

Cartesian Coordinates and Energies

(PBE0-D3(BJ)/def2-QZVP*+SMD(AcOH)/PBE0-D3(BJ)/def2-SVP level of theory)

Intermediate A	N	-0.416716	0.576789	1.417002
E(SMD/def2-QZVP*) = -1322.919154 E _h	C	2.832896	-0.322632	0.471541
$\Delta\Delta G(353) = 0.396571 E_h$	C	1.374669	-1.925694	1.126673
Lowest frequency = 22.96 cm ⁻¹	C	3.320410	-1.576828	0.028247
C 0.870786 0.416361 1.779894	C	3.485920	0.879667	0.185264
C -1.166562 1.483725 2.072342	C	2.380633	-2.573190	0.470666
C -0.652466 2.303816 3.063897	C	4.510303	-1.618962	-0.715069
C 0.690470 2.172181 3.412393	C	4.660534	0.804706	-0.554259
C 1.455151 1.207542 2.771347	H	3.099729	1.842016	0.528456
Ru -1.268052 -0.305841 -0.319330	H	2.456111	-3.649646	0.332145
C 0.252213 0.574196 -1.618035	C	5.167767	-0.430051	-0.997241
C 0.256352 -0.823239 -1.789690	H	4.909621	-2.573295	-1.065189
C -0.953674 -1.524016 -2.093205	H	5.201604	1.723062	-0.791839
C -2.145643 -0.772976 -2.240708	H	6.095552	-0.449268	-1.572522
C -2.134585 0.633390 -2.022135	N	1.632639	-0.557201	1.134385
C -0.942022 1.344918 -1.721047	O	-3.036059	-0.315197	0.832301
H 1.175088 -1.382934 -1.604470	C	-2.748843	-1.437392	1.353166
H -3.087066 1.169690 -2.000182	O	-1.685360	-1.983354	0.936323
H 2.498390 1.029841 3.035477	C	-3.587823	-2.046694	2.417450
H 1.131398 2.796700 4.192389	H	-3.514274	-3.140658	2.382777
H -1.301712 3.033252 3.549681	H	-3.212365	-1.710026	3.396789
H -2.212945 1.541685 1.768767	H	-4.630425	-1.720771	2.318358

H	0.475844	-2.311632	1.602213	C	-1.106710	3.189083	-2.534301
H	1.179015	1.050966	-1.294346	C	-1.751212	1.987104	-2.266877
H	-3.095411	-1.287587	-2.396050	Ru	1.037852	-0.227572	0.196763
C	-0.957445	-3.014481	-2.157654	C	-0.236146	0.012917	1.978062
H	-0.646583	-3.336192	-3.164578	C	0.159116	-1.330534	1.856112
H	-0.248247	-3.434529	-1.431891	C	1.530851	-1.728641	1.732297
H	-1.955135	-3.424836	-1.956921	C	2.496551	-0.701547	1.712874
C	-0.980951	2.843289	-1.521410	C	2.113905	0.669682	1.775914
H	-1.896656	3.056370	-0.942087	C	0.742502	1.048651	1.912881
C	-1.114141	3.524871	-2.886094	H	-0.615912	-2.094540	1.779125
H	-2.003854	3.178461	-3.432268	H	2.874571	1.444008	1.653951
H	-1.196537	4.614741	-2.764171	H	-2.753723	1.775403	-2.639135
H	-0.232260	3.320455	-3.513095	H	-1.620457	3.969688	-3.099535
C	0.210588	3.395622	-0.749412	H	0.760327	4.285047	-2.341820
H	0.068613	4.469583	-0.563499	H	1.873097	2.413911	-1.083697
H	0.342246	2.904222	0.225365	N	0.190336	1.217983	-1.095191
H	1.147209	3.289869	-1.318987	C	-2.771469	-0.577281	-0.665375
Transition state TS1				C	-0.732655	-1.365442	-1.262375
E(SMD/def2-QZVP*) = -1322.898926 E _h				C	-2.710488	-1.959610	-0.336200
$\Delta\Delta G(353) = 0.393381 E_h$				C	-3.873490	0.216307	-0.331315
Lowest frequency = -99.57 cm ⁻¹				C	-1.423549	-2.432469	-0.737584
C	-1.059558	1.015367	-1.546047	C	-3.809288	-2.565851	0.300188
C	0.834108	2.349235	-1.411639	C	-4.935942	-0.410770	0.304412
C	0.212565	3.369332	-2.116505	H	-3.908803	1.282953	-0.557370
				H	-1.045481	-3.451763	-0.684402

C	-4.910331	-1.786843	0.610061
H	-3.788043	-3.629868	0.545243
H	-5.816862	0.177246	0.570876
H	-5.773825	-2.238714	1.101980
N	-1.570000	-0.243721	-1.264603
O	2.569473	-0.016304	-1.158288
C	2.824602	-1.140496	-1.749856
O	2.152726	-2.148858	-1.536857
C	4.003127	-1.130981	-2.681196
H	3.937023	-1.974309	-3.378473
H	4.070405	-0.179618	-3.224498
H	4.924386	-1.239880	-2.088078
H	0.189424	-1.401901	-1.851797
H	-1.299306	0.252649	2.012559
H	3.538960	-0.952977	1.505590
C	1.905354	-3.163285	1.550841
H	2.131502	-3.616461	2.529252
H	1.084839	-3.729218	1.092084
H	2.783529	-3.261353	0.900741
C	0.389311	2.512964	2.014099
H	1.046607	3.045426	1.305160
C	0.741254	2.991752	3.427339
H	1.800563	2.821296	3.668506
H	0.541682	4.068962	3.522311
H	0.133413	2.467857	4.181038

C	-1.057108	2.841140	1.670485
H	-1.201074	3.930761	1.672073
H	-1.349135	2.466788	0.679603
H	-1.754947	2.424526	2.413078

Intermediate **B**

E(SMD/def2-QZVP*) = -1322.902812 E_h

$\Delta\Delta G(353) = 0.394631$ E_h

Lowest frequency = 13.04 cm⁻¹

C	-1.137809	1.022932	-1.663702
C	0.201566	2.774323	-0.952284
C	-0.588835	3.696420	-1.627106
C	-1.703773	3.241359	-2.329103
C	-1.976471	1.876633	-2.369423
Ru	0.913533	0.023873	0.238679
C	-0.390191	-0.480110	1.942280
C	0.595291	-1.489938	1.775268
C	1.985300	-1.212927	1.742477
C	2.360068	0.158463	1.828621
C	1.399855	1.184625	1.982734
C	0.000925	0.873900	2.049392
H	0.266283	-2.519515	1.624357
H	1.724221	2.227196	2.005498
H	-2.794720	1.467539	-2.962721
H	-2.339908	3.942498	-2.873541

H -0.323711 4.754213 -1.607023
 H 1.098749 3.070634 -0.406163
 N -0.095890 1.470896 -0.937130
 C -2.247491 -1.129375 -1.076855
 C -0.035334 -1.083681 -1.574498
 C -1.679680 -2.374806 -0.688289
 C -3.582551 -0.815519 -0.809686
 C -0.295224 -2.329944 -1.027613
 C -2.484855 -3.343059 -0.059736
 C -4.348595 -1.788584 -0.182872
 H -4.015769 0.145879 -1.089162
 H 0.448627 -3.121829 -0.955149
 C -3.812763 -3.040985 0.183727
 H -2.067171 -4.311730 0.223410
 H -5.400718 -1.581251 0.025049
 H -4.460290 -3.777772 0.662622
 N -1.247663 -0.368153 -1.655000
 O 2.415642 0.479398 -1.068826
 C 3.136378 -0.494123 -1.554132
 O 2.886801 -1.677417 -1.376195
 C 4.327172 -0.027643 -2.351993
 H 4.718773 -0.853036 -2.957766
 H 4.065338 0.829701 -2.986109
 H 5.113919 0.306974 -1.658229
 H 0.786122 -0.828696 -2.241934

H -1.445237 -0.754349 1.914257
 H 3.407077 0.431825 1.679522
 C 3.000352 -2.298956 1.600578
 H 3.359207 -2.597330 2.598790
 H 2.572587 -3.179931 1.106586
 H 3.855540 -1.969996 0.998764
 C -0.987214 1.998074 2.241011
 H -0.597526 2.861699 1.675172
 C -0.992862 2.379635 3.725399
 H 0.010797 2.650436 4.084636
 H -1.656153 3.240602 3.893150
 H -1.358792 1.544440 4.342138
 C -2.391180 1.696152 1.739667
 H -3.017880 2.595850 1.817242
 H -2.392590 1.372547 0.689883
 H -2.879384 0.910751 2.336744

Intermediate C

E(SMD/def2-QZVP*) = -1322.921971 E_h

$\Delta\Delta G(353) = 0.395220 E_h$

Lowest frequency = 20.75 cm⁻¹

C 1.119389 -0.908314 1.437209
 C -0.894385 -1.508153 2.449840
 C -0.247396 -2.160753 3.482779
 C 1.149168 -2.185382 3.469362

C	1.841502	-1.564496	2.443049	C	5.358998	0.140367	-0.108161
Ru	-1.185668	0.026387	-0.143312	H	4.302945	-0.661200	1.574783
C	-1.397998	2.170877	0.079001	H	1.112430	1.155853	-2.577167
C	-1.681941	1.806751	-1.277509	C	5.297481	0.722369	-1.381164
C	-2.633259	0.817959	-1.582684	H	4.021173	1.418368	-2.982134
C	-3.438817	0.209783	-0.554866	H	6.330307	-0.019786	0.364206
C	-3.197492	0.583912	0.771484	H	6.222299	1.002905	-1.889179
C	-2.142181	1.500964	1.083061	N	1.655913	-0.263156	0.353111
C	-0.352212	3.215750	0.381622	O	-1.262956	-1.958160	-0.910354
H	-1.081267	2.239041	-2.080541	C	-0.570869	-2.599874	-1.709216
H	-2.758259	0.496234	-2.618710	O	0.499955	-2.138444	-2.275782
H	-3.761825	0.111863	1.578320	H	0.710285	-1.217435	-1.953450
H	-1.900583	1.685645	2.131289	C	-0.929767	-3.993373	-2.092430
H	0.408236	3.122782	-0.411823	H	-1.024687	-4.058973	-3.186121
H	2.925587	-1.602605	2.406318	H	-0.110327	-4.668036	-1.803045
H	1.701829	-2.700392	4.258059	H	-1.861126	-4.300007	-1.606110
H	-0.823980	-2.645417	4.270744	C	0.348589	3.011256	1.717568
H	-1.982984	-1.473406	2.389575	H	1.176409	3.727183	1.818561
N	-0.234664	-0.889186	1.458698	H	-0.327375	3.182290	2.570122
C	2.977074	-0.019406	-0.045547	H	0.769310	1.998448	1.801732
C	0.755125	0.208236	-0.627881	C	-0.988004	4.603718	0.278795
C	2.901896	0.586603	-1.324928	H	-0.227241	5.384980	0.421693
C	4.207011	-0.235579	0.578260	H	-1.457980	4.766652	-0.702724
C	1.504595	0.714739	-1.661957	H	-1.762312	4.740783	1.049994
C	4.073213	0.953399	-1.995372	C	-4.428968	-0.846665	-0.917793

H -5.263679 -0.404200 -1.483703
 H -3.959292 -1.609454 -1.555726
 H -4.837730 -1.342038 -0.027924

Intermediate D

E(SMD/def2-QZVP*) = -1400.244897 E_h

ΔΔG(353) = 0.428333 E_h

Lowest frequency = 9.66 cm⁻¹

C -1.083171 1.168299 0.857600
 C 1.067433 1.675460 1.612911
 C 0.597494 2.630697 2.491564
 C -0.781090 2.864631 2.530643
 C -1.625874 2.139261 1.712865
 Ru 0.940983 -0.516685 -0.456517
 C 0.664743 -2.643154 0.237902
 C 1.214578 -2.617038 -1.072061
 C 2.442691 -1.956920 -1.335585
 C 3.104168 -1.313898 -0.245441
 C 2.499900 -1.252359 1.013476
 C 1.259623 -1.927496 1.291038
 H 0.690469 -3.121342 -1.885661
 H 2.987470 -0.694363 1.816389
 H -2.695412 2.319374 1.725135
 H -1.196274 3.621093 3.199915
 H 1.294866 3.185128 3.119610

H 2.134494 1.483221 1.502827
 N 0.254466 0.954797 0.820424
 C -3.159375 0.184322 -0.217065
 C -1.052528 -0.564314 -0.757053
 C -3.267569 -0.859404 -1.169945
 C -4.291690 0.820749 0.290641
 C -1.932321 -1.303085 -1.490231
 C -4.528913 -1.264724 -1.616814
 C -5.537299 0.398412 -0.169370
 H -4.248816 1.626982 1.019333
 H -1.677847 -2.075072 -2.213627
 C -5.657545 -0.630470 -1.111329
 H -4.621203 -2.066129 -2.352988
 H -6.435117 0.886591 0.214808
 H -6.649507 -0.934226 -1.451935
 N -1.785336 0.351588 0.024094
 C 1.693538 1.118900 -1.713283
 H 2.759397 0.948999 -1.884838
 C 0.716622 0.408394 -2.420723
 H 0.992790 -0.324175 -3.181276
 H -0.259776 0.877623 -2.551432
 C 1.367572 2.492432 -1.234577
 O 0.275191 2.996942 -1.265422
 O 2.459624 3.104530 -0.770988
 H -0.299333 -3.129077 0.391145

H	4.049433	-0.793950	-0.418464	C	1.144630	1.576319	1.713274
C	0.675555	-1.868313	2.681492	C	0.757868	2.647124	2.496555
H	0.870246	-0.845982	3.050617	C	-0.533469	3.151925	2.331535
C	1.430735	-2.846500	3.586418	C	-1.390678	2.558701	1.420552
H	2.513303	-2.649618	3.597284	Ru	0.857050	-0.622098	-0.366952
H	1.064072	-2.767584	4.620065	C	0.132678	-2.640704	0.265559
H	1.279097	-3.884606	3.252424	C	0.739237	-2.701226	-1.022563
C	-0.827919	-2.106288	2.723882	C	2.066669	-2.261272	-1.246260
H	-1.369639	-1.453682	2.023615	C	2.780541	-1.719833	-0.129413
H	-1.083468	-3.150482	2.485796	C	2.155751	-1.597730	1.121544
H	-1.208313	-1.908957	3.735856	C	0.812947	-2.060884	1.349498
C	3.066579	-1.990286	-2.694007	H	0.157679	-3.080170	-1.865481
H	3.503186	-1.019586	-2.968396	H	2.694076	-1.114256	1.940141
H	3.882473	-2.730261	-2.700903	H	-2.379114	2.969633	1.232494
H	2.344500	-2.284730	-3.466340	H	-0.864773	4.024276	2.898637
C	2.287238	4.454829	-0.358421	H	1.463340	3.093424	3.197656
H	3.273711	4.806230	-0.037121	H	2.160764	1.181878	1.749878
H	1.915314	5.067382	-1.191631	N	0.314395	0.976909	0.844796
H	1.565151	4.516080	0.469019	C	-3.074423	0.615563	-0.368214
Transition state TS3				C	-1.031443	-0.141388	-1.089812
E(SMD/def2-QZVP*) = -1400.225382 E _h				C	-3.279236	-0.353287	-1.386269
$\Delta\Delta G(353) = 0.429702 E_h$				C	-4.148095	1.194727	0.309836
Lowest frequency = -294.19 cm ⁻¹				C	-1.992634	-0.804070	-1.820356
C	-0.944450	1.445406	0.700266	C	-4.584742	-0.705707	-1.758718
				C	-5.432537	0.820963	-0.075036

C	1.247148	-0.951890	1.914348	C	0.979659	0.603819	-2.538146
C	-0.184577	-0.937201	2.053807	H	1.092638	0.332545	-3.599385
H	-0.864432	-3.257727	-0.370594	H	1.145885	1.686327	-2.451724
H	1.845719	-0.257229	2.507949	C	3.012848	0.654782	-1.023993
H	-1.843271	3.833691	-1.148074	O	3.026852	1.860019	-0.906785
H	-0.680651	5.225113	0.609139	O	4.024663	-0.118711	-0.589785
H	1.159096	4.154288	1.953321	H	-2.017842	-1.783234	1.250118
H	1.719967	1.769056	1.533079	H	2.985005	-1.754009	0.896418
N	0.228215	1.489234	0.125026	C	-0.818561	-0.003450	3.053927
C	-2.522789	0.553937	-1.296234	H	-0.173975	0.891450	3.098309
C	-0.389827	0.244596	-2.033593	C	-0.786127	-0.664821	4.435366
C	-2.377693	-0.812397	-1.613292	H	0.234032	-0.955406	4.727380
C	-3.702137	1.066804	-0.768404	H	-1.172820	0.026434	5.198396
C	-1.004174	-1.000176	-2.041689	H	-1.412012	-1.570352	4.448952
C	-3.457958	-1.684476	-1.451059	C	-2.220570	0.448542	2.673064
C	-4.763072	0.179444	-0.596344	H	-2.250325	0.874336	1.659754
H	-3.803418	2.121508	-0.507520	H	-2.944272	-0.380166	2.710981
H	-0.604305	-1.879751	-2.544074	H	-2.573273	1.214796	3.377956
C	-4.648343	-1.175558	-0.940665	C	1.831280	-3.629748	-0.774629
H	-3.372161	-2.739873	-1.720333	H	2.773678	-3.200166	-1.141776
H	-5.709090	0.552094	-0.197970	H	2.072569	-4.579951	-0.272417
H	-5.508169	-1.835669	-0.810659	H	1.190449	-3.862433	-1.636364
N	-1.304449	1.206545	-1.567014	C	5.131148	0.565646	-0.021808
C	1.910340	-0.145059	-1.599909	H	5.881167	-0.198943	0.210586
H	2.291976	-1.087688	-2.011174	H	5.542326	1.298533	-0.730072

