3.635427	2.149433	-1.827983	O	0.507961	-1.176862	-3.262463
N	-2.731107	-0.442002	-1.014902				
C	-3.186420	0.577571	-0.247233				
C	-4.555317	0.610670	0.032833				
H	-4.939530	1.390170	0.682183				
C	-5.392904	-0.366750	-0.471144				
H	-6.452876	-0.343567	-0.233601				
C	-4.873673	-1.402255	-1.258892				
H	-5.506761	-2.188807	-1.654396				
C	-3.521241	-1.419804	-1.495323				
H	-3.012816	-2.205341	-2.047102				
C	0.609995	-2.577147	0.285387				
O	1.089467	-3.623852	0.091742				
C	-1.621215	-1.621800	1.375776				
O	-2.528463	-2.044973	1.972866				
TS₁₀₋₁				TS₁₋₁₂			
SCF done: -1176.097918				SCF done: -1176.102677			
C	0.040850	2.258074	-0.392542	C	-0.028414	2.153422	-0.806187
C	0.542170	3.587199	-0.526770	C	-0.422854	3.466711	-1.111642
C	1.886663	3.848626	-0.439578	C	-1.752325	3.831319	-1.003509
C	2.805262	2.817493	-0.203881	C	-2.713225	2.873954	-0.655727
C	2.305015	1.523018	-0.106092	C	-2.287134	1.592266	-0.348043
N	0.980247	1.248588	-0.236959	N	-0.967190	1.276027	-0.328007
H	2.242016	4.873120	-0.530236	H	-2.058718	4.847740	-1.237611
H	-0.174163	4.391442	-0.674788	H	0.323885	4.178515	-1.455661
H	3.862354	3.024455	-0.077567	H	-3.771440	3.117417	-0.680993
Ru	0.358294	-0.763658	-0.217657	Ru	-0.367827	-0.656025	0.161075
H	1.543962	-0.655513	1.244561	H	0.547480	0.212797	-1.493978
P	-1.777180	0.287313	0.095721	P	1.811742	0.212758	-0.013748
C	-1.311673	1.939826	-0.388046	C	1.244518	1.573502	-1.083022
H	-2.040087	2.747939	-0.426730	H	1.981397	2.217707	-1.573868
C	-3.263788	-0.213092	-1.010087	C	0.134208	-2.450988	-0.122040
C	-2.344197	0.340758	1.946970	O	0.412995	-3.569224	-0.289752
C	-4.002774	-1.424492	-0.450423	C	2.620087	0.918487	1.592622
H	-4.746311	-1.763385	-1.186158	C	3.134675	-0.674630	-1.087997
H	-3.325415	-2.266866	-0.259827	C	2.826564	-0.174173	2.639983
H	-4.543813	-1.196643	0.474981	H	3.167101	0.289811	3.577131
C	-4.229293	0.959323	-1.191644	H	1.900828	-0.715196	2.862017
H	-3.734427	1.806547	-1.679425	H	3.585653	-0.905378	2.344992
H	-5.055720	0.639352	-1.842473	C	3.932763	1.655036	1.342650
H	-4.668745	1.309185	-0.252897	H	3.838265	2.400114	0.541874
C	-2.429302	-1.063703	2.539899	H	4.218909	2.193586	2.258000
H	-2.683860	-0.991902	3.607569	H	4.759716	0.978433	1.099086
H	-3.190599	-1.690056	2.063282	C	3.867899	-1.697254	-0.219881
H	-1.467234	-1.585769	2.464339	H	4.503687	-2.322920	-0.861466
C	-1.255149	1.111881	2.691682	H	4.520949	-1.224356	0.522116
				H	3.170867	-2.363971	0.304092
				C	2.476166	-1.416085	-2.252416
				H	3.277065	-1.842387	-2.874100
				H	1.837067	-2.239488	-1.924918
				H	1.880614	-0.749253	-2.884457
				C	1.610945	1.936019	2.130275
				H	1.495658	2.788824	1.451029
				H	0.621340	1.495354	2.294971
				H	1.970965	2.317396	3.096009
				C	4.136356	0.310585	-1.694960
				H	4.659201	0.918791	-0.953756
				H	4.897608	-0.261122	-2.244106
				H	3.656170	0.980856	-2.417107
				N	-2.526982	-0.764419	-0.136092

C	-3.161011	0.441793	-0.162051
C	-4.553244	0.522638	-0.060830
H	-5.032333	1.498021	-0.054891
C	-5.304417	-0.632698	0.032430
H	-6.387320	-0.579865	0.105885
C	-4.648221	-1.865892	0.029465
H	-5.196590	-2.800953	0.089583
C	-3.269863	-1.881699	-0.045476
H	-2.713611	-2.816214	-0.032542
C	-0.582482	-0.835469	2.080606
O	-0.614269	-0.985148	3.229882

TS₁₋₁₂

SCF done: -1252.505914

C	0.033953	2.178755	-0.630330
C	-0.358076	3.524098	-0.799551
C	-1.685876	3.880161	-0.668884
C	-2.653178	2.908218	-0.402636
C	-2.228071	1.599936	-0.208613
N	-0.915497	1.271167	-0.250895
H	-1.984981	4.917214	-0.803100
H	0.396235	4.263328	-1.057989
H	-3.706241	3.169312	-0.369393
Ru	-0.383351	-0.754045	0.121575
H	-0.169201	-0.494145	-1.814060
P	1.814025	0.154539	-0.046975
C	1.329068	1.661316	-0.976190
H	2.099543	2.415207	-1.161181
C	0.042028	-2.510698	-0.342579
O	0.277777	-3.614335	-0.641448
C	2.555306	0.779569	1.637809
C	3.230440	-0.653499	-1.072225
C	2.730882	-0.366783	2.633635
H	3.029950	0.050030	3.606336
H	1.802469	-0.924339	2.788454
H	3.505513	-1.077745	2.333795
C	3.880301	1.521629	1.479454
H	3.814069	2.334860	0.745669
H	4.146971	1.977465	2.444410
H	4.708887	0.861981	1.199033
C	3.993788	-1.645005	-0.195183
H	4.695288	-2.210383	-0.824224
H	4.582515	-1.156978	0.588978
H	3.317085	-2.371633	0.274761
C	2.645096	-1.440259	-2.245905
H	3.479408	-1.906817	-2.789582
H	1.975896	-2.240667	-1.918689
H	2.101317	-0.810002	-2.954050
C	1.541867	1.769663	2.215337
H	1.473248	2.681571	1.610870
H	0.539366	1.335117	2.301490
H	1.868996	2.060660	3.223380
C	4.182076	0.390971	-1.654215
H	4.690189	0.991902	-0.895826
H	4.957458	-0.126410	-2.237238
H	3.658399	1.067320	-2.339663
N	-2.533731	-0.769067	-0.049762
C	-3.127087	0.456208	-0.034839
C	-4.511807	0.577753	0.103565
H	-4.963808	1.564863	0.138745
C	-5.298284	-0.555809	0.204277
H	-6.376013	-0.468829	0.312219
C	-4.683142	-1.806161	0.164008
H	-5.257548	-2.724938	0.231485
C	-3.307592	-1.864084	0.043423
H	-2.779219	-2.814177	0.023437
C	-0.564570	-1.043670	2.086177
O	-0.735843	-1.525192	3.127149
O	0.107987	0.188525	-2.827826
H	-0.715771	0.645779	-3.049646
H	0.733341	0.910060	-2.217991