H	4.838008	1.100130	0.894638	C	3.666259	0.198961	0.265935
				C	2.225327	-1.555729	0.396652
Intermediate F				C	4.286666	-0.930312	-0.317678
E(SMD/def2-QZVP*) = -1629.209186 E _h				C	4.276012	1.454871	0.292912
$\Delta\Delta G(353) = 0.487612 E_h$				C	3.356341	-2.020511	-0.210702
Lowest frequency = 19.48 cm ⁻¹				C	5.563497	-0.792386	-0.880103
C	1.603423	0.534662	1.568561	C	5.543277	1.562502	-0.270323
C	-0.450842	1.381488	2.188538	H	3.784450	2.326362	0.730528
C	0.068598	1.999447	3.311197	H	3.503261	-3.040134	-0.561375
C	1.431936	1.863057	3.573204	C	6.180572	0.451119	-0.847475
C	2.199846	1.118663	2.695083	H	6.060502	-1.649480	-1.339499
Ru	-0.735359	0.171651	-0.510448	H	6.049236	2.530194	-0.265909
C	-0.979122	2.354164	-1.088014	H	7.175487	0.572112	-1.280807
C	0.280953	1.788735	-1.459529	N	2.395451	-0.194701	0.688371
C	0.393590	0.648296	-2.298541	C	-0.021807	-1.834903	-0.515147
C	-0.829317	-0.003714	-2.659429	C	0.921745	-2.232176	0.620157
C	-2.063813	0.472148	-2.184608	H	1.099811	-3.318917	0.620737
C	-2.166471	1.690389	-1.422486	H	0.512061	-1.985632	1.613927
H	1.201132	2.249518	-1.090485	H	-1.000836	3.239393	-0.451873
H	-2.961145	-0.120473	-2.375646	H	-0.809076	-0.952309	-3.199668
H	3.264619	0.954793	2.863530	C	-3.535214	2.145441	-0.982451
H	1.885012	2.317563	4.456805	H	-4.049644	1.236035	-0.626425
H	-0.587562	2.577695	3.962907	C	-4.300506	2.679872	-2.197411
H	-1.506422	1.479574	1.939404	H	-4.356346	1.938361	-3.007749
N	0.286796	0.663122	1.317530	H	-5.329395	2.945212	-1.913686

H	-3.815514	3.582881	-2.599114	
C	-3.525657	3.159302	0.151236	Transition state TS4
H	-2.966706	2.796004	1.026637	E(SMD/def2-QZVP*) = -1629.183552 E _h
H	-3.083615	4.118480	-0.160482	$\Delta\Delta G(353) = 0.483402 E_h$
H	-4.554467	3.371146	0.475962	Lowest frequency = -1167.57 cm ⁻¹
C	1.721323	0.163720	-2.780623	C -1.473983 -0.384325 1.679431
H	1.740224	-0.927807	-2.899479	C 0.521533 -1.297852 2.404378
H	1.933328	0.607267	-3.766526	C -0.033975 -1.705112 3.605076
H	2.530721	0.452644	-2.097096	C -1.376622 -1.425573 3.849538
O	-2.391526	-0.371959	0.813503	C -2.097659 -0.752991 2.874992
C	-2.711535	-0.859846	1.899048	Ru 0.827355 -0.306453 -0.394946
O	-2.207807	-1.955921	2.383264	C 0.593068 -2.371473 -1.044670
H	-1.737747	-2.473988	1.668017	C -0.520767 -1.610882 -1.519410
C	-3.740223	-0.223521	2.772808	C -0.335113 -0.458957 -2.308204
H	-4.617147	-0.885745	2.837702	C 1.014311 -0.029322 -2.548483
H	-3.344852	-0.124581	3.794125	C 2.107385 -0.767551 -2.074210
H	-4.043272	0.750954	2.375599	C 1.917851 -1.980743 -1.329330
C	-1.186129	-2.717811	-0.750991	H -1.536464 -1.903092 -1.241827
O	-1.780664	-2.859443	-1.788552	H 3.113678 -0.362601 -2.196582
O	-1.563639	-3.414996	0.365760	H -3.147538 -0.491638 3.013364
C	-2.649761	-4.328975	0.203185	H -1.851230 -1.715979 4.789229
H	-3.558288	-3.799040	-0.115409	H 0.585066 -2.230574 4.333358
H	-2.395639	-5.080181	-0.555416	H 1.569897 -1.487547 2.174756
H	-2.797492	-4.805151	1.178924	N -0.176163 -0.657271 1.447513
H	0.550685	-1.897519	-1.449573	C -3.438173 -0.261444 0.221568

C	-2.166086	1.617332	0.356339	C	2.838474	-3.744981	0.256479
C	-4.118018	0.781688	-0.450395	H	2.317120	-3.298334	1.115732
C	-3.944592	-1.560784	0.296037	H	2.228527	-4.581342	-0.119918
C	-3.293316	1.952868	-0.339567	H	3.779230	-4.175378	0.627762
C	-5.343350	0.502906	-1.073936	C	-1.494158	0.294417	-2.871856
C	-5.163574	-1.806729	-0.327402	H	-1.313130	1.378150	-2.897647
H	-3.413724	-2.355910	0.824805	H	-1.650036	-0.032117	-3.912755
H	-3.503689	2.940486	-0.745170	H	-2.417840	0.104343	-2.311207
C	-5.853513	-0.786870	-1.005385	O	2.566385	-0.079505	0.731899
H	-5.886028	1.289124	-1.603249	C	2.688133	0.854426	1.580531
H	-5.591601	-2.810605	-0.288233	O	1.751111	1.657817	1.804078
H	-6.807734	-1.016098	-1.484062	H	0.984911	1.491122	0.777702
N	-2.234079	0.256207	0.694287	C	3.987382	1.000980	2.300851
C	0.215077	1.981122	-0.217772	H	4.533927	0.051334	2.329413
C	-0.962224	2.434227	0.655939	H	4.596022	1.734887	1.749176
H	-1.198946	3.485633	0.445526	H	3.820596	1.395204	3.310779
H	-0.696429	2.389140	1.725737	C	1.261942	2.997959	-0.584207
H	0.411621	-3.229974	-0.397193	O	2.192594	2.744089	-1.313153
H	1.202366	0.929811	-3.035705	O	1.064113	4.181734	-0.021864
C	3.131825	-2.723321	-0.831199	C	2.039452	5.181764	-0.289789
H	3.797688	-1.951981	-0.409123	H	3.024999	4.862454	0.077951
C	3.836882	-3.372142	-2.026756	H	2.111513	5.374453	-1.369287
H	4.102670	-2.636304	-2.799913	H	1.708061	6.081414	0.239683
H	4.765250	-3.861115	-1.697878	H	-0.191418	1.677319	-1.185960
H	3.197968	-4.137825	-2.493460				

Intermediate G	C	-4.091256	0.769747	-0.516733			
E(SMD/def2-QZVP*) = -1629.201819 E _h	C	-3.852494	-1.412585	0.605635			
$\Delta\Delta G(353) = 0.485205 E_h$	C	-3.294775	1.961493	-0.609025			
Lowest frequency = 17.72 cm ⁻¹	C	-5.323243	0.369033	-1.056127			
C	-1.395208	0.004595	1.727009	C	-5.078365	-1.780178	0.060974
C	0.574829	-0.900521	2.530167	H	-3.295944	-2.094151	1.253373
C	0.076849	-0.974707	3.820490	H	-3.535884	2.866538	-1.163209
C	-1.217008	-0.524586	4.066953	C	-5.802542	-0.900757	-0.763295
C	-1.956473	-0.024716	3.003935	H	-5.895842	1.047425	-1.692334
Ru	0.774241	-0.462528	-0.420630	H	-5.486958	-2.768835	0.280502
C	0.369805	-2.535618	-0.739099	H	-6.761366	-1.223650	-1.173866
C	-0.699737	-1.811113	-1.348811	N	-2.173432	0.471040	0.654214
C	-0.434702	-0.798851	-2.288327	C	0.203967	2.113712	-0.576128
C	0.940092	-0.507008	-2.590727	C	-0.961187	2.651503	0.246137
C	1.988451	-1.245392	-2.025882	H	-1.230746	3.652530	-0.115531
C	1.724550	-2.291921	-1.080999	H	-0.638223	2.766759	1.293034
H	-1.730036	-1.991191	-1.033603	H	0.139475	-3.251719	0.050615
H	3.018719	-0.934300	-2.207667	H	1.182630	0.355743	-3.215820
H	-2.971660	0.352721	3.133471	C	2.887741	-3.009054	-0.444241
H	-1.640964	-0.551935	5.072989	H	3.577177	-2.211222	-0.119214
H	0.707178	-1.371902	4.617076	C	3.587448	-3.860560	-1.508327
H	1.592010	-1.211160	2.291444	H	3.914143	-3.261911	-2.371228
N	-0.145238	-0.434267	1.495603	H	4.479193	-4.339620	-1.079161
C	-3.373130	-0.137324	0.297724	H	2.922290	-4.655735	-1.879359
C	-2.148488	1.765694	0.110236	C	2.516133	-3.845137	0.770783

H	2.000287	-3.254771	1.541905	E(SMD/def2-QZVP*) = -1629.232680 E _h
H	1.872540	-4.697370	0.500757	$\Delta\Delta G(353) = 0.484414 E_h$
H	3.424988	-4.260580	1.228274	Lowest frequency = 15.80 cm ⁻¹
C	-1.540785	-0.045450	-2.949165	C -0.357013 0.878589 1.824906
H	-1.263473	0.994789	-3.167751	C -0.614787 -1.321201 2.493316
H	-1.762466	-0.530156	-3.914004	C -0.801700 -0.949332 3.816870
H	-2.457229	-0.050203	-2.346110	C -0.772404 0.401711 4.146345
O	2.516952	-0.076903	0.565696	C -0.536830 1.323259 3.133369
C	2.747367	0.966851	1.316461	Ru -0.462177 -1.233126 -0.490180
O	1.886879	1.761898	1.665726	C -2.291908 -0.146200 -0.986531
H	0.717637	1.366932	0.108049	C -1.259654 0.270398 -1.855581
C	4.193828	1.127749	1.695654	C -0.502870 -0.689998 -2.588344
H	4.714764	1.590235	0.842562	C -0.833870 -2.064661 -2.445033
H	4.284543	1.789039	2.565280	C -1.850229 -2.458843 -1.535363
H	4.670012	0.157787	1.888808	C -2.617350 -1.514756 -0.794288
C	1.385940	3.016461	-0.854712	H -0.988007 1.326425 -1.899276
O	2.352154	2.633741	-1.464985	H -1.986543 -3.524119 -1.330157
O	1.226417	4.232321	-0.367705	H -0.475082 2.394465 3.329340
C	2.324725	5.126059	-0.520935	H -0.913933 0.733905 5.177022
H	3.188235	4.757934	0.050902	H -0.968097 -1.719753 4.570923
H	2.606273	5.215542	-1.579061	H -0.618188 -2.370358 2.195862
H	1.990285	6.090961	-0.125926	N -0.417280 -0.430653 1.502990
H	-0.140686	1.736341	-1.543803	C -1.099157 2.684887 0.320213
				C 1.084682 2.068493 0.170745
Intermediate H				C -0.492430 3.451531 -0.705280

C	-2.442270	2.830705	0.675294	H	-4.552965	-0.079589	0.784913
C	0.883302	3.042172	-0.773715	H	-4.791586	-1.413630	1.920758
C	-1.275684	4.383599	-1.404598	C	0.665640	-0.257494	-3.408796
C	-3.190250	3.764976	-0.033187	H	1.436157	-1.037827	-3.452439
H	-2.887694	2.249131	1.486093	H	0.329926	-0.043689	-4.436252
H	1.654491	3.470322	-1.410340	H	1.108537	0.658758	-2.995897
C	-2.613911	4.528279	-1.064324	O	0.523189	-2.876646	0.399525
H	-0.835478	4.989595	-2.199575	C	1.667630	-2.375319	0.164100
H	-4.241064	3.915559	0.223236	O	1.658564	-1.269227	-0.455728
H	-3.230533	5.254677	-1.597531	H	3.068479	0.879338	-1.278964
N	-0.131701	1.819975	0.812302	C	2.928988	-3.034044	0.580123
C	3.443030	1.366103	-0.363279	H	3.591489	-2.287955	1.043614
C	2.338906	1.443427	0.671780	H	2.724720	-3.872395	1.255635
H	2.691433	2.018567	1.547203	H	3.441993	-3.410791	-0.318278
H	2.144948	0.428718	1.039113	C	4.599096	0.530019	0.118685
H	-2.774621	0.616285	-0.374310	O	4.544853	-0.264553	1.026347
H	-0.222898	-2.824696	-2.935082	O	5.693418	0.751208	-0.599794
C	-3.704537	-1.986667	0.143475	C	6.840654	-0.016505	-0.261467
H	-3.313883	-2.890830	0.642860	H	7.121754	0.147589	0.788426
C	-4.931927	-2.392266	-0.676808	H	6.648521	-1.089216	-0.409584
H	-4.689807	-3.165605	-1.420772	H	7.641887	0.320111	-0.928197
H	-5.718501	-2.791371	-0.019863	H	3.820505	2.354466	-0.663617
H	-5.346970	-1.525256	-1.214138				
C	-4.072162	-0.971026	1.217431				
H	-3.196453	-0.643793	1.796999				

Intermediate **A**^{benzene}

E(SMD/def2-QZVP*) = -1165.763414 E_h

$\Delta\Delta G(353) = 0.293233 E_h$

Lowest frequency = 25.71 cm^{-1}

C	0.657195	1.686180	0.107044
C	-1.349097	2.282338	-0.894029
C	-0.901843	3.570292	-1.140928
C	0.387532	3.919379	-0.744510
C	1.168899	2.968055	-0.103838
Ru	-1.324716	-0.642325	-0.277173
C	0.284985	-1.312549	-1.595849
C	0.342209	-2.060555	-0.401883
C	-0.833091	-2.715887	0.063934
C	-2.038058	-2.657193	-0.671331
C	-2.081166	-1.871996	-1.857916
C	-0.923949	-1.209659	-2.336667
H	1.250906	-2.060111	0.202582
H	-3.038827	-1.707417	-2.357042
H	2.171064	3.196043	0.261543
H	0.772759	4.927369	-0.913169
H	-1.562274	4.283360	-1.636004
H	-2.356154	1.966922	-1.170619
N	-0.581226	1.345656	-0.304080
C	2.703185	0.318638	0.294798
C	1.171711	0.093133	1.947593
C	3.206166	-0.602487	1.246407
C	3.398064	0.645253	-0.873338

C	2.217688	-0.714440	2.286330
C	4.453806	-1.203649	1.016479
C	4.629659	0.032474	-1.072511
H	3.002705	1.358284	-1.600428
H	2.286276	-1.314453	3.191189
C	5.151888	-0.879829	-0.137928
H	4.865674	-1.914283	1.736283
H	5.204319	0.267991	-1.970749
H	6.124493	-1.338269	-0.327515
N	1.447880	0.725103	0.737007
O	-3.163107	0.291719	0.123453
C	-2.932690	0.313960	1.373089
O	-1.850548	-0.233876	1.737604
C	-3.850377	0.977224	2.332783
H	-3.803458	0.480929	3.310070
H	-3.526053	2.021713	2.464658
H	-4.875753	0.980543	1.943474
H	0.232709	0.287484	2.460408
H	1.161020	-0.731994	-1.895125
H	-2.949824	-3.107765	-0.276842
H	-0.982535	-0.569311	-3.217889
H	-0.823153	-3.194866	1.045499

Transition state **TS1**^{benzene}

$E(\text{SMD}/\text{def2-QZVP}^*) = -1165.743738 E_h$

$\Delta\Delta G(353) = 0.291709 E_h$

Lowest frequency = -114.98 cm^{-1}

C	0.782371	1.801518	0.333130
C	-1.214413	2.601578	-0.541979
C	-0.739090	3.904568	-0.535573
C	0.559418	4.142881	-0.083843
C	1.330273	3.081660	0.376559
Ru	-1.062850	-0.437224	-0.405677
C	0.015161	-0.611034	-2.289521
C	0.381561	-1.699232	-1.481350
C	-0.634672	-2.507169	-0.881023
C	-1.998711	-2.263263	-1.126657
C	-2.365783	-1.141796	-1.927142
C	-1.366671	-0.311115	-2.500125
H	1.430373	-1.862236	-1.227486
H	-3.416152	-0.856735	-2.011660
H	2.321132	3.233107	0.805418
H	0.959132	5.158940	-0.057840
H	-1.382526	4.718041	-0.872700
H	-2.229033	2.350939	-0.856832
N	-0.450354	1.571450	-0.153619
C	2.681442	0.182578	0.520819
C	0.684258	-0.337650	1.455077
C	2.755030	-1.143982	1.030631
C	3.733453	0.759860	-0.197362

C	1.490957	-1.440318	1.624703
C	3.937414	-1.886883	0.852097
C	4.881320	-0.002519	-0.361176
H	3.667820	1.766749	-0.612018
H	1.202827	-2.344522	2.157715
C	4.987779	-1.307524	0.162630
H	4.018286	-2.900441	1.250468
H	5.726438	0.421692	-0.907638
H	5.914562	-1.865511	0.016145
N	1.422079	0.669860	0.821843
O	-2.717690	0.300686	0.569518
C	-2.880080	-0.368240	1.667111
O	-2.079887	-1.244339	1.996619
C	-4.091507	-0.015123	2.478367
H	-4.047705	-0.507768	3.456170
H	-4.168868	1.074105	2.599182
H	-4.994630	-0.347276	1.944512
H	-0.249055	-0.118308	1.979048
H	0.784124	0.065321	-2.669161
H	-2.760395	-2.838292	-0.599024
H	-1.656582	0.585325	-3.052310
H	-0.352868	-3.267967	-0.151096

Intermediate **B**^{benzene}

E(SMD/def2-QZVP*) = $-1165.748628 E_h$

$\Delta\Delta G(353) = 0.291483 E_h$

Lowest frequency = 27.63 cm^{-1}

C -0.872928 1.840711 -0.482751

C 0.992469 2.805054 0.497802

C 0.454689 4.076939 0.349050

C -0.807215 4.210067 -0.228439

C -1.481642 3.075839 -0.671898

Ru 0.950544 -0.275492 0.464739

C -0.245782 -1.583167 1.740486

C 0.816012 -2.341553 1.148879

C 2.146961 -1.909932 1.267026

C 2.441249 -0.698994 1.965428

C 1.391577 0.049176 2.545131

C 0.039182 -0.406114 2.451831

H 0.591067 -3.208186 0.526630

H 1.609152 1.010222 3.016416

H -2.438547 3.140048 -1.190693

H -1.252845 5.197882 -0.363792

H 1.024056 4.947723 0.676335

H 1.983091 2.641710 0.925920

N 0.321534 1.710320 0.123535

C -2.576312 0.013254 -0.607758

C -0.466530 -0.356930 -1.355652

C -2.446270 -1.375844 -0.908330

C -3.735889 0.532514 -0.020101

C -1.130132 -1.579245 -1.394473

C -3.528918 -2.247370 -0.663702

C -4.776479 -0.353199 0.210551

H -3.828834 1.587896 0.239208

H -0.686145 -2.496012 -1.780082

C -4.682551 -1.726273 -0.113368

H -3.449327 -3.308743 -0.907961

H -5.701835 0.022281 0.653344

H -5.537196 -2.377189 0.079811

N -1.388440 0.625627 -0.931819

O 2.362415 0.237924 -0.912584

C 2.755382 -0.700451 -1.735812

O 2.246433 -1.809750 -1.786420

C 3.906237 -0.287998 -2.616130

H 4.023699 -1.003446 -3.438112

H 3.757894 0.728503 -3.004393

H 4.830050 -0.276308 -2.017610

H 0.359443 -0.060576 -2.003663

H -1.283854 -1.881977 1.581431

H 3.459430 -0.306671 1.974322

H 2.930080 -2.436442 0.720815

H -0.774405 0.205017 2.846955

Intermediate C^{benzene}

E(SMD/def2-QZVP*) = -1165.767420 E_h

$\Delta\Delta G(353) = 0.292779 E_h$

Lowest frequency = 27.29 cm^{-1}

C 0.805244 1.623359 -0.289833
C -1.281538 2.665136 -0.214792
C -0.715260 3.924487 -0.153893
C 0.678737 4.016730 -0.154973
C 1.447692 2.866757 -0.216699
Ru -1.374813 -0.358401 -0.285413
C -1.605765 -1.247295 -2.227323
C -1.781468 -2.268322 -1.245290
C -2.723223 -2.092570 -0.214320
C -3.579290 -0.941849 -0.204382
C -3.441557 0.046871 -1.178688
C -2.399513 -0.079354 -2.154448
H -1.127469 -3.141533 -1.244921
H -2.795598 -2.830158 0.586547
H -4.067506 0.940595 -1.150837
H -2.212038 0.736925 -2.855472
H 2.531069 2.925357 -0.190635
H 1.169416 4.990708 -0.097327
H -1.350708 4.808406 -0.097520
H -2.363008 2.524964 -0.193142
N -0.546771 1.544475 -0.292586
C 2.771541 0.019594 -0.356631
C 0.596594 -0.741408 -0.268046

C 2.787417 -1.394918 -0.268962
C 3.957511 0.747962 -0.464741
C 1.416197 -1.841857 -0.215338
C 4.004933 -2.083148 -0.264773
C 5.156916 0.040488 -0.459809
H 3.985519 1.830136 -0.571305
H 1.091816 -2.879922 -0.160527
C 5.184994 -1.356568 -0.356260
H 4.022381 -3.172876 -0.196083
H 6.094993 0.592760 -0.544685
H 6.145139 -1.876290 -0.355393
N 1.422588 0.400701 -0.335629
O -1.372909 -0.045994 1.814468
C -0.636358 -0.391194 2.746253
O 0.457129 -1.070868 2.595680
H 0.650864 -1.236101 1.631205
C -0.962554 -0.034737 4.154356
H -0.956610 -0.942936 4.773997
H -0.173908 0.624614 4.547231
H -1.934196 0.465812 4.210879
H -4.288991 -0.806293 0.614087
H -0.821387 -1.334835 -2.980050

Intermediate **D**^{benzene}

E(SMD/def2-QZVP*) = -1243.089690 E_h

$\Delta\Delta G(353) = 0.325409 E_h$

Lowest frequency = 13.38 cm^{-1}

C -0.724791 1.230779 0.841234

C 1.519093 1.653520 1.344714

C 1.221608 2.875048 1.913249

C -0.116801 3.284307 1.927458

C -1.093278 2.469343 1.388808

Ru 1.004758 -1.003284 0.016392

C 0.494740 -2.953742 1.026249

C 1.214125 -3.216598 -0.160178

C 2.481114 -2.604601 -0.352710

C 3.083173 -1.823638 0.672798

C 2.326164 -1.515456 1.809269

C 1.013950 -2.054682 1.981612

H 0.787558 -3.854699 -0.935613

H 2.729145 -0.839763 2.567096

H -2.131635 2.783160 1.377842

H -0.395888 4.249256 2.355975

H 2.018919 3.494412 2.324004

H 2.547404 1.300125 1.264938

N 0.574699 0.844872 0.830888

C -2.957437 0.276827 0.109658

C -0.989771 -0.856477 -0.240065

C -3.237291 -0.944399 -0.552264

C -3.977433 1.161843 0.457359

C -1.984132 -1.630338 -0.758731

C -4.556974 -1.274775 -0.874704

C -5.284247 0.810481 0.125818

H -3.802616 2.103914 0.972050

H -1.859281 -2.585823 -1.264935

C -5.573376 -0.390629 -0.533217

H -4.781042 -2.212610 -1.387441

H -6.096408 1.491475 0.387770

H -6.609165 -0.632654 -0.779694

N -1.565081 0.313186 0.291675

C 1.834394 0.126941 -1.683340

H 2.898129 -0.115064 -1.759657

C 0.851321 -0.746255 -2.157531

H 1.123266 -1.691001 -2.633927

H -0.112779 -0.327126 -2.449618

C 1.531374 1.587809 -1.664637

O 0.440591 2.069041 -1.829907

O 2.638915 2.297503 -1.450265

H -0.509731 -3.360567 1.155912

H 4.082139 -1.405402 0.536238

C 2.488097 3.712016 -1.482735

H 3.488157 4.130771 -1.327344

H 2.083908 4.033577 -2.452653

H 1.801936 4.043273 -0.689603

H 0.424041 -1.791417 2.860874

H	3.019472	-2.772060	-1.288694	C	-2.974251	0.546031	-0.081126
				C	-1.066152	-0.625900	-0.580027
Transition state TS3 ^{benzene}				C	-3.337793	-0.669002	-0.720389
E(SMD/def2-QZVP*) = -1243.071195 E _h				C	-3.941679	1.431660	0.396522
$\Delta\Delta G(353) = 0.327083 E_h$				C	-2.132319	-1.377921	-1.021173
Lowest frequency = -293.46 cm ⁻¹				C	-4.692208	-0.972569	-0.923045
C	-0.704984	1.431119	0.583578	C	-5.277674	1.102678	0.187281
C	1.463492	1.656745	1.396683	H	-3.693487	2.346896	0.930314
C	1.233585	2.956224	1.804383	H	-2.063904	-2.318019	-1.565510
C	-0.019410	3.516416	1.545574	C	-5.651688	-0.078825	-0.472309
C	-0.994871	2.757511	0.923031	H	-4.980521	-1.900870	-1.420609
Ru	0.842363	-1.033669	0.131174	H	-6.051208	1.783487	0.548394
C	0.097712	-2.638989	1.517153	H	-6.710899	-0.296998	-0.621848
C	0.441376	-3.176944	0.242586	N	-1.579356	0.563222	-0.019647
C	1.735616	-2.991539	-0.294736	C	1.607987	-0.159162	-1.660736
C	2.702207	-2.233134	0.429195	H	2.336429	-0.870064	-2.059321
C	2.345169	-1.641046	1.652211	C	0.226846	-0.324166	-2.005691
C	1.034632	-1.843161	2.192526	H	-0.035104	-1.165966	-2.649153
H	-0.307786	-3.723629	-0.332496	H	-0.298867	0.607120	-2.243985
H	3.061927	-1.010645	2.181075	C	2.121139	1.229060	-1.550858
H	-1.957125	3.189484	0.661528	O	1.444384	2.225250	-1.626910
H	-0.228566	4.554531	1.811920	O	3.441050	1.243808	-1.348548
H	2.027682	3.524805	2.288725	H	-0.914170	-2.755354	1.908227
H	2.440991	1.188200	1.515579	H	3.689142	-2.046508	0.001501
N	0.518545	0.903763	0.809370	C	4.049508	2.528119	-1.299256

H 5.121351 2.355338 -1.153633
H 3.875047 3.075015 -2.236554
H 3.638707 3.122275 -0.469776
H 0.750694 -1.338953 3.118577
H 1.980459 -3.399286 -1.277275

Intermediate **E^{benzene}**

E(SMD/def2-QZVP*) = -1243.095101 E_h

$\Delta\Delta G(353) = 0.329739 E_h$

Lowest frequency = 30.38 cm⁻¹

C -0.610975 2.017348 -0.138733
C 1.208184 1.926952 1.282994
C 1.100824 3.282278 1.562107
C 0.091364 4.019813 0.950716
C -0.773316 3.378567 0.067728
Ru 0.350065 -0.822535 0.141856
C -0.835138 -1.714481 1.868602
C -0.750909 -2.622933 0.787503
C 0.498066 -3.004441 0.223884
C 1.690722 -2.425928 0.725042
C 1.629021 -1.479813 1.777575
C 0.360825 -1.116862 2.321372
H -1.673502 -3.018169 0.357840
H 2.543734 -1.003110 2.132916
H -1.546497 3.915268 -0.482520

H -0.006147 5.091468 1.136263
H 1.819032 3.750707 2.235873
H 2.010281 1.328594 1.713917
N 0.349437 1.290904 0.475141
C -2.643841 0.733696 -0.576864
C -0.690175 0.219195 -1.628343
C -2.713803 -0.621151 -0.961496
C -3.662482 1.350160 0.140784
C -1.447222 -0.944879 -1.588034
C -3.862793 -1.367444 -0.681162
C -4.791871 0.585635 0.427393
H -3.593542 2.392405 0.456446
H -1.225507 -1.845450 -2.159661
C -4.898291 -0.750764 0.013064
H -3.949095 -2.407820 -1.003956
H -5.618727 1.043079 0.974804
H -5.808599 -1.309986 0.237686
N -1.408425 1.254639 -1.005955
C 1.602746 -0.401911 -1.521774
H 1.849981 -1.358549 -1.998804
C 0.628557 0.451644 -2.313651
H 0.567019 0.191075 -3.381362
H 0.910971 1.511231 -2.244552
C 2.831855 0.284786 -1.064165
O 2.975979 1.482113 -0.964394

O	3.794409	-0.587641	-0.717456	C	1.009191	1.160495	3.020865
H	-1.803437	-1.419639	2.274521	H	-2.123399	0.628315	1.735440
H	2.651227	-2.635641	0.251079	H	2.530349	-0.409730	3.200740
C	5.016952	-0.021064	-0.269505	H	-2.857226	1.806148	-2.511301
H	5.699588	-0.859755	-0.092029	H	-1.822720	4.073396	-2.837979
H	5.434944	0.655372	-1.028141	H	0.349970	4.572798	-1.638170
H	4.870445	0.552214	0.658617	H	1.344627	2.808771	-0.205513
H	0.311571	-0.329318	3.077429	N	-0.139649	1.408972	-0.559538
H	0.533424	-3.697452	-0.617760	C	-3.252654	-0.249744	-0.584645
				C	-1.356308	-1.338699	-1.212075
Intermediate F^{benzene}				C	-3.513153	-1.640840	-0.571628
E(SMD/def2-QZVP*) = -1472.052792 E _h				C	-4.206242	0.692931	-0.194400
$\Delta\Delta G(353) = 0.384520 E_h$				C	-2.302023	-2.298160	-0.982279
Lowest frequency = 30.36 cm ⁻¹				C	-4.780251	-2.092560	-0.176076
C	-1.308306	1.144586	-1.181972	C	-5.453058	0.215039	0.196524
C	0.416246	2.624197	-0.746964	H	-3.995080	1.764373	-0.192659
C	-0.148592	3.607891	-1.538659	H	-2.150534	-3.368214	-1.110048
C	-1.350901	3.331863	-2.189779	C	-5.737983	-1.160628	0.200997
C	-1.930039	2.086376	-2.010166	H	-5.006203	-3.160945	-0.161538
Ru	0.694338	0.208434	1.004912	H	-6.223935	0.924720	0.503936
C	-0.296231	1.456796	2.621219	H	-6.728851	-1.499169	0.510373
C	-1.134648	0.400649	2.140252	N	-1.921840	-0.083583	-0.969168
C	-0.702789	-0.943763	2.167504	C	0.941959	-1.470395	-0.311461
C	0.623745	-1.240251	2.612521	C	0.076321	-1.482047	-1.575105
C	1.482719	-0.192233	2.987264	H	0.207578	-2.431552	-2.114309

H	0.363879	-0.700496	-2.303094	Lowest frequency = -1117.34 cm ⁻¹
H	-0.641381	2.491696	2.584064	C 1.253463 -0.997443 -1.341474
H	1.012748	-2.258681	2.567259	C -0.275499 -2.686942 -0.939548
O	2.613591	0.978121	0.477699	C 0.277346 -3.494052 -1.920186
C	3.293038	0.976963	-0.546910	C 1.361537 -3.014359 -2.650645
O	2.801262	0.663434	-1.720001	C 1.849863 -1.749589 -2.355218
H	1.877782	0.368499	-1.612142	Ru -0.686616 -0.444781 0.998428
C	4.738806	1.305535	-0.535457	C 0.326119 -1.668697 2.491851
H	5.270341	0.368078	-0.301750	C 1.179825 -0.583422 2.120589
H	5.076984	1.670519	-1.512213	C 0.719163 0.743103 2.202649
H	4.958140	2.024209	0.262420	C -0.619136 0.996270 2.640973
C	2.372325	-1.873538	-0.516469	C -1.471958 -0.062693 2.996612
O	3.220919	-1.874778	0.346828	C -0.989118 -1.404112 2.919526
O	2.624269	-2.256312	-1.772964	H 2.174306 -0.777560 1.712243
C	3.952255	-2.663634	-2.065813	H -2.518341 0.136207 3.230811
H	4.300406	-3.413823	-1.342976	H 2.691555 -1.314690 -2.895688
H	3.929988	-3.082626	-3.077857	H 1.816172 -3.613173 -3.442718
H	4.633216	-1.799630	-2.036013	H -0.145011 -4.482910 -2.103264
H	0.552338	-2.287940	0.315931	H -1.128331 -3.020187 -0.347340
H	-1.359116	-1.728311	1.785444	N 0.195825 -1.461467 -0.646111
H	1.698753	1.966112	3.280551	C 3.110163 0.390804 -0.537021
Transition state TS4 ^{benzene}				C 1.245323 1.504595 -1.206051
E(SMD/def2-QZVP*) = -1472.030998 E _h				C 3.356363 1.779095 -0.412687
ΔΔG(353) = 0.379853 E _h				C 4.056401 -0.574543 -0.184233
				C 2.164974 2.453344 -0.849116