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SCF done: -1176.170369

C	-0.032068	2.310492	-0.435107
C	-0.415863	3.631139	-0.401926
C	-1.780096	3.956101	-0.277926
C	-2.704184	2.938556	-0.233466
C	-2.274930	1.601688	-0.266198
N	-0.938022	1.297077	-0.312649
H	-2.096911	4.994610	-0.242371
H	0.336198	4.410176	-0.504140
H	-3.764822	3.163564	-0.160905
Ru	-0.425593	-0.701796	0.069964
P	1.774943	0.150528	-0.134736
C	-0.047091	-2.445234	-0.545578
O	0.164157	-3.545089	-0.875714
C	2.771065	0.457647	1.481787
C	2.944726	-0.477973	-1.527670
C	2.954389	-0.865419	2.225858
H	3.447651	-0.669933	3.188404
H	1.999438	-1.355679	2.438289
H	3.582674	-1.570751	1.671411
C	4.136805	1.105900	1.270297
H	4.086441	2.018278	0.662562
H	4.546089	1.391432	2.249898
H	4.859392	0.421406	0.812040
C	3.650631	-1.749578	-1.058777
H	4.156597	-2.217549	-1.914685
H	4.415175	-1.545290	-0.300559
H	2.945918	-2.486398	-0.652854
C	2.064706	-0.831038	-2.729233
H	2.714898	-1.143132	-3.559058
H	1.376444	-1.650793	-2.505359
H	1.462351	0.016244	-3.080689
C	1.921198	1.398414	2.340109
H	1.841332	2.402973	1.905781
H	0.908484	1.011794	2.497991
H	2.396363	1.503899	3.325166
C	3.981141	0.549041	-1.986884
H	4.690568	0.827657	-1.204551
H	4.561639	0.111970	-2.811656
H	3.522157	1.466042	-2.375714
N	-2.511280	-0.761128	-0.183196
C	-3.143564	0.457911	-0.227662
C	-4.548029	0.531853	-0.231756
H	-5.029030	1.505662	-0.267139
C	-5.305545	-0.614408	-0.201949
H	-6.390553	-0.559438	-0.213181
C	-4.648079	-1.856047	-0.160164
H	-5.201464	-2.789906	-0.140528
C	-3.275545	-1.879396	-0.146991
H	-2.728343	-2.817956	-0.110388
C	-0.455298	-1.074582	1.951310
O	-0.536822	-1.488730	3.035788
C	1.374366	1.892468	-0.731908
H	1.471104	1.842921	-1.826435
H	2.106200	2.633007	-0.385368

TS₁₂₋₁₃

SCF done: -1176.114604

C	0.461165	0.906148	0.000000
C	0.218219	2.140000	0.593573
C	-1.059087	2.402034	1.085561
C	-2.027372	1.408709	1.034773
C	-1.701094	0.211823	0.398830
N	-0.508572	-0.005055	-0.167162
H	-1.276279	3.356717	1.558481
H	1.022376	2.864685	0.702654
H	-3.002516	1.530841	1.497203
Ru	0.124550	-1.694226	1.686726
P	2.145861	-1.187611	0.679158
C	0.407858	-3.546279	1.683013

O	0.622050	-4.668049	1.953487	C	-3.068798	0.582240	2.606320
C	3.617835	-0.715440	1.818670	H	-3.082318	1.165842	3.537776
C	2.718370	-2.416515	-0.694037	H	-4.108454	0.470094	2.278102
C	3.670883	-1.744691	2.950005	H	-2.669653	-0.412197	2.846874
H	4.524529	-1.512967	3.602312	C	-0.835222	1.555516	2.224876
H	2.758817	-1.725302	3.555384	H	-0.978363	2.160868	3.131605
H	3.799716	-2.768546	2.578955	H	-0.353818	0.613710	2.517547
C	4.967026	-0.662348	1.106614	H	-0.146808	2.103121	1.569598
H	4.957932	0.014123	0.242340	C	-3.288727	-1.139654	-1.961402
H	5.717582	-0.278291	1.811979	H	-3.197899	-0.348507	-2.715266
H	5.310286	-1.648844	0.777512	H	-2.380000	-1.755320	-1.989420
C	3.310854	-3.677532	-0.064131	H	-4.139185	-1.769334	-2.256245
H	3.527681	-4.400522	-0.863082	C	-2.825227	2.651821	1.220616
H	4.256449	-3.480258	0.455610	H	-3.793671	2.557835	0.718755
H	2.624148	-4.163429	0.635757	H	-2.988414	3.225751	2.144451
C	1.466323	-2.798481	-1.490904	H	-2.164324	3.253979	0.584832
H	1.757379	-3.516873	-2.270160	N	4.385946	0.760633	-0.228835
H	0.702371	-3.262109	-0.858247	C	3.135144	0.606879	0.225016
H	1.002949	-1.936543	-1.987704	C	2.798683	-0.299569	1.233814
C	3.357414	0.670777	2.414427	H	1.773370	-0.368849	1.597079
H	3.490485	1.470378	1.675263	C	3.798232	-1.119682	1.745351
H	2.365698	0.773050	2.862242	H	3.566203	-1.844483	2.521681
H	4.093551	0.844988	3.211171	C	5.086332	-0.998519	1.245728
C	3.739261	-1.834099	-1.677068	H	5.895426	-1.626124	1.608999
H	4.715534	-1.642838	-1.226541	C	5.327924	-0.035283	0.267954
H	3.894803	-2.571046	-2.477488	H	6.332547	0.099487	-0.134067
H	3.399452	-0.912172	-2.162390	C	1.655461	-1.927498	-1.064395
N	-3.002591	-1.349273	1.658646	O	2.555064	-2.394614	-1.630168
C	-2.555922	-1.003081	0.442743				
C	-2.754475	-1.787431	-0.696751				
H	-2.344093	-1.461412	-1.648910	TS₁₃₋₁₄			
C	-3.446287	-2.980192	-0.564734	SCF done: -1176.152573			
H	-3.619144	-3.616344	-1.429474	C	0.039459	2.078607	0.885437
C	-3.902035	-3.358185	0.694931	C	-0.291728	3.418312	0.993056
H	-4.433027	-4.293612	0.846126	C	-1.611539	3.816804	0.751634
C	-3.653503	-2.512109	1.768313	C	-2.553920	2.875232	0.396941
H	-3.987482	-2.778188	2.770760	C	-2.164017	1.535222	0.279388
C	0.353899	-0.517055	3.176385	N	-0.889305	1.157026	0.536030
O	0.523178	-0.104826	4.257245	H	-1.886417	4.865584	0.834258
C	1.816395	0.390223	-0.360681	H	0.474810	4.140758	1.262072
H	1.817986	0.076995	-1.409552	H	-3.589762	3.122349	0.184975
H	2.613927	1.127717	-0.221244	Ru	-0.431579	-0.916121	0.194518
				H	2.163800	2.369767	1.107052
				P	1.779952	0.140269	-0.053434
				C	1.421693	1.562722	1.130876
				H	1.455400	1.109869	2.130659
				C	-0.098714	-2.672608	-0.358407
				O	0.088026	-3.756446	-0.731090
				C	3.367400	-0.662446	0.666196
				C	2.177878	1.043302	-1.710173
				C	3.531782	-2.033810	0.006000
				H	4.401737	-2.541356	0.445670
				H	2.653028	-2.666669	0.176543
				H	3.699055	-1.971188	-1.074377
				C	4.640186	0.159770	0.492586
				H	4.541450	1.166091	0.919251
				H	5.463471	-0.340054	1.023181
				H	4.942900	0.253093	-0.555994
				C	2.845524	0.047148	-2.657263
				H	2.918940	0.491494	-3.659640
				H	3.861600	-0.217871	-2.342590
				H	2.256700	-0.876125	-2.748030
				C	0.851159	1.473330	-2.342773
				H	1.062827	1.927008	-3.321409
				H	0.177246	0.623013	-2.495063
				H	0.320371	2.223277	-1.742602
				C	3.144560	-0.886365	2.163647
				H	3.188326	0.048835	2.734688
				H	2.191889	-1.383861	2.377742
				H	3.947468	-1.532589	2.543946
				C	3.042563	2.293248	-1.550087
				H	4.024518	2.095866	-1.111456