C	4.598624	2.206257	0.080649	O	-2.720425	2.749770	-1.490051
C	5.277205	-0.120316	0.303807	C	-4.007961	3.353321	-1.556355
H	3.858116	-1.643439	-0.292778	H	-4.154665	4.046464	-0.716484
H	2.007367	3.528499	-0.909592	H	-4.044291	3.890822	-2.509798
C	5.544483	1.253701	0.434265	H	-4.791440	2.583093	-1.521059
H	4.815730	3.271643	0.183833	H	-0.590658	1.883203	0.448849
H	6.043441	-0.845559	0.585604	H	1.358833	1.557099	1.853103
H	6.515281	1.573468	0.818224	H	-1.678313	-2.233239	3.090591
N	1.806519	0.240434	-1.002112				
C	-1.081305	1.424705	-0.413635	Intermediate G^{benzene}			
C	-0.171812	1.669982	-1.621612	E(SMD/def2-QZVP*) = -1472.048548 E _h			
H	-0.313273	2.695040	-1.990091	$\Delta\Delta G(353) = 0.382223$ E _h			
H	-0.433645	1.000491	-2.457488	Lowest frequency = 23.86 cm ⁻¹			
H	0.662891	-2.699739	2.369502	C	-1.094181	-0.339352	1.674458
H	-1.024310	2.010190	2.617260	C	0.387513	-2.113315	1.811824
O	-2.460897	-1.383850	0.477437	C	-0.005841	-2.405413	3.108478
C	-3.007448	-1.169852	-0.649398	C	-0.974341	-1.609571	3.711852
O	-2.464776	-0.434282	-1.506932	C	-1.521842	-0.561888	2.981647
H	-1.614302	0.251481	-0.783053	Ru	0.543946	-0.822428	-0.887678
C	-4.333830	-1.795522	-0.923814	C	-0.506447	-2.478227	-1.726790
H	-5.108589	-1.070144	-0.628262	C	-1.413300	-1.371757	-1.694732
H	-4.447981	-1.995025	-1.996146	C	-1.047502	-0.146015	-2.274450
H	-4.473389	-2.706256	-0.330106	C	0.232744	-0.021996	-2.894252
C	-2.447439	2.062158	-0.392555	C	1.122551	-1.112095	-2.972674
O	-3.200715	1.942996	0.544087	C	0.746849	-2.345754	-2.372486

H	-2.353505	-1.442967	-1.143583	H	-0.750859	-3.403273	-1.201166
H	2.126645	-0.975832	-3.375844	H	0.566469	0.953812	-3.254935
H	-2.283512	0.098232	3.398486	O	2.345363	-1.475792	-0.225840
H	-1.297260	-1.797456	4.738044	C	3.034339	-0.924055	0.740944
H	0.456152	-3.242476	3.633346	O	2.586838	-0.075085	1.497892
H	1.160474	-2.691485	1.304147	H	1.295879	0.603958	0.139536
N	-0.145405	-1.106043	1.101852	C	4.455375	-1.404722	0.815929
C	-3.038442	0.583254	0.501515	H	5.038862	-0.812295	0.093348
C	-1.204260	1.920157	0.570131	H	4.859289	-1.230197	1.820180
C	-3.354628	1.798201	-0.152552	H	4.543095	-2.460914	0.532120
C	-3.956778	-0.462172	0.631828	C	2.580167	2.106901	-0.263566
C	-2.180396	2.622006	-0.086260	O	3.350214	1.649517	-1.068328
C	-4.636851	1.959239	-0.701595	O	2.873388	3.013645	0.648465
C	-5.217406	-0.273170	0.076395	C	4.238958	3.412337	0.729806
H	-3.705677	-1.386335	1.157884	H	4.853616	2.563381	1.061033
H	-2.072341	3.637051	-0.463927	H	4.599686	3.759884	-0.247769
C	-5.551933	0.922639	-0.584602	H	4.277426	4.220553	1.467488
H	-4.908529	2.887248	-1.209393	H	0.719875	1.807114	-1.210947
H	-5.963970	-1.065548	0.162112	H	-1.697918	0.724185	-2.158726
H	-6.552898	1.036143	-1.005628	H	1.478987	-3.152063	-2.297665
N	-1.712840	0.663096	0.912730				
C	1.129218	1.674699	-0.204959				
C	0.209964	2.298360	0.835873				
H	0.297753	3.392121	0.787195				
H	0.538743	1.996610	1.842327				

Intermediate **H**^{benzene}

E(SMD/def2-QZVP*) = -1472.077144 E_h

$\Delta\Delta G(353) = 0.381587$ E_h

Lowest frequency = 15.97 cm⁻¹

C	-0.794504	0.462369	1.773284	C	-4.475922	2.293862	0.077915
C	-0.419628	-1.722563	2.441071	H	-3.635580	0.976806	1.580661
C	-0.594274	-1.396081	3.778370	H	0.139800	3.513134	-1.553440
C	-0.883094	-0.078573	4.116777	C	-4.221312	3.182002	-0.982556
C	-0.977426	0.859685	3.095912	H	-2.737657	4.160558	-2.209559
Ru	-0.409404	-1.613604	-0.543313	H	-5.506201	2.114735	0.392587
C	-2.510892	-1.146346	-0.938434	H	-5.060942	3.671310	-1.480301
C	-1.708234	-0.442812	-1.864459	N	-0.922712	1.414850	0.753693
C	-0.742093	-1.159554	-2.620610	C	2.553090	2.111177	-0.588355
C	-0.599504	-2.560809	-2.481861	C	1.529293	1.848051	0.498049
C	-1.396125	-3.239923	-1.519616	H	1.716929	2.521757	1.353976
C	-2.369509	-2.545532	-0.756887	H	1.685853	0.831106	0.877060
H	-1.771374	0.644772	-1.929423	H	-3.182102	-0.576176	-0.293192
H	-1.195626	-4.292226	-1.305646	H	0.189033	-3.092313	-3.016313
H	-1.185830	1.911629	3.294990	O	1.079191	-2.839331	0.289935
H	-1.022517	0.218268	5.158487	C	1.989597	-1.992642	0.018758
H	-0.499872	-2.175155	4.536057	O	1.590873	-0.952419	-0.588271
H	-0.171152	-2.740274	2.138652	H	2.311961	1.514047	-1.483667
N	-0.529572	-0.821377	1.446931	C	3.410767	-2.203985	0.376970
C	-2.136607	1.923637	0.313480	H	3.828659	-1.270200	0.781851
C	0.120265	2.030595	0.055643	H	3.511951	-3.037442	1.081415
C	-1.853619	2.828065	-0.739954	H	3.971000	-2.440485	-0.541189
C	-3.437463	1.650515	0.743081	C	3.936587	1.699306	-0.158998
C	-0.424343	2.874591	-0.877336	O	4.177246	0.907796	0.721363
C	-2.924511	3.457983	-1.394402	O	4.872597	2.292931	-0.888176

C	6.219977	1.942280	-0.600682	H	-3.074447	1.892867	-1.174224
H	6.463768	2.166574	0.447381	H	2.392380	-0.979814	3.035424
H	6.389278	0.870411	-0.778971	H	0.860771	-0.394551	4.942453
H	6.842293	2.541409	-1.274077	H	-1.586013	-0.011732	4.430996
H	2.577899	3.162857	-0.908283	H	-2.345212	-0.175763	2.062108
H	-0.038723	-0.607305	-3.247573	N	-0.461741	-0.567534	1.300758
H	-2.943463	-3.067121	0.010147	C	2.881864	-0.491137	0.222947
				C	1.557474	-2.242271	-0.332325
Intermediate A ^t -Bubenzene				C	3.489312	-1.187283	-0.850838
E(SMD/def2-QZVP*) = -1322.908834 E _h				C	3.434549	0.669449	0.771898
ΔΔG(353) = 0.398323 E _h				C	2.632726	-2.299337	-1.169383
Lowest frequency = 22.09 cm ⁻¹				C	4.695915	-0.702841	-1.379129
C	0.834918	-0.820055	1.569199	C	4.629175	1.124971	0.225817
C	-1.296882	-0.317362	2.328037	H	2.958593	1.199632	1.599395
C	-0.866836	-0.236203	3.642339	H	2.806484	-3.062701	-1.924765
C	0.483098	-0.445030	3.918904	C	5.253108	0.446136	-0.836012
C	1.337645	-0.755881	2.871102	H	5.185931	-1.223386	-2.204757
Ru	-1.223673	-0.278056	-0.665643	H	5.093799	2.025103	0.633858
C	0.278332	1.231108	-1.161254	H	6.192732	0.832098	-1.236315
C	0.316478	0.212800	-2.132239	N	1.689516	-1.145551	0.517435
C	-0.884600	-0.168230	-2.796802	O	-2.994029	-1.082561	0.148315
C	-2.093980	0.486281	-2.496873	C	-2.608269	-2.273565	-0.069457
C	-2.109795	1.491031	-1.485964	O	-1.493669	-2.391203	-0.658087
C	-0.932677	1.905811	-0.809048	C	-3.396565	-3.449226	0.380337
H	1.243059	-0.337073	-2.304467	H	-3.179671	-4.320061	-0.250106

H	-3.107157	-3.691362	1.415265	C	-1.231163	0.312804	2.492654
H	-4.468638	-3.216362	0.371704	C	-0.746898	0.311717	3.790747
H	0.686586	-2.889058	-0.252838	C	0.514400	-0.234375	4.033204
H	1.194797	1.437865	-0.607794	C	1.237041	-0.776581	2.979519
H	-3.030573	0.148477	-2.942896	Ru	-1.242738	-0.003224	-0.517048
C	-0.955011	3.048297	0.201740	C	0.189705	1.091330	-1.788001
C	-0.783024	4.339036	-0.616882	C	-0.667947	0.273765	-2.572221
H	-1.600105	4.465455	-1.343094	C	-2.075703	0.376659	-2.491641
H	-0.785122	5.212913	0.051985	C	-2.621659	1.261514	-1.532438
H	0.167905	4.338392	-1.171042	C	-1.772062	2.044909	-0.704799
C	0.192053	2.940504	1.210418	C	-0.345771	2.009563	-0.851524
H	0.124446	3.771774	1.926659	H	-0.228206	-0.503888	-3.198683
H	0.148363	2.003368	1.784208	H	-2.224821	2.660437	0.071863
H	1.179674	3.013028	0.732500	H	2.190579	-1.279690	3.137780
C	-2.282185	3.098715	0.963365	H	0.918827	-0.269148	5.047116
H	-3.135549	3.332113	0.310620	H	-1.356761	0.720248	4.597155
H	-2.491182	2.149206	1.477887	H	-2.224694	0.688576	2.244381
H	-2.240734	3.892563	1.722781	N	-0.509656	-0.156104	1.462902
H	-0.883293	-1.031111	-3.465815	C	2.636386	-1.165568	0.187368
Transition state TS1 ^t -Bubenzene				C	0.568658	-1.849934	-0.445536
E(SMD/def2-QZVP*) = -1322.888185 E _h				C	2.724945	-1.719121	-1.118391
$\Delta\Delta G(353) = 0.397227 E_h$				C	3.745131	-0.600584	0.825080
Lowest frequency = -120.90 cm ⁻¹				C	1.412336	-2.153636	-1.485180
C	0.689749	-0.721450	1.696297	C	3.965714	-1.736223	-1.779753
				C	4.953742	-0.625872	0.142831

H	3.679414	-0.149494	1.815534
H	1.125004	-2.684464	-2.390954
C	5.067285	-1.191962	-1.142112
H	4.053020	-2.170555	-2.777859
H	5.839574	-0.198808	0.617770
H	6.039809	-1.197835	-1.638089
N	1.310835	-1.268118	0.585989
O	-2.897428	-0.793022	0.426176
C	-3.087997	-2.001340	0.006916
O	-2.313550	-2.523717	-0.797101
C	-4.308586	-2.698933	0.530229
H	-4.210558	-3.781873	0.391933
H	-4.479571	-2.453578	1.586389
H	-5.185805	-2.351281	-0.037034
H	-0.449724	-2.239333	-0.282412
H	1.266925	0.942233	-1.860907
H	-3.695689	1.255380	-1.337057
C	0.553727	2.972613	-0.084343
C	0.852875	4.100766	-1.090763
H	-0.071972	4.574157	-1.453553
H	1.462135	4.877140	-0.604104
H	1.410148	3.726166	-1.962185
C	1.865815	2.326385	0.359521
H	2.514126	3.093480	0.806838
H	1.692513	1.555883	1.122062

H	2.431036	1.872453	-0.465676
H	-2.714466	-0.306840	-3.051105
C	-0.139128	3.569833	1.142057
H	-1.011458	4.184246	0.875839
H	-0.457142	2.793457	1.853380
H	0.564222	4.230574	1.668545

Intermediate **B^t-Bubenzene**

E(SMD/def2-QZVP*) = -1322.893220 E_h

$\Delta\Delta G(353) = 0.395954$ E_h

Lowest frequency = 20.33 cm⁻¹

C	0.640233	-0.657360	1.863584
C	-1.030843	0.768277	2.600602
C	-0.526076	0.753973	3.893378
C	0.616549	0.000074	4.158109
C	1.203161	-0.736093	3.134197
Ru	-1.126695	0.117366	-0.384505
C	0.091789	1.038218	-1.951129
C	-0.978042	0.295881	-2.542884
C	-2.309477	0.530334	-2.168197
C	-2.577304	1.499672	-1.158414
C	-1.516034	2.225263	-0.572005
C	-0.152183	2.034796	-0.982126
H	-0.756334	-0.519212	-3.232624
H	-1.744547	2.913697	0.241441

C	-0.350308	-1.648899	3.717896	C	3.949513	1.285621	-1.877914
C	1.014314	-1.374600	3.834266	C	5.128572	1.087304	0.230619
C	1.701022	-0.819173	2.767342	H	4.049547	0.378575	1.939876
Ru	-1.217507	-0.427039	-0.349723	H	1.094367	0.772054	-2.733333
C	-2.053944	1.593226	-0.287275	C	5.112021	1.421039	-1.130156
C	-1.862718	1.183220	-1.642258	H	3.929873	1.555210	-2.935958
C	-2.412879	-0.017853	-2.145076	H	6.049021	1.212849	0.804393
C	-3.214216	-0.832928	-1.294246	H	6.021676	1.797294	-1.602375
C	-3.460387	-0.454736	0.033427	N	1.538771	0.010940	0.447296
C	-2.819958	0.714012	0.533412	O	-0.732466	-2.472975	-0.684348
C	-1.524418	2.912734	0.271982	C	0.160417	-3.062369	-1.304015
H	-1.212487	1.770736	-2.289476	O	1.146425	-2.467314	-1.899838
H	-2.200844	-0.330934	-3.168050	H	1.116565	-1.482075	-1.747573
H	-4.055949	-1.089051	0.691378	C	0.169101	-4.547352	-1.412259
H	-2.916780	0.945952	1.596373	H	0.221419	-4.836796	-2.471789
H	2.766801	-0.626640	2.837191	H	1.078484	-4.936300	-0.930162
H	1.548626	-1.603752	4.758759	H	-0.720970	-4.974084	-0.939489
H	-0.919746	-2.093214	4.534342	C	-0.761876	2.687295	1.581702
H	-2.028910	-1.564952	2.356699	H	-0.464872	3.656863	2.007113
N	-0.320321	-0.798483	1.484790	H	-1.364076	2.171457	2.344223
C	2.829218	0.452003	0.122686	H	0.151274	2.101619	1.405871
C	0.692712	0.110781	-0.677584	C	-2.748256	3.807252	0.526072
C	2.796525	0.802186	-1.250795	H	-2.424866	4.793090	0.892288
C	3.994179	0.602797	0.876908	H	-3.327842	3.962953	-0.396562
C	1.451642	0.577989	-1.722861	H	-3.421963	3.373997	1.281158

C	-0.590689	3.610869	-0.717584	H	-0.280482	2.876393	3.932328
H	-0.219051	4.544568	-0.271578	H	2.115780	2.193168	3.494594
H	0.282227	2.987458	-0.962150	H	2.595730	0.842692	1.452059
H	-1.106522	3.883931	-1.650705	N	0.616626	0.732676	0.858389
H	-3.579362	-1.794866	-1.660469	C	-2.922029	0.698361	-0.028140
Intermediate D^f-Bubenzene				C	-0.976678	-0.136666	-0.926302
E(SMD/def2-QZVP*) = -1400.235611 E _h				C	-3.226240	-0.009439	-1.217933
$\Delta\Delta G(353) = 0.430170 E_h$				C	-3.923437	1.300349	0.733062
Lowest frequency = 16.98 cm ⁻¹				C	-1.987342	-0.515165	-1.758101
C	-0.671920	1.094069	1.071594	C	-4.553322	-0.108100	-1.647185
C	1.577472	1.136848	1.707510	C	-5.237862	1.187149	0.285115
C	1.306452	1.895409	2.828092	H	-3.727933	1.848572	1.651901
C	-0.021790	2.268631	3.062644	H	-1.881164	-1.086114	-2.678602
C	-1.014612	1.876270	2.185248	C	-5.551577	0.493473	-0.890096
Ru	1.001388	-0.474749	-0.767413	H	-4.797014	-0.648708	-2.564263
C	0.435500	-2.649376	-0.937905	H	-6.035889	1.652975	0.866605
C	1.209147	-2.282247	-2.057615	H	-6.592466	0.426850	-1.213152
C	2.485476	-1.697006	-1.860205	N	-1.529300	0.612803	0.131427
C	3.025849	-1.581599	-0.552740	C	1.900162	1.327583	-1.661983
C	2.211991	-1.900867	0.541994	H	2.961619	1.128793	-1.833727
C	0.886220	-2.427386	0.389919	C	0.916347	0.834177	-2.525027
H	0.810612	-2.410517	-3.065165	H	1.188726	0.248690	-3.406199
H	2.593730	-1.720966	1.548047	H	-0.031868	1.370303	-2.587116
H	-2.044870	2.175375	2.346081	C	1.620227	2.591128	-0.921871
				O	0.541792	3.119407	-0.836459

O	2.733648	3.071212	-0.366406	Lowest frequency = -293.65 cm ⁻¹			
H	-0.571684	-3.032361	-1.101952	C	0.395343	-1.444878	0.940635
H	4.027995	-1.176924	-0.399967	C	-1.667475	-0.848428	1.837984
C	0.068977	-2.903090	1.590129	C	-1.555037	-1.777428	2.853980
C	0.450498	-4.379368	1.797934	C	-0.422795	-2.595085	2.877244
H	1.525985	-4.494317	2.003200	C	0.556008	-2.440419	1.910907
H	-0.103372	-4.792583	2.654222	Ru	-0.861871	0.695423	-0.636380
H	0.205943	-4.986145	0.912820	C	0.236342	2.589192	-0.953491
C	-1.436536	-2.794994	1.329544	C	-0.750245	2.458577	-1.968916
H	-1.741245	-1.763570	1.103768	C	-2.097176	2.245083	-1.609776
H	-1.773836	-3.438917	0.504880	C	-2.469747	2.187568	-0.240450
H	-1.982390	-3.122390	2.225744	C	-1.459885	2.296958	0.740633
C	2.604154	4.314169	0.312938	C	-0.084968	2.537345	0.424203
H	3.607442	4.577608	0.664763	H	-0.458354	2.476564	-3.020273
H	2.221022	5.087143	-0.367692	H	-1.740839	2.156938	1.785184
H	1.909907	4.218388	1.160657	H	1.416086	-3.103632	1.875349
C	0.399100	-2.114874	2.860585	H	-0.314060	-3.369935	3.638909
H	1.448284	-2.224825	3.172381	H	-2.349123	-1.875610	3.594372
H	0.174971	-1.044743	2.750088	H	-2.554080	-0.221506	1.733744
H	-0.213384	-2.497310	3.689300	N	-0.712403	-0.672489	0.910358
H	3.068623	-1.365560	-2.722467	C	2.659876	-1.414974	-0.175124
Transition state TS3^f-Bubenzene				C	0.867683	-0.345667	-1.129853
E(SMD/def2-QZVP*) = -1400.216070 E _h				C	3.093902	-0.761967	-1.359538
ΔΔG(353) = 0.428204 E _h				C	3.559792	-2.082980	0.656670
				C	1.959142	-0.108727	-1.935057

C	-0.976389	1.950542	-2.180475	C	-2.044148	-0.910848	-1.434993
C	-1.689209	2.149708	-0.964091	H	-2.336107	-0.578117	-2.438402
C	-0.973445	2.242689	0.250782	C	-1.261405	-2.212350	-1.418110
C	0.464759	2.209944	0.306311	H	-1.374737	-2.816074	-2.331707
H	0.977664	1.601142	-3.038666	H	-1.577225	-2.832710	-0.568086
H	-1.540795	2.352237	1.174511	C	-3.209218	-0.868486	-0.522392
H	1.054453	-3.528767	2.210835	O	-3.373642	-1.577671	0.445299
H	-0.250485	-2.894576	4.277005	O	-4.086911	0.090741	-0.864057
H	-1.841686	-0.948589	4.131035	H	2.225003	1.844773	-0.905889
H	-2.014500	0.301479	1.990092	H	-2.779727	2.156531	-0.961655
N	-0.550110	-0.801814	1.029064	C	1.252129	2.453939	1.593317
C	2.253896	-1.706159	-0.328675	C	2.041608	3.758217	1.385217
C	0.167236	-1.778482	-1.240397	H	1.371311	4.599204	1.151360
C	2.320690	-1.084538	-1.592886	H	2.594004	4.010582	2.302799
C	3.360720	-1.797610	0.507553	H	2.771521	3.667077	0.567538
C	0.979546	-1.107576	-2.143047	C	2.222343	1.299420	1.860847
C	3.538693	-0.578627	-2.057960	H	1.680739	0.363552	2.058561
C	4.562458	-1.275973	0.033770	H	2.906435	1.119395	1.019719
H	3.299326	-2.263802	1.492098	H	2.837821	1.527388	2.743608
H	0.705875	-0.894062	-3.175109	C	-5.247811	0.189479	-0.052532
C	4.654728	-0.680248	-1.233675	H	-5.875646	0.965434	-0.505030
H	3.613992	-0.118734	-3.046128	H	-5.787137	-0.767733	-0.025315
H	5.455330	-1.344074	0.658829	H	-4.986980	0.466536	0.980196
H	5.618592	-0.299681	-1.577333	C	0.339771	2.631944	2.807289
N	0.931934	-2.138551	-0.115532	H	-0.345372	3.485111	2.690247

H -0.251011 1.729213 3.018886
 H 0.954321 2.831205 3.696905
 H -1.508750 1.829725 -3.124706

Intermediate **F^M-Bubenzene**

E(SMD/def2-QZVP*) = -1629.196825 E_h

ΔΔG(353) = 0.489014 E_h

Lowest frequency = 23.99 cm⁻¹

C -1.742208 0.146503 1.635824
 C 0.271487 -0.493546 2.574460
 C -0.300203 -0.681019 3.820158
 C -1.663282 -0.428810 3.973444
 C -2.385850 -0.007065 2.869240
 Ru 0.567549 -0.263140 -0.403151
 C 0.384851 -2.528209 -0.458067
 C -0.785345 -1.855974 -0.924706
 C -0.730106 -0.927820 -1.987300
 C 0.548157 -0.611592 -2.535298
 C 1.710635 -1.194040 -1.999612
 C 1.651352 -2.199005 -0.970119
 H -1.748995 -2.054731 -0.449904
 H 2.674068 -0.832614 -2.354882
 H -3.448999 0.227225 2.933542
 H -2.152208 -0.547282 4.942735
 H 0.318301 -1.020701 4.651751

H 1.328186 -0.703117 2.410196
 N -0.420901 -0.089236 1.489841
 C -3.671867 -0.088451 0.118169
 C -2.246231 1.637371 -0.285832
 C -4.170476 0.653159 -0.979533
 C -4.298376 -1.246544 0.583687
 C -3.255511 1.739635 -1.201681
 C -5.346363 0.225424 -1.612420
 C -5.461270 -1.648283 -0.065726
 H -3.902425 -1.821787 1.423326
 H -3.341005 2.522805 -1.952361
 C -5.981293 -0.918629 -1.147858
 H -5.751984 0.782968 -2.459389
 H -5.978885 -2.547524 0.274658
 H -6.898217 -1.261773 -1.631254
 N -2.485927 0.523504 0.523978
 C 0.143160 1.785457 -0.895930
 C -1.011469 2.448437 -0.137465
 H -1.202666 3.453573 -0.540793
 H -0.790751 2.610874 0.934364
 H 0.292385 -3.243426 0.359869
 H 0.650244 0.157383 -3.302799
 C 2.909425 -2.898084 -0.459767
 C 2.885040 -4.316243 -1.055751
 H 2.846902 -4.286717 -2.155177

H 3.795665 -4.860908 -0.763596
 H 2.016248 -4.890717 -0.700811
 C 2.919701 -2.980535 1.070004
 H 2.967559 -1.974074 1.509943
 H 2.040407 -3.501516 1.475556
 H 3.806448 -3.539235 1.403303
 O 2.377851 0.309641 0.569017
 C 2.736975 1.281291 1.230154
 O 1.893986 2.165342 1.702451
 H 0.998590 1.960215 1.373238
 C 4.165973 1.547404 1.525882
 H 4.572497 2.085025 0.653307
 H 4.283780 2.175112 2.416692
 H 4.714980 0.603437 1.623747
 C 1.366935 2.635891 -1.060280
 O 2.397798 2.274791 -1.582647
 O 1.204995 3.872308 -0.573648
 C 2.309503 4.755776 -0.687735
 H 2.685242 4.782818 -1.719586
 H 1.947187 5.743608 -0.382238
 H 3.126261 4.437480 -0.022208
 H -0.214507 1.680449 -1.932491
 C 4.183611 -2.184497 -0.917138
 H 4.304548 -2.212435 -2.009982
 H 4.196489 -1.135086 -0.589476

H 5.059423 -2.690330 -0.485462
 H -1.637917 -0.425351 -2.326127

Transition state **TS4^t-Bubenzene**

E(SMD/def2-QZVP*) = -1629.175555 E_h

$\Delta\Delta G(353) = 0.484630 E_h$

Lowest frequency = -1175.27 cm⁻¹

C -1.711688 0.028889 1.668362
 C 0.240309 -0.779396 2.607638
 C -0.355786 -0.932883 3.848614
 C -1.691616 -0.570372 3.999695
 C -2.372128 -0.082175 2.893442
 Ru 0.628750 -0.299450 -0.324155
 C 0.517534 -2.461518 -0.624057
 C -0.695124 -1.850712 -1.063351
 C -0.674506 -0.815216 -2.013959
 C 0.589726 -0.368253 -2.499881
 C 1.788638 -0.952698 -2.053997
 C 1.774848 -2.037514 -1.117154
 H -1.648533 -2.147948 -0.620838
 H 2.731593 -0.514926 -2.375983
 H -3.417390 0.224657 2.947605
 H -2.194453 -0.660689 4.964886
 H 0.228453 -1.329645 4.679837
 H 1.283890 -1.048799 2.447038

N	-0.414130	-0.309902	1.530571	H	2.274814	-4.696640	-1.263712
C	-3.535985	-0.251419	0.051976	C	3.048043	-3.060409	0.818820
C	-2.303164	1.646676	-0.153021	H	3.006946	-2.139419	1.416245
C	-4.081585	0.517693	-1.003773	H	2.212960	-3.715739	1.106171
C	-4.056163	-1.494067	0.422097	H	3.973057	-3.594964	1.078597
C	-3.287033	1.710510	-1.102519	O	2.344548	0.110695	0.773972
C	-5.187928	0.016731	-1.706821	C	2.441302	1.160197	1.479253
C	-5.151394	-1.964776	-0.294411	O	1.484553	1.965369	1.583283
H	-3.632488	-2.074554	1.244991	H	0.763737	1.652551	0.555648
H	-3.434174	2.538700	-1.793038	C	3.736703	1.439591	2.165017
C	-5.710084	-1.217891	-1.346307	H	4.344896	2.055293	1.483198
H	-5.629562	0.591011	-2.524140	H	3.568972	2.014899	3.083426
H	-5.587559	-2.930590	-0.030807	H	4.285101	0.512557	2.369518
H	-6.571527	-1.617869	-1.884911	C	1.199487	2.956259	-0.946709
N	-2.436081	0.443838	0.546795	O	2.213914	2.589935	-1.491346
C	0.096844	2.003858	-0.565129	O	0.940654	4.214509	-0.622080
C	-1.165734	2.570530	0.092779	C	1.954539	5.166994	-0.920511
H	-1.406922	3.548604	-0.345134	H	2.180589	5.169156	-1.995865
H	-1.007729	2.743453	1.170228	H	1.560944	6.140196	-0.608393
H	0.470919	-3.231882	0.145683	H	2.874304	4.931057	-0.366476
H	0.649990	0.496496	-3.164401	H	-0.207432	1.590247	-1.530074
C	3.060485	-2.728526	-0.676289	C	4.297450	-1.880733	-0.982338
C	3.119725	-4.030709	-1.495935	H	4.448164	-1.741580	-2.062951
H	3.107272	-3.826662	-2.577331	H	4.233980	-0.895050	-0.500741
H	4.050971	-4.569610	-1.265164	H	5.191695	-2.394194	-0.600927

H	-1.602629	-0.315883	-2.300729	C	-3.491409	-0.180297	0.085454
				C	-2.287213	1.628195	-0.573787
Intermediate G^{\ddagger} -Bubenzene				C	-4.040272	0.294556	-1.130273
E(SMD/def2-QZVP*) = -1629.194335 E _h				C	-4.005067	-1.292044	0.758836
$\Delta\Delta G(353) = 0.486437 E_h$				C	-3.262993	1.438086	-1.516477
Lowest frequency = 12.91 cm ⁻¹				C	-5.136842	-0.381400	-1.689303
C	-1.678340	0.491743	1.589780	C	-5.090220	-1.940138	0.179970
C	0.231603	-0.209261	2.690887	H	-3.585213	-1.633882	1.707940
C	-0.326150	0.055805	3.931859	H	-3.420079	2.070512	-2.388186
C	-1.612277	0.582412	3.991025	C	-5.647347	-1.491240	-1.031329
C	-2.293575	0.803333	2.800401	H	-5.581099	-0.035442	-2.625158
Ru	0.570470	-0.497016	-0.273342	H	-5.522542	-2.809799	0.679340
C	0.481178	-2.616283	-0.099524	H	-6.501173	-2.024212	-1.454455
C	-0.790113	-2.160848	-0.566809	N	-2.406315	0.629792	0.398045
C	-0.878453	-1.354731	-1.712279	C	0.105404	2.043098	-1.060339
C	0.327434	-0.993845	-2.371926	C	-1.195083	2.638374	-0.540436
C	1.585503	-1.473236	-1.945171	H	-1.483239	3.488749	-1.173107
C	1.686215	-2.317639	-0.801004	H	-1.032109	3.036208	0.473067
H	-1.691667	-2.363104	0.015211	H	0.527895	-3.178562	0.832936
H	2.483664	-1.113771	-2.443961	H	0.294930	-0.278838	-3.197331
H	-3.304090	1.213209	2.779178	C	3.023345	-2.870786	-0.329763
H	-2.078928	0.821600	4.948941	C	3.083822	-4.297604	-0.907294
H	0.254190	-0.141418	4.833977	H	3.013482	-4.292910	-2.005536
H	1.244584	-0.599728	2.593548	H	4.042795	-4.761960	-0.632428
N	-0.426251	-0.002325	1.539390	H	2.274736	-4.931732	-0.513719