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SCF done: -1176.166112

C	-0.056153	1.884660	-1.096691
C	0.243271	3.210573	-1.388130
C	1.539444	3.674505	-1.199103
C	2.489665	2.805698	-0.696354
C	2.122847	1.494602	-0.386906
N	0.873887	1.028720	-0.609619
H	1.797551	4.704546	-1.432492
H	-0.538188	3.860930	-1.773420
H	3.517721	3.105203	-0.520359
Ru	0.169108	-1.104671	-0.223639
H	-2.153395	2.165816	-1.458892
P	-1.896463	0.150978	0.066011
C	-1.433986	1.350406	-1.313166
H	-1.430995	0.732067	-2.219647
C	-0.549114	-2.767466	0.100649
O	-1.027759	-3.809839	0.323480
C	-3.551337	-0.582534	-0.558995
C	-2.200895	1.304499	1.576407
C	-3.953490	-1.757385	0.338102
H	-4.862779	-2.216376	-0.074964
H	-3.180343	-2.532719	0.370616
H	-4.181448	-1.455934	1.364855
C	-4.692468	0.428119	-0.630591
H	-4.442180	1.300933	-1.247453
H	-5.567001	-0.053047	-1.091676
H	-5.004159	0.782138	0.359191

H	3.211945	2.733863	-2.543219
H	2.541223	3.060373	-0.945830
N	-4.349959	0.750673	-0.304035
C	-3.043598	0.473049	-0.165967
C	-2.439152	-0.787703	-0.440513
H	-1.310073	-0.648624	-1.281788
C	-3.331509	-1.789540	-0.886076
H	-2.949350	-2.778331	-1.136596
C	-4.678471	-1.517044	-0.997622
H	-5.377538	-2.286593	-1.317465
C	-5.146258	-0.226045	-0.703031
H	-6.205802	0.012055	-0.802529
C	-0.399667	-1.403300	2.065371
O	-0.428550	-1.733292	3.176504

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SCF done: -1176.171486			
C	0.011426	2.241211	-0.566528
C	-0.356082	3.581329	-0.610365
C	-1.700748	3.919603	-0.466196
C	-2.648326	2.921151	-0.323233
C	-2.221419	1.594981	-0.270762
N	-0.908082	1.287789	-0.334132
H	-2.004341	4.963511	-0.493872
H	0.401774	4.342230	-0.779841
H	-3.713712	3.118484	-0.255243
Ru	-0.447817	-0.793476	-0.041435
H	-0.426504	-0.836905	-1.702672
P	1.828541	0.111300	-0.146867
C	-0.149738	-2.631287	-0.214252
O	0.032740	-3.760276	-0.405912
C	2.676485	0.591948	1.507385
C	3.122547	-0.578686	-1.383856
C	2.798385	-0.658785	2.379629
H	3.186451	-0.373440	3.367397
H	1.829286	-1.146283	2.531737
H	3.486686	-1.398590	1.957460
C	4.046931	1.245878	1.361310
H	4.025696	2.127045	0.707709
H	4.384517	1.586803	2.350591
H	4.806643	0.551496	0.986283
C	3.861356	-1.742101	-0.722346
H	4.459395	-2.265868	-1.480773
H	4.550475	-1.413970	0.064959
H	3.164695	-2.474077	-0.291480
C	2.350897	-1.130843	-2.584352
H	3.075258	-1.514586	-3.316807
H	1.680117	-1.948372	-2.302478
H	1.743082	-0.369085	-3.086822
C	1.747063	1.586982	2.208451
H	1.698741	2.552752	1.690298
H	0.726232	1.204869	2.313381
H	2.132182	1.777710	3.219606
C	4.121358	0.460147	-1.893455
H	4.745220	0.886173	-1.103587
H	4.794493	-0.023384	-2.615503
H	3.628180	1.284939	-2.422262
C	-3.120144	0.441396	-0.202202
C	-5.253701	-0.352628	-0.207330
H	-6.323304	-0.138763	-0.208076
C	-4.795220	-1.670781	-0.209076
H	-5.506855	-2.493717	-0.217528
C	-3.427080	-1.910119	-0.193632
H	-3.060590	-2.936421	-0.184273
C	-0.683444	-0.848807	1.914516
O	-0.896808	-0.977144	3.042132
C	-2.525819	-0.840550	-0.189419
N	-4.437425	0.693129	-0.206331
C	1.402368	1.785890	-0.893757
H	1.431952	1.619132	-1.980984
H	2.148604	2.559108	-0.670761

TS₁₄₋₁₅

SCF done: -1360.707320			
C	-0.082952	2.434912	-0.459107
C	0.279609	3.767636	-0.300015
C	1.612527	4.083199	-0.042326
C	2.554915	3.073212	0.042735
C	2.136957	1.752990	-0.112082
N	0.837770	1.460108	-0.340878
H	1.909149	5.121501	0.085818
H	-0.476255	4.543924	-0.388211
H	3.607750	3.256921	0.233536
Ru	0.385944	-0.641914	-0.360618
H	0.677678	-0.486601	1.398783
P	-1.897084	0.299319	-0.181656
C	0.099733	-2.502371	-0.189073
O	-0.051187	-3.648159	-0.205730
C	-3.250520	-0.384513	-1.366016
C	-2.606254	0.669072	1.564449
C	-3.220596	-1.908411	-1.213270
H	-4.026915	-2.347162	-1.817279
H	-2.271711	-2.332110	-1.560169
C	-3.368600	-2.232302	-0.175546
H	-4.668377	0.117841	-1.111099
H	-4.732255	1.212921	-1.092125
H	-5.316518	-0.234874	-1.925891
C	-5.085924	-0.275549	-0.178555
H	-2.893943	-0.665198	2.251412
H	-3.166744	-0.481295	3.299923
H	-3.736742	-1.193563	1.787271
H	-2.022713	-1.333768	2.244406
C	-1.513272	1.416824	2.334269
H	-1.839891	1.525141	3.377512
H	-0.553440	0.893774	2.343448
C	-1.353490	2.428338	1.939156
H	-2.880841	-0.030818	-2.806795
H	-3.075734	1.024256	-3.036099
H	-1.838349	-0.257505	-3.054208
C	-3.508905	-0.627555	-3.482257
H	-3.851993	1.554898	1.597124
H	-4.756301	1.047118	1.257883
H	-4.027359	1.861125	2.637865
C	-3.732422	2.476125	1.012199
H	3.033317	0.596240	-0.042738
C	5.147611	-0.204516	0.226926
H	6.204994	0.007164	0.389902
C	4.700586	-1.520992	0.106988
H	5.407833	-2.344296	0.178450
C	3.346935	-1.757190	-0.097591
H	2.984128	-2.781211	-0.182951
C	0.492084	-0.792647	-2.270075
O	0.658693	-0.921310	-3.407308
C	2.456912	-0.684079	-0.183076
N	4.335598	0.842435	0.156474
C	-1.482728	2.026261	-0.821409
H	-2.208085	2.788150	-0.508466
H	-1.540010	1.961224	-1.916126
N	0.685235	-1.706488	3.030907
N	1.133943	-0.670282	2.696980
O	0.002143	-2.638220	2.655201