C	3.114013	-2.928772	1.198184	
H	3.025090	-1.920602	1.625278	Intermediate H[†]-Bubenzene
H	2.355134	-3.586099	1.647484	E(SMD/def2-QZVP*) = -1629.222437 E _h
H	4.092942	-3.338963	1.484423	$\Delta\Delta G(353) = 0.486591 E_h$
O	2.274283	0.119868	0.636898	Lowest frequency = 15.77 cm ⁻¹
C	2.473628	1.297154	1.173991	C -0.213619 0.905275 1.741566
O	1.588677	2.112425	1.384412	C -0.499456 -1.304956 2.359413
H	0.521093	1.423627	-0.208985	C -0.696597 -0.961223 3.688758
C	3.919141	1.579044	1.474243	C -0.662859 0.382169 4.047679
H	4.383269	1.929392	0.538582	C -0.404218 1.322117 3.058088
H	4.000952	2.372855	2.226138	Ru -0.366631 -1.142933 -0.632159
H	4.452736	0.675666	1.796530	C -2.093471 0.101178 -1.130152
C	1.292121	2.958117	-1.278316	C -1.018452 0.451808 -1.976757
O	2.353815	2.549636	-1.673852	C -0.353737 -0.567487 -2.706026
O	1.019132	4.216273	-0.986731	C -0.783011 -1.910108 -2.608436
C	2.103337	5.135913	-1.072072	C -1.844845 -2.231794 -1.720216
H	2.854387	4.895991	-0.306053	C -2.544509 -1.240354 -0.973630
H	2.572615	5.090859	-2.064247	H -0.653608 1.479983 -1.997386
H	1.677524	6.127964	-0.888993	H -2.067565 -3.285411 -1.546793
H	-0.056578	1.500014	-1.996599	H -0.328172 2.387528 3.279217
C	4.197801	-2.048642	-0.865876	H -0.813265 0.693551 5.083585
H	4.108360	-0.995153	-0.566488	H -0.874121 -1.747339 4.423826
H	5.136146	-2.448433	-0.455786	H -0.502553 -2.347570 2.040816
H	4.281435	-2.107454	-1.961132	N -0.290375 -0.395958 1.387999
H	-1.836335	-0.928143	-2.017106	C -0.873318 2.804344 0.312661

C	1.276546	2.084506	0.125071	H	-3.073023	-0.424700	1.643841
C	-0.231324	3.581780	-0.682421	H	-4.228810	0.432175	0.584741
C	-2.205261	3.006185	0.682676	H	-4.794050	-0.862397	1.644541
C	1.121932	3.107217	-0.774506	O	0.502943	-2.871839	0.212635
C	-0.967219	4.582283	-1.337160	C	1.679033	-2.428343	0.015052
C	-2.905739	4.007965	0.019182	O	1.741688	-1.304022	-0.566694
H	-2.677340	2.415712	1.471305	H	3.174916	0.844632	-1.387239
H	1.911306	3.521130	-1.397995	C	2.894200	-3.169087	0.428787
C	-2.294422	4.782742	-0.982723	H	3.608372	-2.466877	0.883480
H	-0.498667	5.197346	-2.108598	H	2.636477	-3.988851	1.109016
H	-3.945744	4.203033	0.289379	H	3.372723	-3.587214	-0.470565
H	-2.873960	5.562489	-1.481019	C	4.694000	0.347722	-0.018765
N	0.049121	1.867861	0.759829	O	4.606038	-0.460849	0.873791
C	3.587350	1.270286	-0.457515	O	5.785468	0.511802	-0.756680
C	2.500074	1.377922	0.592685	C	6.886129	-0.336564	-0.459669
H	2.892638	1.907250	1.479860	H	7.196029	-0.218300	0.588288
H	2.256432	0.364814	0.933325	H	6.622328	-1.390501	-0.630807
H	-2.520601	0.890178	-0.511729	H	7.695565	-0.035365	-1.133410
H	-0.230814	-2.705980	-3.110076	H	4.023263	2.243775	-0.726049
C	-3.730436	-1.601444	-0.085466	C	-3.532132	-2.966108	0.580871
C	-4.960817	-1.651609	-1.005837	H	-3.501265	-3.791197	-0.144979
H	-4.842865	-2.412336	-1.792412	H	-2.606063	-2.996427	1.173560
H	-5.859481	-1.904275	-0.423012	H	-4.374703	-3.172336	1.256314
H	-5.134494	-0.680993	-1.494746	H	0.552065	-0.327208	-3.266402
C	-3.958741	-0.548644	1.002447				

***p*-cymene**E(SMD/def2-QZVP*) = -389.215198 E_h $\Delta\Delta G(353) = 0.166011 E_h$ Lowest frequency = 16.58 cm⁻¹

C	-1.600312	-1.198595	0.000014
C	-2.200051	0.062573	0.000039
C	-1.356630	1.181970	0.000060
C	0.026381	1.042771	0.000040
C	0.628296	-0.222973	0.000005
C	-0.212377	-1.337511	-0.000007
H	-2.230566	-2.092538	0.000018
H	-1.795719	2.184133	0.000100
H	0.650550	1.940901	0.000063
H	0.228153	-2.338955	-0.000021
C	2.134365	-0.379194	-0.000024
H	2.340459	-1.463515	-0.000059
C	2.762952	0.209817	-1.262510
H	3.850355	0.035097	-1.278393
H	2.329689	-0.237467	-2.169545
H	2.600785	1.298244	-1.317518
C	2.762997	0.209744	1.262474
H	2.329774	-0.237600	2.169498
H	3.850403	0.035036	1.278305
H	2.600821	1.298166	1.317556
C	-3.692672	0.224603	-0.000047

H -4.034532 0.783068 -0.886198

H -4.203394 -0.748599 0.000895

H -4.034476 0.784795 0.885025

benzeneE(SMD/def2-QZVP*) = -232.072172 E_h $\Delta\Delta G(353) = 0.067643 E_h$ Lowest frequency = 416.11 cm⁻¹

C	0.018893	-1.394571	-0.000000
C	1.217192	-0.680925	-0.000003
C	1.198298	0.713649	0.000002
C	-0.018892	1.394571	-0.000001
C	-1.217192	0.680926	-0.000002
C	-1.198298	-0.713648	0.000003
H	0.033690	-2.487177	-0.000001
H	2.170810	-1.214419	0.000002
H	2.137118	1.272770	0.000006
H	-0.033688	2.487174	0.000004
H	-2.170807	1.214417	-0.000006
H	-2.137122	-1.272770	0.000005

***t*-Bubenzene**E(SMD/def2-QZVP*) = -389.210794 E_h $\Delta\Delta G(353) = 0.170727 E_h$ Lowest frequency = 49.22 cm⁻¹

C	-2.207105	1.201807	0.000021	Alkene 3a			
C	-0.811318	1.217179	0.000047	E(SMD/def2-QZVP*) = -306.263685 E _h			
C	-0.071178	0.029813	0.000053	$\Delta\Delta G(353) = 0.058388 E_h$			
C	-0.786734	-1.177639	0.000038	Lowest frequency = 98.57 cm ⁻¹			
C	-2.177786	-1.199472	0.000009	C	-0.039118	0.113460	-0.000001
C	-2.898430	-0.005321	0.000001	O	0.060969	1.314493	0.000005
H	-2.755331	2.147332	0.000021	O	1.014277	-0.714085	0.000034
H	-0.300304	2.180549	0.000071	C	2.284595	-0.090371	0.000079
H	-0.246178	-2.127529	0.000039	H	3.026256	-0.897672	0.000105
H	-2.703861	-2.157462	-0.000005	H	2.410819	0.543173	-0.890819
H	-3.990894	-0.018238	-0.000020	H	2.410756	0.543173	0.890986
C	1.459174	0.005706	0.000013	C	-1.311072	-0.647737	-0.000047
C	1.952917	-0.729681	1.254479	C	-2.481310	-0.007576	-0.000086
H	3.054094	-0.761141	1.273383	H	-1.236107	-1.738033	-0.000046
H	1.608476	-0.221395	2.168125	H	-3.431251	-0.546877	-0.000120
H	1.588017	-1.766749	1.290519	H	-2.501012	1.086327	-0.000084
C	1.952693	-0.729267	-1.254788				
H	1.608137	-0.220620	-2.168191	HOAc			
H	3.053866	-0.760802	-1.273881	E(SMD/def2-QZVP*) = -228.952262 E _h			
H	1.587679	-1.766286	-1.291142	$\Delta\Delta G(353) = 0.029151 E_h$			
C	2.057973	1.412672	0.000189	Lowest frequency = 79.73 cm ⁻¹			
H	1.759077	1.984535	-0.891561	C	-0.092792	0.121673	-0.000005
H	1.759182	1.984263	0.892150	O	-0.637637	1.192942	-0.000033
H	3.156800	1.348758	0.000109	O	-0.776657	-1.033953	-0.000017
				H	-1.715791	-0.792741	-0.000050

C 1.388081 -0.110577 0.000048
 H 1.673345 -0.698450 0.884681
 H 1.673400 -0.698526 -0.884515
 H 1.911661 0.851229 0.000025

HCl

E(SMD/def2-QZVP*) = -460.684264 E_h

$\Delta\Delta G(353) = -0.014961 E_h$

Lowest frequency = 3018.19 cm⁻¹

Cl 0.000000 0.000000 0.071392
 H 0.000000 0.000000 -1.213660

[RuCl₂(*p*-cymene)]₂

E(SMD/def2-QZVP*) = -2808.883869 E_h

$\Delta\Delta G(353) = 0.357479 E_h$

Lowest frequency = 9.69 cm⁻¹

C -3.196188 -0.881133 -1.724727
 C -2.371988 -1.963468 -1.260467
 C -2.269199 -2.159877 0.134134
 C -2.946720 -1.292237 1.044799
 C -3.760441 -0.219736 0.599562
 C -3.875624 -0.038364 -0.819662
 Ru -1.811333 -0.089646 -0.293817
 Cl 0.001572 0.128449 -1.916935
 Ru 1.809584 0.132269 -0.273456

Cl -0.004440 -0.066608 1.344309
 C -1.560623 -2.786344 -2.207202
 C -4.409728 0.767555 1.538076
 C -5.859333 0.356010 1.795703
 C 3.763883 0.127707 0.618783
 C 3.871526 0.130798 -0.812916
 C 3.195636 1.089471 -1.597373
 C 2.382693 2.109581 -0.992661
 C 2.289094 2.124351 0.416242
 C 2.963022 1.140788 1.204020
 C 1.572043 3.053204 -1.819882
 C 4.407444 -0.979552 1.416745
 C 5.867609 -0.627189 1.701042
 Cl 1.733421 -2.245157 -0.408586
 Cl -1.759048 2.286406 -0.143414
 C 3.640625 -1.331765 2.683813
 C -3.629077 0.972261 2.828988
 H 3.195710 0.984858 -2.684214
 H 4.373563 -0.703630 -1.307028
 H 2.745271 1.096065 2.271915
 H 1.573127 2.796338 0.892809
 H 2.087522 4.024532 -1.891154
 H 0.580044 3.198613 -1.367041
 H 1.422809 2.659663 -2.833339
 H 4.373735 -1.866664 0.762902

H	6.423475	-0.414491	0.774940	C	1.948116	0.134342	0.046793
H	6.372464	-1.459410	2.214608	C	1.733976	-1.254545	0.339047
H	5.939667	0.262356	2.347470	H	2.096856	-2.011710	-0.357625
H	3.683510	-0.524377	3.432535	C	0.932686	-1.661312	1.424001
H	4.079562	-2.226550	3.149109	H	0.698693	-2.719857	1.552988
H	2.587783	-1.548344	2.450087	C	0.274448	-0.688223	2.244652
H	-1.544442	-2.881035	0.516197	C	0.513839	0.684570	1.989350
H	-2.723097	-1.383268	2.108609	H	-0.052312	1.452960	2.514923
H	-4.387192	0.848501	-1.199421	C	1.344993	1.083413	0.902232
H	-3.204023	-0.638008	-2.789120	H	1.373534	2.143201	0.647368
H	-0.566714	-2.986507	-1.780037	C	2.744866	0.588941	-1.153850
H	-1.417225	-2.262506	-3.160795	H	2.358278	1.589742	-1.409287
H	-2.072935	-3.741979	-2.403382	C	4.216354	0.732049	-0.762631
H	-4.401041	1.729943	1.000161	H	4.344863	1.423145	0.083907
H	-3.646673	0.076588	3.470675	H	4.806856	1.114565	-1.609114
H	-4.075563	1.793313	3.408956	H	4.640670	-0.242036	-0.469803
H	-2.583653	1.235456	2.610407	C	2.566628	-0.304916	-2.376032
H	-5.906636	-0.609163	2.325395	H	3.048622	-1.286051	-2.236428
H	-6.426357	0.251912	0.857858	H	3.040052	0.160676	-3.253223
H	-6.369247	1.107450	2.417440	H	1.503065	-0.473675	-2.598974
				C	-0.715403	-1.123843	3.277534
[Ru(OAc)₂(<i>p</i>-cymene)]				H	-1.316700	-1.965832	2.907200
E(SMD/def2-QZVP*) = -940.928367 E _h				H	-1.395654	-0.302600	3.538442
ΔΔG(353) = 0.254300 E _h				H	-0.192136	-1.445779	4.192271
Lowest frequency = 19.80 cm ⁻¹				C	-1.793125	-1.555271	-1.199943

C -1.543438 2.359108 -0.138215
 Ru -0.169599 -0.273890 0.189433
 O -0.699321 -1.150383 -1.686672
 O -1.958619 -1.426229 0.046955
 O -1.434034 1.127062 -0.533233
 O -0.879858 2.900389 0.732549
 C -2.625426 3.106886 -0.890170
 H -3.592036 2.602419 -0.744958
 H -2.686081 4.143242 -0.537347
 H -2.410705 3.086849 -1.968746
 C -2.866062 -2.119944 -2.069395
 H -3.483799 -2.831178 -1.507062
 H -3.507634 -1.287688 -2.397780
 H -2.432121 -2.593490 -2.958806

Acetate

E(SMD/def2-QZVP*) = -228.467675 E_h

$\Delta\Delta G(353) = 0.014592 E_h$

Lowest frequency = 40.43 cm⁻¹

C 0.220014 0.001633 -0.000009
 O 0.802620 -1.099484 -0.000016
 O 0.692779 1.155456 -0.000035
 C -1.346982 -0.054735 0.000046
 H -1.737753 0.480214 0.883510
 H -1.737817 0.480304 -0.883334

H -1.725813 -1.089684 0.000013

Pyridyl indole

E(SMD/def2-QZVP*) = -610.478575 E_h

$\Delta\Delta G(353) = 0.154933 E_h$

Lowest frequency = 56.61 cm⁻¹

C 1.116100 -0.091876 0.012371
 C 2.186608 0.835163 -0.106455
 C 3.509840 0.375742 -0.057932
 C 3.747838 -0.978842 0.126283
 C 2.680891 -1.878725 0.281726
 C 1.358517 -1.452177 0.232279
 C 0.249841 1.981677 -0.178029
 C 1.601870 2.141166 -0.228519
 H 4.338883 1.080918 -0.153375
 H 4.774280 -1.350352 0.166538
 H 2.890060 -2.937108 0.453332
 H 0.550751 -2.165992 0.389938
 H -0.559897 2.704483 -0.224131
 H 2.130227 3.085459 -0.339015
 N -0.067497 0.636142 -0.052808
 C -1.389186 0.173129 -0.028504
 C -1.731098 -1.108442 -0.486307
 N -2.294466 1.042187 0.410039
 C -3.065099 -1.489573 -0.422054

H	-0.979707	-1.768399	-0.916311
C	-3.568702	0.670774	0.448794
C	-4.013671	-0.591983	0.065073
H	-3.363486	-2.481210	-0.770769
H	-4.279138	1.422572	0.810986
H	-5.070723	-0.854871	0.129829

Cartesian Coordinates and Energies

(PW6B95-D3(BJ)/def2-QZVP*+SMD(AcOH)/M06-D3/def2-SVP level of theory

Intermediate A	N	-0.383033	0.558450	1.453862
E(SMD/def2-QZVP*) = -1325.968745 E _h	C	2.844475	-0.361818	0.448324
$\Delta\Delta G(353) = 0.389382 E_h$	C	1.381064	-1.974175	1.073172
Lowest frequency = 24.16 cm ⁻¹	C	3.316735	-1.604828	-0.034748
C 0.902682 0.359349 1.805232	C	3.502071	0.843558	0.187843
C -1.108515 1.462816 2.141668	C	2.374604	-2.607099	0.387968
C -0.573185 2.235614 3.159156	C	4.498398	-1.633398	-0.790989
C 0.765833 2.057592 3.500197	C	4.667881	0.782351	-0.565555
C 1.507027 1.100317 2.822941	H	3.123827	1.800035	0.563914
Ru -1.281489 -0.281513 -0.330966	H	2.442450	-3.680797	0.217892
C 0.242927 0.582488 -1.656670	C	5.161529	-0.442594	-1.046887
C 0.197937 -0.811612 -1.853116	H	4.887737	-2.581365	-1.172562
C -1.037459 -1.472607 -2.141422	H	5.213272	1.704506	-0.783408
C -2.211388 -0.684721 -2.245051	H	6.084268	-0.452546	-1.632752
C -2.153308 0.717050 -2.008841	N	1.645783	-0.603488	1.117803
C -0.932742 1.385577 -1.716480	O	-3.045454	-0.290544	0.867659
H 1.102276 -1.408120 -1.694092	C	-2.763629	-1.425459	1.364343
H -3.088777 1.285578 -1.952097	O	-1.720470	-1.989659	0.921249
H 2.548626 0.889069 3.076555	C	-3.589975	-2.028778	2.438547
H 1.222606 2.643303 4.301951	H	-3.496384	-3.122269	2.431719
H -1.203389 2.964088 3.672509	H	-3.226928	-1.661236	3.411900
H -2.157161 1.560332 1.845551	H	-4.639756	-1.724689	2.334891

H	0.485076	-2.366763	1.554421	C	-1.380864	3.363237	-2.281947
H	1.193267	1.025370	-1.339945	C	-1.852829	2.056078	-2.258335
H	-3.180593	-1.173080	-2.381005	Ru	1.030605	-0.128723	0.220437
C	-1.088705	-2.959176	-2.208240	C	-0.392077	-0.345103	1.902916
H	-0.851900	-3.297623	-3.230540	C	0.280698	-1.563591	1.687914
H	-0.348298	-3.403448	-1.525943	C	1.706951	-1.667277	1.658000
H	-2.084988	-3.341115	-1.943868	C	2.441547	-0.470857	1.818959
C	-0.936046	2.875328	-1.469987	C	1.783052	0.779633	1.984207
H	-1.838598	3.085978	-0.861030	C	0.354387	0.860690	2.036912
C	-1.082299	3.597159	-2.808376	H	-0.311337	-2.456392	1.463878
H	-1.992258	3.291293	-3.348220	H	2.372520	1.702927	2.011417
H	-1.129625	4.686778	-2.659120	H	-2.777742	1.762183	-2.759824
H	-0.217389	3.384474	-3.459673	H	-1.957642	4.144869	-2.782820
C	0.283047	3.381589	-0.717102	H	0.270291	4.664369	-1.731874
H	0.170937	4.453468	-0.495262	H	1.541437	2.801762	-0.630455
H	0.439180	2.858865	0.241197	N	0.075768	1.387010	-1.002667
H	1.202442	3.276233	-1.318969	C	-2.551327	-0.808666	-0.932255
Transition state TS1				C	-0.449406	-1.241675	-1.654467
E(SMD/def2-QZVP*) = -1325.948371 E _h				C	-2.270351	-2.179561	-0.695333
$\Delta\Delta G(353) = 0.389554 E_h$				C	-3.733391	-0.206614	-0.494363
Lowest frequency = -111.19 cm ⁻¹				C	-0.947396	-2.428973	-1.177522
C	-1.086594	1.090844	-1.611057	C	-3.223276	-2.972182	-0.031332
C	0.558484	2.634767	-1.082391	C	-4.648831	-1.013450	0.166946
C	-0.148045	3.656747	-1.700204	H	-3.938507	0.854103	-0.664466
				H	-0.415269	-3.380510	-1.204554

C -4.401009 -2.381563 0.392696
 H -3.032287 -4.034078 0.147616
 H -5.589067 -0.577204 0.514777
 H -5.154173 -2.981471 0.909589
 N -1.442357 -0.256314 -1.560890
 O 2.619241 0.416627 -1.010148
 C 3.042991 -0.638166 -1.629977
 O 2.484226 -1.728119 -1.495747
 C 4.253322 -0.444612 -2.491859
 H 4.389399 -1.305263 -3.158290
 H 4.176026 0.485353 -3.072308
 H 5.142544 -0.349875 -1.849299
 H 0.443647 -1.079559 -2.260371
 H -1.485571 -0.326618 1.854126
 H 3.526695 -0.489563 1.673640
 C 2.373957 -2.969722 1.376379
 H 2.526952 -3.527512 2.315195
 H 1.761621 -3.588845 0.705155
 H 3.349585 -2.822228 0.893684
 C -0.291368 2.204060 2.260634
 H 0.311918 2.943529 1.697142
 C -0.174066 2.536075 3.749113
 H 0.871266 2.536119 4.095397
 H -0.598735 3.530495 3.955097
 H -0.730293 1.801030 4.355208

C -1.734787 2.302448 1.798974
 H -2.097660 3.334599 1.918483
 H -1.862243 2.023823 0.740896
 H -2.400251 1.659416 2.400111

Intermediate B

E(SMD/def2-QZVP*) = -1325.951899 E_h

$\Delta\Delta G(353) = 0.388463$ E_h

Lowest frequency = 31.67 cm⁻¹

C -1.185912 1.010742 -1.674563
 C 0.117517 2.788510 -0.964760
 C -0.706729 3.697718 -1.615176
 C -1.818653 3.220236 -2.306653
 C -2.054778 1.850042 -2.361228
 Ru 0.916205 0.016344 0.232307
 C -0.371457 -0.459745 1.971139
 C 0.572987 -1.499483 1.775378
 C 1.973351 -1.268492 1.714445
 C 2.399461 0.084969 1.807109
 C 1.477332 1.143935 1.985109
 C 0.070391 0.881662 2.074024
 H 0.207233 -2.519645 1.620123
 H 1.835073 2.178818 2.005013
 H -2.870016 1.423067 -2.949674
 H -2.481804 3.911230 -2.833158

H -0.469939 4.762843 -1.586807
 H 1.017562 3.105313 -0.428284
 N -0.146634 1.477046 -0.957498
 C -2.262291 -1.150949 -1.074099
 C -0.058089 -1.098062 -1.611035
 C -1.686573 -2.395194 -0.702807
 C -3.584585 -0.829680 -0.758481
 C -0.310155 -2.346547 -1.069476
 C -2.472395 -3.357465 -0.041836
 C -4.330856 -1.795065 -0.098210
 H -4.020902 0.137095 -1.023755
 H 0.438342 -3.137668 -1.002465
 C -3.787616 -3.048241 0.252011
 H -2.046730 -4.327016 0.232343
 H -5.373662 -1.580652 0.151141
 H -4.419611 -3.780254 0.760555
 N -1.277472 -0.384259 -1.677426
 O 2.406786 0.527787 -1.099852
 C 3.145531 -0.429274 -1.591090
 O 2.918086 -1.618617 -1.420264
 C 4.321866 0.066079 -2.387187
 H 4.762240 -0.755955 -2.965033
 H 4.028224 0.891026 -3.051429
 H 5.083185 0.464645 -1.698360
 H 0.755123 -0.834038 -2.289011

H -1.439770 -0.697756 1.963714
 H 3.454935 0.318841 1.632255
 C 2.942781 -2.383880 1.520910
 H 3.315595 -2.729919 2.499383
 H 2.473442 -3.237104 1.011040
 H 3.797208 -2.067934 0.907456
 C -0.873903 2.036151 2.292146
 H -0.441179 2.906685 1.760682
 C -0.880401 2.355673 3.787659
 H 0.129156 2.573469 4.170097
 H -1.516134 3.230830 3.991791
 H -1.282433 1.504999 4.363646
 C -2.284705 1.813647 1.776363
 H -2.880563 2.730208 1.903933
 H -2.304987 1.547070 0.707157
 H -2.805559 1.016086 2.333370

Transition state **TS2**

$E(\text{SMD/def2-QZVP}^*) = -1325.941160 E_h$

$\Delta\Delta G(353) = 0.385173 E_h$

Lowest frequency = -985.57 cm^{-1}

C 0.748172 -1.666426 0.855463
 C -1.279880 -1.852430 1.981049
 C -0.810677 -2.901750 2.752404
 C 0.498384 -3.340850 2.545938

C	1.287165	-2.731102	1.582343	C	5.111465	-0.718543	-0.169314
Ru	-1.171928	0.411726	-0.100130	H	3.830956	-1.697149	1.260236
C	-0.154914	2.255844	0.572043	H	1.219954	0.806970	-2.923149
C	-0.709884	2.436281	-0.732191	C	5.221075	0.032341	-1.356228
C	-2.070994	2.187645	-1.014567	H	4.172386	0.997656	-2.978150
C	-2.956177	1.749246	0.018422	H	6.019610	-0.981600	0.379807
C	-2.422925	1.550964	1.312959	H	6.210970	0.329078	-1.711352
C	-1.038459	1.782115	1.572503	N	1.398598	-0.997660	-0.159298
C	1.301817	2.559707	0.821280	O	-2.499284	-1.005884	-0.887798
H	-0.037577	2.707217	-1.553415	C	-2.183671	-1.956908	-1.676948
H	-2.440305	2.272150	-2.040344	O	-1.029881	-2.152023	-2.106624
H	-3.066225	1.150457	2.102643	H	-0.222893	-1.102308	-1.659320
H	-0.639842	1.523498	2.558986	C	-3.292967	-2.858342	-2.124703
H	1.847376	2.237231	-0.087245	H	-3.660607	-2.499554	-3.099066
H	2.287722	-3.098899	1.352129	H	-2.913892	-3.877789	-2.273785
H	0.896930	-4.180484	3.121055	H	-4.128773	-2.847846	-1.414108
H	-1.463000	-3.373333	3.489053	C	1.893366	1.826750	2.013654
H	-2.305871	-1.482667	2.074071	H	2.982625	1.983322	2.049074
N	-0.510920	-1.231165	1.073852	H	1.486053	2.201473	2.968500
C	2.742006	-0.778303	-0.399924	H	1.719571	0.738235	1.967656
C	0.608567	-0.329095	-1.141644	C	1.472136	4.070263	0.967995
C	2.832375	0.009027	-1.580810	H	2.533588	4.330373	1.101036
C	3.884175	-1.133792	0.326444	H	1.099533	4.616406	0.086670
C	1.503397	0.269148	-2.016759	H	0.921691	4.440815	1.849732
C	4.093577	0.402310	-2.064540	C	-4.368347	1.402205	-0.297371

H	-4.992328	2.310862	-0.268802	H	0.083874	3.307139	-0.447171
H	-4.449183	0.965366	-1.302933	H	2.996063	-1.532660	2.374594
H	-4.776776	0.681762	0.425252	H	1.819173	-2.688677	4.221231
Intermediate C				H	-0.707015	-2.698228	4.263957
E(SMD/def2-QZVP*) = -1325.963398 E _h				H	-1.918352	-1.532790	2.414081
$\Delta\Delta G(353) = 0.385144 E_h$				N	-0.192900	-0.888431	1.468276
Lowest frequency = 11.67 cm ⁻¹				C	2.990434	0.117171	-0.032167
C	1.160627	-0.871788	1.433279	C	0.760072	0.298867	-0.606897
C	-0.825426	-1.538405	2.458868	C	2.892124	0.781176	-1.279051
C	-0.151850	-2.188255	3.475349	C	4.229319	-0.092123	0.575978
C	1.244369	-2.176818	3.445175	C	1.491498	0.878189	-1.611298
C	1.909683	-1.524208	2.421747	C	4.048972	1.216834	-1.932634
Ru	-1.197418	-0.004669	-0.163616	C	5.365990	0.352642	-0.092937
C	-1.577869	2.117264	0.057611	H	4.344542	-0.568131	1.549619
C	-1.806863	1.744529	-1.305631	H	1.084446	1.348590	-2.508314
C	-2.671928	0.684390	-1.632953	C	5.281610	0.995100	-1.334336
C	-3.455592	0.017198	-0.626373	H	3.977333	1.727893	-2.896754
C	-3.274363	0.402509	0.706768	H	6.344609	0.197851	0.368863
C	-2.296236	1.390484	1.045699	H	6.196150	1.329653	-1.830668
C	-0.635675	3.246103	0.391426	N	1.675653	-0.190812	0.358154
H	-1.218676	2.225463	-2.094103	O	-1.084052	-2.036949	-0.939049
H	-2.748677	0.351026	-2.672719	C	-0.319087	-2.659369	-1.679522
H	-3.818204	-0.121384	1.498967	O	0.733846	-2.141737	-2.244301
H	-2.088968	1.587253	2.103157	H	0.850877	-1.190664	-1.988821
				C	-0.538299	-4.092792	-2.004150

H	-0.591362	-4.218124	-3.095917	Ru	1.062380	-0.421968	-0.441454
H	0.330216	-4.677046	-1.664142	C	0.842029	-2.641139	-0.001977
H	-1.452808	-4.465207	-1.530122	C	1.592656	-2.457226	-1.187229
C	0.158932	3.033477	1.668724	C	2.798030	-1.698916	-1.179904
H	0.865461	3.864603	1.813987	C	3.239595	-1.141425	0.055307
H	-0.488095	3.010892	2.562505	C	2.431260	-1.237394	1.189729
H	0.745781	2.100917	1.637804	C	1.202117	-1.986596	1.192793
C	-1.435974	4.545577	0.438549	H	1.249296	-2.908727	-2.123401
H	-0.771132	5.406937	0.605805	H	2.732651	-0.728638	2.112776
H	-1.989470	4.722591	-0.497606	H	-2.821756	2.013079	1.847860
H	-2.169989	4.522512	1.262730	H	-1.449507	3.312022	3.446376
C	-4.347174	-1.111833	-1.013320	H	1.071006	3.100504	3.371143
H	-5.246108	-0.732066	-1.526309	H	2.072106	1.595297	1.652533
H	-3.832908	-1.790279	-1.711670	N	0.243909	0.957678	0.904393
H	-4.671745	-1.693950	-0.139542	C	-3.089564	0.029777	-0.283390
Intermediate D				C	-0.922807	-0.490456	-0.856682
E(SMD/def2-QZVP*) = -1403.482404 E _h				C	-3.100712	-0.885167	-1.363765
$\Delta\Delta G(353) = 0.423396 E_h$				C	-4.275224	0.499556	0.280286
Lowest frequency = 24.43 cm ⁻¹				C	-1.730478	-1.187484	-1.701586
C	-1.108261	1.061839	0.929375	C	-4.319500	-1.323769	-1.888696
C	0.987226	1.689251	1.757131	C	-5.476534	0.046068	-0.258839
C	0.429553	2.533502	2.694818	H	-4.305566	1.196470	1.117711
C	-0.965243	2.644845	2.728728	H	-1.402183	-1.850006	-2.504279
C	-1.738953	1.917656	1.845537	C	-5.501277	-0.852377	-1.331409
				H	-4.336975	-2.027247	-2.725799

H	-6.416514	0.404034	0.168992
H	-6.462106	-1.185498	-1.732336
N	-1.734284	0.270293	0.015127
C	1.732245	1.349987	-1.588462
H	2.829375	1.368739	-1.569029
C	1.030330	0.498347	-2.447503
H	1.560956	-0.157639	-3.143426
H	0.017339	0.781622	-2.746837
C	1.085599	2.619205	-1.154256
O	-0.071341	2.904933	-1.321959
O	1.969349	3.413548	-0.540534
H	-0.098369	-3.196549	-0.054414
H	4.170307	-0.565553	0.087041
C	0.405790	-2.092820	2.471108
H	0.427712	-1.083746	2.932162
C	1.113342	-3.062232	3.417091
H	2.154842	-2.766633	3.621534
H	0.584557	-3.115739	4.380942
H	1.130501	-4.078298	2.987377
C	-1.046022	-2.492949	2.265962
H	-1.573602	-1.841127	1.550109
H	-1.133313	-3.533312	1.908865
H	-1.586428	-2.444602	3.223122
C	3.635896	-1.565717	-2.408111
H	4.030395	-0.544821	-2.529424

H	4.505264	-2.239445	-2.332508
H	3.085599	-1.844994	-3.317809
C	1.480121	4.682122	-0.124836
H	2.316756	5.199605	0.358159
H	1.122428	5.262612	-0.988079
H	0.641810	4.562572	0.580610

Transition state **TS3**

E(SMD/def2-QZVP*) = -1403.462204 E_h

$\Delta\Delta G(353) = 0.423437 E_h$

Lowest frequency = -262.37 cm⁻¹

C	-0.930400	1.481992	0.698631
C	1.135607	1.594761	1.760407
C	0.744914	2.675961	2.526150
C	-0.535506	3.195562	2.325187
C	-1.379801	2.605392	1.401226
Ru	0.873907	-0.629788	-0.351212
C	0.112972	-2.685190	0.145198
C	0.832396	-2.697464	-1.083635
C	2.173741	-2.244203	-1.163439
C	2.783818	-1.750679	0.033191
C	2.040101	-1.668163	1.220762
C	0.683314	-2.139317	1.307845
H	0.335559	-3.047949	-1.994613
H	2.492187	-1.205325	2.105421