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SCF done: -1360.740519			
C	0.102699	2.189371	-0.729589
C	-0.233560	3.526365	-0.901994
C	-1.559490	3.921964	-0.735552
C	-2.526277	2.981191	-0.421444
C	-2.135217	1.658765	-0.234663
N	-0.837133	1.296489	-0.360498
H	-1.835334	4.964550	-0.873335
H	0.534162	4.239826	-1.190318

H	-3.579428	3.223334	-0.316944	H	-4.558737	-1.490060	0.424033
Ru	-0.421525	-0.719241	0.308695	C	-4.488712	0.550717	-1.446166
H	-0.902259	0.261558	-2.179100	H	-4.088997	1.440411	-1.947483
P	1.930881	0.124247	-0.063142	H	-5.224980	0.104130	-2.129505
C	-0.145625	-2.502438	0.875005	H	-5.030504	0.875274	-0.554830
O	0.015132	-3.595361	1.202145	C	-2.498208	-0.803929	2.520291
C	2.806903	0.858313	1.481668	H	-2.827498	-0.622012	3.553150
C	3.188254	-0.769007	-1.192086	H	-3.132527	-1.599116	2.111201
C	2.858642	-0.222148	2.564675	H	-1.461185	-1.154882	2.551591
H	3.329627	0.192486	3.466710	C	-1.680060	1.542993	2.360909
H	1.860425	-0.573587	2.845808	H	-1.956022	1.648388	3.419569
H	3.446897	-1.093960	2.256367	H	-0.633498	1.226252	2.317522
C	4.219556	1.377709	1.226096	H	-1.791699	2.533146	1.900233
H	4.255246	2.124473	0.423242	C	-2.790995	-0.919169	-2.485480
H	4.582398	1.868997	2.140117	H	-2.289341	-0.101520	-3.017778
H	4.928341	0.577547	0.989167	H	-2.074653	-1.738341	-2.360382
C	3.868476	-1.865693	-0.372385	H	-3.596589	-1.281098	-3.139317
H	4.462847	-2.497324	-1.046501	C	-4.037222	1.038118	1.805852
H	4.550325	-1.468699	0.388545	H	-4.787530	0.309903	1.479538
H	3.134537	-2.517045	0.121824	H	-4.258011	1.277129	2.855882
C	2.382542	-1.439734	-2.305974	H	-4.173244	1.963417	1.231126
H	3.081408	-1.984272	-2.955812	C	2.974116	0.660620	-0.224688
H	1.640392	-2.145730	-1.920981	C	5.129526	-0.054493	-0.070974
H	1.844755	-0.722767	-2.939012	H	6.184337	0.199921	0.036500
C	1.968578	2.037201	1.984394	C	4.731591	-1.387976	-0.168608
H	2.033559	2.904425	1.316040	H	5.474238	-2.181503	-0.132287
H	0.910879	1.794470	2.124246	C	3.379018	-1.679543	-0.298769
H	2.357988	2.353471	2.961858	H	3.052883	-2.717518	-0.356293
C	4.231380	0.143109	-1.835394	C	0.381367	-0.836505	-2.201699
H	4.917166	0.604146	-1.120353	O	0.475559	-0.923175	-3.351376
H	4.838868	-0.460459	-2.524358	C	2.447631	-0.642349	-0.330964
H	3.771819	0.937274	-2.436064	N	4.273665	0.960051	-0.096844
C	-3.055408	0.552253	0.044819	C	-1.637938	1.876836	-0.753046
C	-5.197935	-0.204003	0.171876	H	-2.378184	2.622879	-0.437701
H	-6.263805	0.024165	0.145351	H	-1.745521	1.765861	-1.842820
C	-4.761773	-1.514550	0.374299	N	1.135632	-1.740547	2.557876
H	-5.486790	-2.317167	0.487208	N	2.110765	-1.292234	3.074788
C	-3.397352	-1.769654	0.434353	O	0.652282	-0.455460	1.746210
H	-3.040295	-2.785720	0.596517				
C	-0.571157	-0.146285	2.091948				
O	-0.774753	0.149302	3.192033				
C	-2.493470	-0.719988	0.276775				
N	-4.367940	0.818292	0.006260				
C	1.467157	1.658372	-1.054865				
H	1.445025	1.324087	-2.104180				
H	2.226598	2.447595	-0.990672				
N	-0.816016	-1.481083	-2.786593				
N	-0.974081	-0.280380	-3.063586				
O	-0.564980	-1.863024	-1.559389				

TS₁₅₋₁₆

SCF done: -1360.702981

C	-0.242137	2.352653	-0.472468
C	0.065704	3.702162	-0.340977
C	1.393828	4.081188	-0.158838
C	2.388366	3.118081	-0.119954
C	2.025383	1.779155	-0.245090
N	0.731134	1.427330	-0.400850
H	1.647287	5.133363	-0.053116
H	-0.729361	4.441873	-0.388745
H	3.439625	3.354927	0.011417
Ru	0.376756	-0.682497	-0.320291
H	1.787149	-0.246406	2.418892
P	-1.976885	0.159738	-0.044342
C	0.134073	-2.546412	-0.107137
O	-0.027518	-3.684028	-0.003702
C	-3.401513	-0.482563	-1.152999
C	-2.610444	0.502836	1.729675
C	-4.007255	-1.722869	-0.493505
H	-4.714242	-2.191259	-1.192077
H	-3.238985	-2.470133	-0.252172

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SCF done: -1251.375584

C	0.041580	2.222194	-0.593426
C	-0.313786	3.564246	-0.704524
C	-1.649563	3.926638	-0.557597
C	-2.608708	2.949297	-0.345225
C	-2.193333	1.626072	-0.226656
N	-0.886069	1.301064	-0.288512
H	-1.941293	4.971123	-0.639032
H	0.449480	4.305596	-0.927561
H	-3.670680	3.164270	-0.278388
Ru	-0.457174	-0.785484	-0.008189
H	-1.256204	-0.948660	-2.377459
P	1.876229	0.116723	-0.093226
C	-0.174664	-2.640493	-0.042706
O	-0.009816	-3.780630	-0.135431
C	2.635759	0.657953	1.583027
C	3.225985	-0.590689	-1.252475
C	2.720230	-0.563061	2.501324
H	3.087621	-0.247378	3.487848
H	1.743811	-1.036180	2.648070
H	3.410608	-1.323914	2.121850
C	4.013680	1.304983	1.478141
H	4.031278	2.145783	0.773724
H	4.294238	1.701442	2.464463
H	4.791052	0.590588	1.187193
C	3.872306	-1.787279	-0.553971
H	4.526343	-2.307656	-1.266838
H	4.492023	-1.495062	0.302221
H	3.120804	-2.510431	-0.209592
C	2.522242	-1.092452	-2.516235
H	3.267330	-1.614348	-3.133680

H	1.684992	-1.764308	-2.306945	C	-4.718538	-1.619097	-0.101741
H	2.105978	-0.273940	-3.113429	H	-5.441481	-2.421461	0.028074
C	1.683989	1.682444	2.207833	C	-3.401587	-1.762345	0.322566
H	1.670783	2.629247	1.653741	H	-3.081697	-2.691969	0.794111
H	0.654178	1.319545	2.286283	C	-0.651649	-0.324435	2.258267
H	2.029468	1.906177	3.226589	O	-0.790640	-0.208951	3.409209
C	4.298319	0.412853	-1.675608	C	-2.490663	-0.716464	0.148941
H	4.945602	0.732991	-0.855588	N	-4.275483	0.599651	-0.883998
H	4.939647	-0.065039	-2.429734	C	1.398074	2.090719	0.387027
H	3.867723	1.305684	-2.144655	H	2.177552	2.762619	0.006893
C	-3.107233	0.483314	-0.104233	H	1.299178	2.284939	1.463825
C	-5.248659	-0.288564	-0.040386	O	-0.180239	-2.071830	-1.244743
H	-6.314959	-0.060206	-0.024812				
C	-4.808783	-1.610945	-0.012473				
H	-5.530197	-2.424278	0.022194	18			
C	-3.441540	-1.865799	-0.019563	SCF done: -1251.375607			
H	-3.085417	-2.895237	0.017899	C	0.031608	2.217722	-0.695847
C	-0.662237	-0.773594	1.877191	C	-0.341387	3.542758	-0.903534
O	-0.879785	-0.796124	3.015345	C	-1.675359	3.902678	-0.731391
C	-2.533185	-0.806366	-0.067922	C	-2.608483	2.944646	-0.366802
N	-4.419883	0.748508	-0.087527	C	-2.176506	1.637458	-0.161142
C	1.428830	1.747684	-0.910951	N	-0.875502	1.306841	-0.306954
H	1.442221	1.517574	-1.986123	H	-1.983895	4.933464	-0.890452
H	2.171702	2.535739	-0.732819	H	0.404042	4.272838	-1.208810
O	-0.363101	-0.766530	-2.069392	H	-3.662733	3.165438	-0.230516

TS₁₆₋₁₈

SCF done: -1251.357874

C	0.067978	2.376209	-0.249446	Ru	-0.401763	-0.720767	0.234728
C	-0.235584	3.595424	-0.846932	H	-0.963307	-0.902236	-3.345975
C	-1.518203	3.797095	-1.353540	P	1.849425	0.186034	0.052211
C	-2.470243	2.795212	-1.247871	C	-0.621514	-1.440522	-1.593291
C	-2.105688	1.591760	-0.647517	O	-0.600810	-2.593014	-1.963617
N	-0.855923	1.403786	-0.180125	C	2.467183	0.862849	1.734373
H	-1.771202	4.743326	-1.826189	C	3.275649	-0.595360	-0.946216
H	0.521947	4.372836	-0.906276	C	2.592827	-0.308580	2.712790
H	-3.485457	2.902197	-1.617563	H	2.801808	0.083261	3.718350
H	-3.485457	2.902197	-1.617563	H	1.665135	-0.892369	2.765893
Ru	-0.442445	-0.634051	0.469050	H	3.404849	-0.994741	2.452635
H	-1.054111	-2.342284	-1.562909	C	3.777552	1.639566	1.683203
P	1.848435	0.259623	0.257939	H	3.750290	2.457485	0.951907
C	-0.176132	-2.527777	0.359973	H	3.970836	2.089298	2.667981
O	-0.073563	-3.673342	0.611253	C	4.633321	0.995727	1.449723
C	3.150367	-0.048026	1.626950	H	3.961508	-1.650738	-0.080522
C	2.618198	0.126542	-1.491361	H	4.635756	-2.248371	-0.709493
C	3.147826	-1.557912	1.885404	H	4.568501	-1.206908	0.717228
H	3.905406	-1.794147	2.645645	H	3.236229	-2.341123	0.371587
H	2.174908	-1.900397	2.256510	C	2.622951	-1.309706	-2.132121
H	3.383119	-2.141679	0.987614	H	3.409222	-1.794719	-2.727481
C	4.562950	0.423310	1.298909	H	1.915501	-2.082143	-1.808527
H	4.592345	1.485465	1.024116	H	2.089223	-0.620824	-2.799080
H	5.194250	0.296891	2.190077	C	1.361376	1.787068	2.253194
H	5.024763	-0.160155	0.494571	H	1.246521	2.692928	1.645303
C	3.119379	-1.305023	-1.682184	H	0.385228	1.282986	2.297876
H	3.450878	-1.433344	-2.722303	H	1.612684	2.104639	3.274726
H	3.976378	-1.536253	-1.037502	C	4.300625	0.407732	-1.467267
H	2.322801	-2.035579	-1.494740	H	4.809806	0.953722	-0.667108
C	1.483938	0.384853	-2.491512	H	5.070473	-0.132154	-2.037013
H	1.884161	0.245417	-3.505828	H	3.853558	1.139356	-2.150739
H	0.654422	-0.317659	-2.359696	C	-3.059173	0.522084	0.209185
H	1.103922	1.413112	-2.433106	C	-5.170349	-0.221094	0.618672
C	2.695336	0.659247	2.905165	H	-6.232495	0.009304	0.712668
H	2.843598	1.744970	2.853334	C	-4.713383	-1.527905	0.791044
H	1.648822	0.456774	3.159658	H	-5.419641	-2.325290	1.012509
H	3.306371	0.292403	3.741325	C	-3.353118	-1.786517	0.671524
C	3.734462	1.125735	-1.789421	H	-2.981430	-2.803737	0.795544
H	4.646724	0.947959	-1.215577	C	-0.086788	-2.459406	0.831426
H	3.999628	1.039570	-2.852716	O	0.105792	-3.535397	1.223983
H	3.420664	2.164852	-1.626809	C	-2.459395	-0.746564	0.387775
C	-3.012728	0.447924	-0.463435	N	-4.365635	0.795281	0.327612
C	-5.105676	-0.421693	-0.701174	C	1.432484	1.736934	-0.941960
H	-6.130656	-0.283427	-1.047511	H	1.488804	1.412425	-1.991293
				H	2.162656	2.547383	-0.815449
				O	-0.829563	-0.436319	-2.503661