H	-2.360359	3.027136	1.184825	O	1.374384	3.057256	-0.903589
H	-0.868783	4.077290	2.878093	O	3.404635	2.112787	-0.736385
H	1.438670	3.118336	3.242866	H	-0.938457	-2.986010	0.143369
H	2.148030	1.184416	1.832098	H	3.800404	-1.345840	-0.004557
N	0.319344	0.999290	0.873778	C	-0.064909	-2.013184	2.611114
C	-3.057183	0.677854	-0.411504	H	0.278486	-1.065293	3.072376
C	-1.013029	-0.113084	-1.096282	C	0.338809	-3.162371	3.532516
C	-3.257070	-0.283414	-1.434693	H	1.427793	-3.200693	3.696102
C	-4.132609	1.264545	0.255813	H	-0.146351	-3.061775	4.515521
C	-1.967894	-0.752849	-1.848114	H	0.029799	-4.130093	3.102021
C	-4.560193	-0.617639	-1.827289	C	-1.573874	-1.939025	2.444008
C	-5.415594	0.908389	-0.148643	H	-1.881688	-1.157566	1.727851
H	-4.004288	1.968764	1.078756	H	-1.993527	-2.899212	2.098872
H	-1.769032	-1.462899	-2.652692	H	-2.051889	-1.716751	3.409808
C	-5.629535	-0.012862	-1.184170	C	2.922350	-2.293638	-2.454194
H	-4.725322	-1.350962	-2.621373	H	3.759038	-1.579568	-2.471499
H	-6.273660	1.358911	0.356946	H	3.348812	-3.298826	-2.605151
H	-6.652298	-0.262168	-1.478065	H	2.262076	-2.085948	-3.311124
N	-1.671824	0.793542	-0.232363	C	3.912274	3.325436	-0.197709
C	1.723449	0.828308	-1.697477	H	4.975990	3.159096	0.006779
H	2.546590	0.312526	-2.203369	H	3.789390	4.152163	-0.913161
C	0.397819	0.696496	-2.215595	H	3.383295	3.595228	0.730131
H	0.258863	0.077209	-3.108077				
H	-0.195812	1.620402	-2.214566				
C	2.110998	2.119367	-1.086035				

Intermediate **E**

E(SMD/def2-QZVP*) = -1403.486541 E_h

$$\Delta\Delta G(353) = 0.426426 E_h$$

Lowest frequency = 28.13 cm⁻¹

C -0.648696 2.112464 -0.583715

C 1.005826 2.184309 1.025346

C 0.763189 3.529320 1.267285

C -0.228808 4.175303 0.536702

C -0.936001 3.459256 -0.424820

Ru 0.452831 -0.681574 -0.141373

C -0.927707 -1.813767 1.286699

C -0.419074 -2.655978 0.259339

C 0.969151 -2.823145 0.009089

C 1.861935 -2.044169 0.801973

C 1.367378 -1.157347 1.783605

C -0.040658 -1.034478 2.049335

H -1.131428 -3.187811 -0.381320

H 2.074440 -0.534394 2.343396

H -1.683193 3.926149 -1.070086

H -0.430732 5.238113 0.690854

H 1.366653 4.062562 2.003699

H 1.810255 1.657811 1.546501

N 0.287453 1.469814 0.148841

C -2.536976 0.690625 -1.196246

C -0.464319 0.280778 -2.049079

C -2.492546 -0.668411 -1.566018

C -3.644631 1.247177 -0.567638

C -1.158895 -0.918623 -2.070876

C -3.610405 -1.482797 -1.361754

C -4.740955 0.415407 -0.351987

H -3.662255 2.296740 -0.260888

H -0.823764 -1.812311 -2.602293

C -4.730666 -0.928603 -0.752788

H -3.602772 -2.532720 -1.670620

H -5.634222 0.824493 0.127400

H -5.617956 -1.544435 -0.585726

N -1.299040 1.285658 -1.516930

C 1.858107 -0.154199 -1.683500

H 2.259531 -1.097154 -2.085258

C 0.900036 0.567936 -2.612316

H 0.961477 0.230075 -3.660057

H 1.095464 1.651578 -2.608037

C 2.936929 0.671929 -1.104332

O 2.954956 1.880940 -1.052259

O 3.918222 -0.084283 -0.571320

H -2.010092 -1.712312 1.410167

H 2.933698 -2.059748 0.581628

C -0.514758 -0.100755 3.133754

H 0.262320 0.680790 3.244364

C -0.575009 -0.884931 4.444529

H 0.389029 -1.361222 4.684100

H -0.843290 -0.221805 5.281317

H	-1.337440	-1.680148	4.385279	C	0.297159	1.981695	-1.230913
C	-1.836280	0.587703	2.834648	C	0.421010	0.970137	-2.224252
H	-1.808022	1.150182	1.886219	C	-0.794091	0.367045	-2.680197
H	-2.673507	-0.128600	2.775535	C	-2.034485	0.767588	-2.149575
H	-2.082760	1.296244	3.640193	C	-2.148392	1.867836	-1.227500
C	1.472195	-3.746386	-1.050492	H	1.215363	2.389727	-0.791613
H	2.432707	-3.400188	-1.461672	H	-2.932370	0.199939	-2.418455
H	1.637367	-4.755506	-0.638589	H	3.259520	0.492076	3.014779
H	0.752357	-3.844489	-1.877817	H	1.862940	1.587704	4.789583
C	4.990856	0.622526	0.029909	H	-0.603852	1.928802	4.322659
H	5.722961	-0.126842	0.353367	H	-1.509320	1.173549	2.145089
H	5.455455	1.318863	-0.683884	N	0.293486	0.453610	1.414432
H	4.643553	1.206932	0.897971	C	3.677923	0.149423	0.310954
				C	2.245055	-1.612584	0.181136
Intermediate F				C	4.299520	-0.876394	-0.435299
E(SMD/def2-QZVP*) = -1632.962863 E _h				C	4.279030	1.392542	0.515921
$\Delta\Delta G(353) = 0.480600 E_h$				C	3.375570	-1.975544	-0.488502
Lowest frequency = 26.52 cm ⁻¹				C	5.568551	-0.646184	-0.982924
C	1.608013	0.283791	1.654366	C	5.538392	1.593546	-0.037791
C	-0.451367	1.029455	2.380724	H	3.782606	2.187745	1.081265
C	0.057541	1.459691	3.591875	H	3.523303	-2.933206	-0.987805
C	1.417995	1.279526	3.840184	C	6.176669	0.584343	-0.776680
C	2.194673	0.682938	2.863285	H	6.067092	-1.423506	-1.568521
Ru	-0.717904	0.234704	-0.520904	H	6.037427	2.556021	0.102922
C	-0.966865	2.484190	-0.793608	H	7.166563	0.776146	-1.198958

C	-0.374865	-0.768662	-2.256406	C	0.179482	1.984003	-0.370359
C	0.935170	-0.272779	-2.562321	C	-1.008329	2.517051	0.438604
C	2.090831	-0.891677	-2.058732	H	-1.255207	3.540309	0.115143
C	1.999202	-2.044299	-1.211347	H	-0.746282	2.596396	1.510813
H	-1.453194	-2.182614	-1.024977	H	0.600404	-3.303369	-0.122103
H	3.067908	-0.430573	-2.236441	H	1.041448	0.653667	-3.136504
H	-3.179403	-0.129392	3.057569	C	3.270477	-2.658355	-0.690892
H	-1.913390	-1.203146	4.951572	H	3.929729	-1.809646	-0.429207
H	0.499371	-1.849464	4.549426	C	3.917656	-3.447643	-1.829540
H	1.506226	-1.363829	2.330780	H	4.105406	-2.822598	-2.716752
N	-0.220454	-0.559544	1.514373	H	4.882343	-3.866103	-1.504225
C	-3.453103	-0.232737	0.225495	H	3.273695	-4.288298	-2.139090
C	-2.204932	1.666540	0.220164	C	3.092511	-3.525079	0.541301
C	-4.138256	0.743589	-0.531439	H	2.602587	-2.983081	1.366015
C	-3.935450	-1.532600	0.387761	H	2.503786	-4.432946	0.324158
C	-3.328479	1.929610	-0.508535	H	4.073072	-3.863852	0.907920
C	-5.346107	0.394455	-1.152174	C	-1.591351	-0.145018	-2.850689
C	-5.135638	-1.850479	-0.238254	H	-1.495282	0.947365	-2.951707
H	-3.394137	-2.276449	0.982535	H	-1.739059	-0.548322	-3.866430
H	-3.542211	2.880520	-0.996758	H	-2.498597	-0.366938	-2.268209
C	-5.831355	-0.897214	-1.000383	O	2.550408	-0.006480	0.757055
H	-5.894178	1.128683	-1.749129	C	2.648394	1.002134	1.522695
H	-5.544536	-2.859062	-0.134279	O	1.694964	1.798096	1.689091
H	-6.771965	-1.180802	-1.479764	H	0.910586	1.549017	0.646202
N	-2.255444	0.332616	0.668232	C	3.950768	1.244910	2.207129

H	4.512807	0.312345	2.341587	C	0.854924	-1.005287	-2.412288
H	4.547152	1.912404	1.564090	C	2.063720	-1.455711	-1.853445
H	3.793035	1.756910	3.164942	C	2.051291	-2.362031	-0.752059
C	1.258364	2.944719	-0.780117	H	-1.402222	-2.720776	-0.492205
O	2.202469	2.613674	-1.458541	H	3.007180	-0.989745	-2.155389
O	1.085363	4.165123	-0.289274	H	-2.804033	1.482950	2.790397
C	2.117330	5.107067	-0.552767	H	-1.517273	1.172587	4.943986
H	3.069536	4.760865	-0.122579	H	0.620343	-0.168791	4.863767
H	2.253140	5.247170	-1.635174	H	1.420367	-1.006914	2.663257
H	1.810161	6.047829	-0.082729	N	-0.199238	-0.272284	1.597402
H	-0.202997	1.582879	-1.316873	C	-3.232008	-0.308065	0.270749
				C	-2.345490	1.715094	-0.260318
Intermediate G				C	-4.115521	0.337581	-0.621363
E(SMD/def2-QZVP*) = -1632.965014 E _h				C	-3.498823	-1.561678	0.821096
ΔΔG(353) = 0.479009 E _h				C	-3.527609	1.611108	-0.935488
Lowest frequency = 27.00 cm ⁻¹				C	-5.283807	-0.329192	-1.015840
C	-1.358773	0.404525	1.639119	C	-4.666498	-2.199808	0.414562
C	0.472337	-0.468308	2.743913	H	-2.820039	-2.024503	1.546402
C	0.032102	0.019061	3.963759	H	-3.925247	2.366546	-1.613687
C	-1.147636	0.755852	4.003858	C	-5.542542	-1.592968	-0.501008
C	-1.856318	0.938415	2.824151	H	-5.982157	0.140936	-1.713781
Ru	0.803465	-0.679445	-0.266550	H	-4.910674	-3.185377	0.820159
C	0.776972	-2.794468	-0.265071	H	-6.451139	-2.122094	-0.800166
C	-0.437326	-2.408794	-0.905684	N	-2.121466	0.520115	0.456468
C	-0.418903	-1.512133	-1.988078	C	-0.228699	2.300670	-1.360468

C	-1.280785	2.750006	-0.354205	H	3.540430	2.860561	2.092702
H	-1.724273	3.706478	-0.670301	H	4.328503	1.243221	1.899782
H	-0.793734	2.922570	0.619237	C	1.085681	3.029518	-1.393602
H	0.729182	-3.404622	0.642086	O	2.115167	2.520485	-1.765877
H	0.882637	-0.197704	-3.152612	O	0.961427	4.293149	-1.014492
C	3.357278	-2.749477	-0.114510	C	2.154370	5.061401	-0.954692
H	3.970775	-1.829090	-0.105942	H	2.818309	4.667132	-0.169667
C	4.032711	-3.785246	-1.014592	H	2.687919	5.036109	-1.916022
H	4.185442	-3.411446	-2.039247	H	1.856622	6.086987	-0.709858
H	5.017809	-4.058013	-0.606450	H	-0.646355	2.311120	-2.386078
H	3.428580	-4.706381	-1.076777				
C	3.235804	-3.256838	1.310035	Intermediate H			
H	2.726571	-2.533539	1.966637	E(SMD/def2-QZVP*) = -1632.988615 E _h			
H	2.698402	-4.219270	1.362243	$\Delta\Delta G(353) = 0.478226 E_h$			
H	4.236785	-3.429762	1.732329	Lowest frequency = 23.25 cm ⁻¹			
C	-1.669960	-1.051945	-2.653311	C	-0.308437	0.877812	1.860823
H	-1.692094	0.042592	-2.773671	C	-0.614725	-1.328533	2.488132
H	-1.723484	-1.491782	-3.663027	C	-0.788116	-0.977479	3.819242
H	-2.568193	-1.359239	-2.099324	C	-0.733815	0.366674	4.171261
O	2.412023	0.188909	0.607590	C	-0.479326	1.302871	3.176690
C	2.344853	1.417050	1.051967	Ru	-0.534243	-1.182521	-0.537079
O	1.304869	2.056916	1.110672	C	-2.401380	-0.093225	-0.944055
H	0.034780	1.234646	-1.182046	C	-1.410284	0.341014	-1.851092
C	3.674019	1.992391	1.434182	C	-0.676581	-0.601793	-2.629267
H	4.162663	2.325347	0.503006	C	-0.990289	-1.981971	-2.490318

C	-1.966520	-2.397684	-1.546734	H	2.749103	1.857898	1.662095
C	-2.700858	-1.467368	-0.753870	H	2.181043	0.321673	1.032122
H	-1.147133	1.403145	-1.892583	H	-2.856884	0.659036	-0.293298
H	-2.085129	-3.468494	-1.343637	H	-0.388081	-2.729357	-3.015120
H	-0.394502	2.370975	3.391542	C	-3.714374	-1.965504	0.247776
H	-0.869187	0.682419	5.208723	H	-3.256860	-2.849797	0.736582
H	-0.965781	-1.757515	4.561895	C	-4.966715	-2.424764	-0.496129
H	-0.644343	-2.375599	2.173190	H	-4.744084	-3.203722	-1.242363
N	-0.403166	-0.423278	1.513790	H	-5.708480	-2.834725	0.206373
C	-0.976428	2.719233	0.348288	H	-5.435991	-1.577444	-1.024570
C	1.190516	2.038677	0.232801	C	-4.066691	-0.948316	1.321128
C	-0.332273	3.462284	-0.669106	H	-3.179907	-0.567693	1.856286
C	-2.322579	2.895583	0.673669	H	-4.606445	-0.084009	0.896314
C	1.031977	3.013806	-0.715222	H	-4.734562	-1.402566	2.068344
C	-1.082002	4.401979	-1.393096	C	0.468063	-0.149033	-3.466780
C	-3.038885	3.833060	-0.062047	H	1.229277	-0.935978	-3.565719
H	-2.796233	2.327064	1.482222	H	0.114383	0.118101	-4.476297
H	1.826209	3.413877	-1.345417	H	0.937068	0.743486	-3.024438
C	-2.425127	4.573388	-1.087211	O	0.488359	-2.855052	0.296150
H	-0.612619	4.992086	-2.185287	C	1.628577	-2.359801	0.026924
H	-4.093735	4.005015	0.168518	O	1.622045	-1.248558	-0.583863
H	-3.016642	5.304881	-1.643991	H	3.175393	0.946017	-1.246182
N	-0.041985	1.827698	0.864183	C	2.886805	-3.024733	0.431077
C	3.540087	1.319071	-0.271126	H	3.356503	-2.428433	1.229600
C	2.410576	1.355949	0.733824	H	2.699048	-4.048945	0.775212

H	3.597973	-3.019363	-0.407740
C	4.640141	0.389540	0.157142
O	4.551547	-0.427469	1.040363
O	5.731212	0.561016	-0.584191
C	6.833513	-0.288232	-0.300871
H	7.158205	-0.173040	0.744085
H	6.568013	-1.343787	-0.466901
H	7.640266	0.006637	-0.981338
H	3.972479	2.313614	-0.471349

Alkene 3a

E(SMD/def2-QZVP*) = -306.978933 E_h

$\Delta\Delta G(353) = 0.057218 E_h$

Lowest frequency = 98.10 cm⁻¹

C	-0.041115	0.115962	-0.000001
O	0.056877	1.316312	0.000005
O	1.014428	-0.712454	0.000034
C	2.285179	-0.092297	0.000079
H	3.031048	-0.896465	0.000102
H	2.415626	0.542922	-0.890398

H	2.415565	0.542917	0.890568
C	-1.309380	-0.648391	-0.000046
C	-2.479582	-0.011171	-0.000087
H	-1.230126	-1.740092	-0.000044
H	-3.431146	-0.548690	-0.000120
H	-2.502018	1.083925	-0.000087

HOAc

E(SMD/def2-QZVP*) = -229.469374 E_h

$\Delta\Delta G(353) = 0.028749 E_h$

Lowest frequency = 91.72 cm⁻¹

C	-0.092892	0.124244	-0.000006
O	-0.646051	1.190449	-0.000050
O	-0.766277	-1.039274	-0.000003
H	-1.709529	-0.809639	-0.000040
C	1.384835	-0.103073	0.000051
H	1.672718	-0.692564	0.883434
H	1.672778	-0.692617	-0.883278
H	1.911001	0.858393	0.000041