TS₁₄₋₁₆			Ru	0.4177370	-0.650656	-0.386068
SCF done:	-1360.682533		H	0.9434660	-1.761278	1.328783
C	0.011426	2.241211	P	-1.9208030	0.128081	0.033463
C	-0.356082	3.581329	C	0.1195220	-2.473959	-0.784522
C	-1.700748	3.919603	O	-0.0697530	-3.591281	-1.007447
C	-2.648326	2.921151	C	-2.7942920	0.997540	-1.442577
C	-2.221419	1.594981	C	-3.1908630	-0.890303	1.045805
N	-0.908082	1.287789	C	-2.9545100	0.013951	-2.603185
H	-2.004341	4.963511	H	-3.3770300	0.546513	-3.466546
H	0.401774	4.342230	H	-1.9959490	-0.409595	-2.920863
H	-3.713712	3.118484	H	-3.6287950	-0.815419	-2.368412
Ru	-0.447817	-0.793476	C	-4.1546850	1.597140	-1.090537
H	-0.425567	-0.838814	H	-4.0995770	2.289482	-0.241090
P	1.828541	0.111300	H	-4.5177720	2.174701	-1.952533
C	-0.149738	-2.631287	H	-4.9126230	0.837423	-0.872057
O	0.032740	-3.760276	C	-3.9792870	-1.783497	0.088937
C	2.676485	0.591948	H	-4.5813750	-2.486877	0.679845
C	3.122547	-0.578686	H	-4.6704460	-1.224055	-0.550915
C	2.798385	-0.658785	H	-3.3138230	-2.381275	-0.549497
H	3.186451	-0.373440	C	-2.4191230	-1.801792	2.003381
H	1.829286	-1.146283	H	-3.1481070	-2.401163	2.566326
H	3.486686	-1.398590	H	-1.7681060	-2.499922	1.461849
C	4.046931	1.245878	H	-1.7936360	-1.249847	2.712839
H	4.025696	2.127045	C	-1.8879050	2.144212	-1.901652
H	4.384517	1.586803	H	-1.8148130	2.946041	-1.157296
H	4.806643	0.551496	H	-0.8732860	1.814345	-2.147757
C	3.861356	-1.742101	H	-2.3158130	2.584442	-2.812686
H	4.459395	-2.265868	C	-4.1381530	-0.020223	1.870393
H	4.550475	-1.413970	H	-4.7611100	0.642868	1.263381
H	3.164695	-2.474077	H	-4.8133290	-0.678172	2.434932
C	2.350897	-1.130843	H	-3.5989740	0.586926	2.606715
H	3.075258	-1.514586	C	3.0454580	0.647959	-0.130921
H	1.680117	-1.948372	C	5.1940020	-0.044119	-0.430879
H	1.743082	-0.369085	H	6.2550040	0.207090	-0.428966
C	1.747063	1.586982	C	4.7766080	-1.339741	-0.733273
H	1.698741	2.552752	H	5.5094770	-2.109814	-0.961846
H	0.726232	1.204869	C	3.4154920	-1.621281	-0.743523
H	2.132182	1.777710	H	3.0741870	-2.625882	-0.991926
C	4.121358	0.460147	C	0.5244150	-0.237144	-2.191598
H	4.745220	0.886173	O	0.6772930	-0.063400	-3.325946
H	4.794493	-0.023384	C	2.4989430	-0.617989	-0.428480
H	3.628180	1.284939	N	4.3515100	0.939041	-0.133792
C	-3.120144	0.441396	C	-1.4658280	1.563752	1.149550
C	-5.253701	-0.352628	H	-1.3771920	1.105180	2.146183
H	-6.323304	-0.138763	H	-2.2423210	2.337942	1.185270
C	-4.795220	-1.670781	O	0.2370620	-0.372329	2.500493
H	-5.506855	-2.493717	N	0.7745890	-1.550208	2.456902
C	-3.427080	-1.910119	N	1.0726850	-2.359467	3.260895
H	-3.060590	-2.936421				
C	-0.683444	-0.848807				
O	-0.896808	-0.977144				
C	-2.525819	-0.840550				
N	-4.437425	0.693129				
C	1.402368	1.785890				
H	1.431952	1.619132				
H	2.148604	2.559108				
O	-0.844360	-0.519528				
N	-1.009817	-1.265784				
N	-1.467917	-0.689505				
TS₁₄₋₁₇			17			
SCF done:	-1360.668923		SCF done:	-1360.719313		
C	-0.1170030	2.141091	C	0.077581	2.252197	-0.300507
C	0.2127970	3.444399	C	-0.281489	3.596071	-0.298969
C	1.5308630	3.874201	C	-1.619824	3.944402	-0.145443
C	2.5015400	2.991726	C	-2.577668	2.952378	-0.012348
C	2.1128430	1.707318	C	-2.161228	1.625633	0.014040
N	0.8183830	1.328423	N	-0.854061	1.304045	-0.093193
H	1.8002550	4.889631	H	-1.913012	4.991536	-0.151249
H	-0.5550850	4.098414	H	0.483181	4.353210	-0.452601
H	3.5541630	3.248934	H	-3.639585	3.159845	0.074829
			Ru	-0.428401	-0.783764	0.167703
			H	-1.470513	-0.735290	-3.572475
			P	1.918747	0.126540	-0.009464
			C	-0.131961	-2.645495	0.274681
			O	0.045409	-3.785231	0.300386
			C	2.809793	0.530464	1.643896
			C	3.172726	-0.545713	-1.290269
			C	2.867089	-0.739325	2.495730
			H	3.363913	-0.513170	3.449488
			H	1.868703	-1.123119	2.728565
			H	3.431906	-1.543063	2.011132

C	4.221743	1.087926	1.478084	H	3.307428	0.528972	-3.061609
H	4.251041	1.978861	0.838986	C	0.933585	1.161770	2.086568
H	4.599210	1.387079	2.466382	H	0.417883	2.000410	1.603171
H	4.924217	0.349873	1.076556	H	0.238741	0.309532	2.137759
C	3.883889	-1.752697	-0.679580	H	1.155729	1.465580	3.119621
H	4.486383	-2.243348	-1.456265	C	4.679593	0.044544	-0.829316
H	4.563105	-1.480666	0.137090	H	4.948488	-0.067649	0.226036
H	3.167098	-2.496027	-0.304036	H	5.482402	-0.422750	-1.416960
C	2.360528	-1.028027	-2.493434	H	4.679819	1.113397	-1.079960
H	3.050075	-1.497490	-3.209241	C	-2.966648	0.536525	0.312896
H	1.587738	-1.752413	-2.215667	C	-4.782505	-0.034754	1.563569
H	1.853764	-0.202854	-3.007513	H	-5.646641	0.297924	2.140034
C	1.980152	1.587554	2.378088	C	-4.517520	-1.395290	1.419618
H	2.017391	2.563215	1.878936	H	-5.166555	-2.130681	1.888065
H	0.929429	1.307772	2.497904	C	-3.424349	-1.774400	0.651998
H	2.395469	1.721280	3.386547	H	-3.209057	-2.829107	0.483541
C	4.186391	0.486129	-1.782121	C	0.183291	-2.518866	0.328306
H	4.871924	0.832652	-1.004858	O	0.513871	-3.558660	0.732954
H	4.795050	0.025775	-2.573363	C	-2.601972	-0.805764	0.063012
H	3.695518	1.360266	-2.226664	N	-4.026421	0.923021	1.031617
C	-3.073045	0.480463	0.124904	C	1.385151	1.629235	-1.382983
C	-5.210092	-0.304798	0.178188	H	1.318537	1.236827	-2.406588
H	-6.277883	-0.082745	0.178379	H	2.154381	2.411529	-1.374586
C	-4.763931	-1.624517	0.232177	O	-1.792669	-1.458129	-2.380921
H	-5.481286	-2.441318	0.269064				
C	-3.395619	-1.871983	0.244389				
H	-3.031312	-2.897743	0.292260	19			
C	-0.534242	-0.652638	2.032608	SCF done: -1062.859162			
O	-0.701889	-0.617086	3.177500	C	-0.051494	2.086330	-0.885133
C	-2.500426	-0.805114	0.190936	C	-0.440489	3.421419	-0.876666
N	-4.387882	0.736638	0.123709	C	-1.778117	3.738792	-0.644306
C	1.455354	1.811536	-0.678503	C	-2.697534	2.725101	-0.423420
H	1.391022	1.647883	-1.765458	C	-2.249293	1.406770	-0.445361
H	2.205277	2.585574	-0.476079	N	-0.953879	1.106295	-0.672288
O	-0.702999	-1.247377	-1.903971	H	-2.095305	4.778678	-0.629072
N	-0.867026	-0.271382	-2.859558	H	0.300753	4.199165	-1.044074
N	-0.429300	0.833956	-2.933563	H	-3.744389	2.916858	-0.209840
				Ru	-0.369954	-0.910565	-0.237757
				H	-1.878846	-1.267112	-1.270992
				P	1.700136	0.104337	-0.026527
TS₁₈₋₁₉				C	2.043935	0.874718	1.704555
SCF done: -1251.340054				C	3.300047	-0.613433	-0.799692
C	0.046008	2.154664	-0.979253	C	2.739915	-0.163811	2.582106
C	-0.253464	3.512004	-0.939714	H	2.755329	0.192630	3.622004
C	-1.516592	3.914178	-0.514509	H	2.210886	-1.125921	2.568431
C	-2.444481	2.962626	-0.121126	H	3.780281	-0.333230	2.280283
C	-2.089581	1.616928	-0.180120	C	2.852861	2.167953	1.686425
N	-0.870454	1.234462	-0.615403	H	2.319035	2.978471	1.174257
H	-1.767095	4.971532	-0.476372	H	3.016483	2.502506	2.721275
H	0.500143	4.238559	-1.232659	H	3.837503	2.054713	1.221428
H	-3.428188	3.220995	0.257728	C	3.579481	-1.979835	-0.170361
Ru	-0.314262	-0.820346	-0.238254	H	4.457749	-2.420788	-0.663165
H	-2.174607	-1.136540	-1.146318	H	3.801367	-1.920910	0.899463
P	1.817120	0.107383	-0.345598	H	2.739369	-2.669255	-0.305769
C	-0.537064	-1.551757	-2.174468	C	2.999635	-0.840662	-2.283714
O	0.374477	-1.940791	-2.868786	H	3.785522	-1.476814	-2.713326
C	2.252537	0.792342	1.393297	H	2.034341	-1.346172	-2.422646
C	3.363090	-0.631526	-1.203367	H	2.993058	0.094501	-2.857002
C	2.892604	-0.334036	2.206768	C	0.669902	1.169747	2.316882
H	3.017946	-0.000429	3.246378	H	0.127485	1.954346	1.772657
H	2.256405	-1.228471	2.221071	H	0.036005	0.272130	2.334126
H	3.880966	-0.625676	1.836839	H	0.807780	1.522008	3.349886
C	3.140348	2.033507	1.380283	C	4.526112	0.283658	-0.665354
H	2.660778	2.868776	0.852911	H	4.865513	0.375800	0.372932
H	3.307992	2.364227	2.415344	H	5.356364	-0.156090	-1.237084
H	4.121523	1.859968	0.930564	H	4.355618	1.291665	-1.066117
C	3.391773	-2.117370	-0.841625	C	-3.113826	0.251853	-0.165668
H	4.275802	-2.580356	-1.301472	C	-5.048890	-0.541420	0.750707
H	3.446998	-2.293456	0.239225	H	-6.018395	-0.309362	1.192707
H	2.502030	-2.625174	-1.229867	C	-4.646947	-1.869076	0.599448
C	3.187234	-0.506397	-2.718692	H	-5.289115	-2.677321	0.938743
H	3.978297	-1.096751	-3.201548	C	-3.428682	-2.124309	-0.009598
H	2.224922	-0.905172	-3.055478				

H	-3.087428	-3.142836	-0.183536	N	-0.959094	1.217024	-0.335526
C	0.146342	-2.660289	0.029954	H	-2.148380	4.868089	-0.377549
O	0.472267	-3.777390	0.175229	H	0.273137	4.320409	-0.664418
C	-2.620402	-1.054313	-0.410178	H	-3.803002	2.978217	-0.106111
N	-4.303928	0.499537	0.388323	Ru	-0.451089	-0.855106	-0.053269
C	1.354528	1.633858	-1.104636	H	-0.482223	-1.155775	-1.578902
H	1.440084	1.258336	-2.132108	P	1.770725	0.092910	-0.062881
H	2.072867	2.453822	-0.984243	C	2.428702	0.493129	1.691034

TS₁₉₋₂₀

SCF done: -1062.856513

C	-0.051364	2.207793	-0.567036
C	-0.462386	3.537494	-0.555506
C	-1.816021	3.827857	-0.403280
C	-2.729585	2.795398	-0.260989
C	-2.259151	1.485194	-0.266736
N	-0.944326	1.212744	-0.415921
H	-2.152235	4.862023	-0.393386
H	0.273248	4.329707	-0.671235
H	-3.793872	2.961744	-0.126074
Ru	-0.419319	-0.861829	-0.175048
H	-1.603758	-1.230830	-1.254349
P	1.770902	0.114715	-0.041264
C	2.361154	0.518218	1.729527
C	3.192287	-0.502398	-1.153496
C	2.475734	-0.791297	2.512203
H	2.680484	-0.562187	3.567713
H	1.544562	-1.369161	2.463156
H	3.288309	-1.429829	2.151155
C	3.666028	1.299692	1.824171
H	3.654328	2.218714	1.223693
H	3.831804	1.598960	2.869312
H	4.533515	0.702057	1.521793
C	3.806873	-1.750808	-0.521722
H	4.477607	-2.228519	-1.249270
H	4.406020	-1.517158	0.366309
H	3.040667	-2.486193	-0.243458
C	2.537326	-0.909822	-2.476573
H	3.309212	-1.319352	-3.143646
H	1.761942	-1.669859	-2.325917
H	2.072410	-0.062631	-2.996546
C	1.233297	1.342335	2.358416
H	1.116137	2.328069	1.890266
H	0.269291	0.818243	2.301802
H	1.462384	1.508227	3.420465
C	4.278089	0.533713	-1.431507
H	4.837248	0.815519	-0.534105
H	4.999682	0.110013	-2.144732
H	3.878412	1.448268	-1.886012
C	-3.113372	0.307505	-0.081261
C	-5.176402	-0.538535	0.397796
H	-6.228520	-0.342268	0.607019
C	-4.693560	-1.847574	0.363217
H	-5.365684	-2.681343	0.552169
C	-3.354129	-2.061672	0.077238
H	-2.955483	-3.073751	0.024646
C	-0.019849	-2.652946	0.026863
O	0.222662	-3.789960	0.156364
C	-2.495336	-0.971457	-0.142556
N	-4.406078	0.522472	0.182502
C	1.383535	1.817725	-0.774486
H	1.559709	1.713185	-1.854368
H	2.063441	2.603811	-0.419132

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SCF done: -1062.870764

C	-0.061961	2.202288	-0.518254
C	-0.465202	3.534370	-0.526315
C	-1.817137	3.832095	-0.372421
C	-2.737064	2.806931	-0.221040
C	-2.276439	1.493068	-0.205121

H	-0.959094	1.217024	-0.335526
H	-2.148380	4.868089	-0.377549
H	0.273137	4.320409	-0.664418
H	-3.803002	2.978217	-0.106111
Ru	-0.451089	-0.855106	-0.053269
H	-0.482223	-1.155775	-1.578902
P	1.770725	0.092910	-0.062881
C	2.428702	0.493129	1.691034
C	3.182889	-0.486508	-1.213134
C	2.560613	-0.818917	2.466990
H	2.789873	-0.596805	3.518942
H	1.628453	-1.397121	2.437121
H	3.362529	-1.457391	2.083264
C	3.742446	1.262939	1.746701
H	3.709972	2.197335	1.171555
H	3.960774	1.533908	2.790111
H	4.588794	0.666199	1.387636
C	2.501926	-0.975855	-2.494471
H	3.272688	-1.315042	-3.201046
H	1.822257	-1.811733	-2.295547
H	1.922051	-0.189482	-2.994567
C	4.197997	0.596365	-1.573795
H	4.942714	0.172561	-2.262927
H	3.734700	1.446950	-2.088599
H	4.740875	0.979642	-0.704395
C	1.333000	1.325030	2.364439
H	1.195025	2.308063	1.896692
H	0.363461	0.807220	2.358752
H	1.606692	1.495822	3.415083
C	3.892243	-1.676451	-0.568885
H	3.179342	-2.440538	-0.230097
H	4.554190	-2.146685	-1.309396
H	4.516924	-1.379337	0.282008
C	-3.140052	0.315168	-0.051878
H	-5.246453	-0.516556	0.168699
C	-6.316896	-0.322980	0.252084
C	-4.760743	-1.824495	0.184454
H	-5.453371	-2.658676	0.277055
C	-3.391606	-2.036983	0.083100
H	-3.002915	-3.055311	0.098299
C	-0.122410	-2.664080	0.132478
O	0.077109	-3.811019	0.205772
C	-2.507490	-0.953440	-0.034337
N	-4.456466	0.544575	0.052702
C	1.363651	1.801122	-0.766107
H	1.499998	1.702140	-1.852672
H	2.059969	2.582997	-0.434554

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SCF done: -1364.667517

C	0.063301	2.221746	-0.774700
C	-0.309881	3.530790	-1.061468
C	-1.649762	3.893830	-0.952223
C	-2.591464	2.942893	-0.596774
C	-2.159538	1.651518	-0.304938
N	-0.847353	1.334394	-0.340097
H	-1.956269	4.913713	-1.172643
H	0.440899	4.242877	-1.394916
H	-3.655526	3.151370	-0.543409
Ru	-0.395521	-0.665929	0.300762
H	-1.116143	0.481961	-2.024577
P	1.902479	0.205963	-0.037577
C	-0.472152	-1.248034	-1.732127
O	-0.171465	-2.331926	-2.201141
C	2.772072	1.016665	1.478411
C	3.138069	-0.829899	-1.101543
C	3.068684	-0.084601	2.494476
H	3.483840	0.358016	3.410692
H	2.163819	-0.640002	-2.770860
H	3.804991	-0.804279	2.114392
C	4.050638	1.802288	1.176939

H	3.941188	2.481802	0.322207	C	1.273670	2.142592	1.888303
H	4.288601	2.425149	2.050558	H	1.230705	2.935249	1.132243
H	4.916650	1.163867	0.996832	H	0.279774	1.690887	1.973375
C	2.909970	-2.293939	-0.710972	H	1.500514	2.623748	2.849405
H	3.668045	-2.914533	-1.208983	C	4.124387	-1.506282	0.408055
H	3.004996	-2.462883	0.369960	H	3.439573	-2.154754	0.970644
H	1.924035	-2.643971	-1.036161	H	4.886395	-2.156412	-0.042298
C	2.810294	-0.666071	-2.586516	H	4.640694	-0.844359	1.111423
H	3.392861	-1.410727	-3.146250	C	-3.025042	0.553978	0.008083
H	1.756752	-0.852201	-2.816979	C	-4.923245	0.085039	1.176056
H	3.100470	0.322294	-2.965115	H	-5.825407	0.465215	1.656572
C	1.776647	2.017057	2.073492	C	-4.646849	-1.280921	1.185505
H	1.628634	2.884079	1.417376	H	-5.322174	-1.971784	1.682951
H	0.796456	1.583338	2.284301	C	-3.508846	-1.724077	0.526917
H	2.181818	2.391177	3.023557	H	-3.279756	-2.787908	0.475288
C	4.610695	-0.483732	-0.911446	C	0.210858	-2.589502	0.132065
H	4.964404	-0.693730	0.104257	O	0.555089	-3.693460	0.203774
H	5.202278	-1.112037	-1.592090	C	-2.657363	-0.808848	-0.103644
H	4.831654	0.561443	-1.158083	N	-4.134219	0.995874	0.608019
C	-3.062127	0.536914	0.001050	C	1.509785	1.522525	-1.237816
C	-5.196791	-0.232908	0.193307	H	1.553728	1.005778	-2.208512
H	-6.265229	-0.014629	0.176308	H	2.256265	2.325545	-1.220239
C	-4.744410	-1.531471	0.426689	O	-1.575589	-1.527575	-2.393605
H	-5.458615	-2.336436	0.585342	C	-0.727798	-0.625782	1.988654
C	-3.376030	-1.772598	0.456614	O	-1.185704	-0.748204	3.040630
H	-3.010720	-2.782002	0.644297				
C	-0.137581	-2.493658	0.665718	TS₂₁₋₁₄			
O	-0.013534	-3.625906	0.855384	SCF done:	-1364.591820		
C	-2.478687	-0.724763	0.243201	C	0.181252	2.162300	-1.089216
N	-4.377733	0.790086	-0.019434	C	-0.073356	3.490918	-0.858334
C	1.452092	1.723340	-1.056015	C	-1.392321	3.907710	-0.590603
H	1.455788	1.396282	-2.103475	C	-2.427863	2.995264	-0.490268
H	2.192626	2.528895	-0.970119	C	-2.158114	1.641088	-0.672128
O	-0.939330	-0.288885	-2.593096	N	-0.877068	1.290951	-1.022376
C	-0.600056	-0.312216	2.222668	H	-1.589427	4.963802	-0.425024
O	-0.827086	-0.207867	3.348433	H	0.742348	4.207883	-0.883648
				H	-3.440650	3.281850	-0.225243
TS₂₁₋₁₃				Ru	-0.406676	-0.639850	0.393919
SCF done:	-1364.616527			H	-0.789760	0.421426	-1.615064
C	0.117838	2.052306	-1.088948	P	1.904924	0.151900	-0.037685
C	-0.231662	3.351449	-1.444351	C	-0.808731	-1.897936	-1.752379
C	-1.552787	3.765483	-1.307146	O	-1.099325	-3.051977	-1.736018
C	-2.506113	2.877704	-0.831017	C	2.816715	1.119899	1.358102
C	-2.106571	1.585913	-0.507123	C	3.179770	-0.913203	-1.008473
N	-0.816001	1.208218	-0.612367	C	2.858963	0.208910	2.587484
H	-1.834989	4.780309	-1.576234	H	3.317859	0.754885	3.423540
H	0.530097	4.025121	-1.828228	H	1.855412	-0.098894	2.899880
H	-3.548102	3.149678	-0.695956	H	3.452244	-0.695530	2.418446
Ru	-0.304594	-0.779097	0.022191	C	4.228870	1.594867	1.023725
H	-2.103504	-1.240356	-1.163071	H	4.261868	2.233760	0.131787
P	1.869949	0.151799	-0.004823	H	4.598708	2.201205	1.863067
C	-0.420852	-1.038310	-2.177968	H	4.939100	0.772897	0.889442
O	0.413842	-0.653810	-2.982900	C	2.400573	-1.830896	-1.952272
C	2.368187	1.112363	1.594741	H	3.122055	-2.446481	-2.507664
C	3.405639	-0.758637	-0.715128	H	1.733487	-2.508159	-1.406582
C	2.462666	0.161339	2.789182	H	1.795260	-1.287047	-2.685646
H	2.636346	0.753675	3.698134	C	4.173620	-0.106066	-1.842436
H	1.538506	-0.404585	2.941728	H	4.854192	-0.805138	-2.348291
H	3.285937	-0.552552	2.703601	H	3.677065	0.474360	-2.629667
C	3.686161	1.874030	1.450968	H	4.789295	0.574731	-1.249724
H	3.681013	2.570024	0.602728	C	1.987228	2.359506	1.697506
H	3.838355	2.477110	2.357222	H	2.046753	3.119404	0.908828
H	4.555486	1.215642	1.356911	H	0.932498	2.129458	1.882995
C	2.951826	-1.796355	-1.742579	H	2.390387	2.810251	2.614719
C	3.852150	-2.277175	-2.150272	C	3.919089	-1.808409	-0.011978
H	2.337815	-2.580400	-1.288479	H	3.222403	-2.366184	0.628059
H	2.377691	-1.363750	-2.565123	H	4.507661	-2.548127	-0.571706
C	4.363499	0.209409	-1.411604	H	4.616931	-1.257866	0.628242
H	5.237209	-0.360389	-1.756935	C	-3.045694	0.536687	-0.360770
H	3.906935	0.661975	-2.299311	C	-5.191149	-0.200282	-0.196624
H	4.731061	1.009368	-0.762570	H	-6.256881	0.000637	-0.312910

CO2
SCF done: -188.498060
C 0.000000 0.000000 0.000000
O 0.000000 0.000000 1.164705
O 0.000000 0.000000 -1.164705

CO
SCF done: -113.248634
C 0.000000 0.000000 -0.649957
O 0.000000 0.000000 0.487468