Supporting Information

Z-Selective Ethenolysis With a Ruthenium Metathesis Catalyst: Experiment and Theory

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Computational Details

The geometries of all intermediates and transition states were optimized with B3LYP in gas phase. A mixed basis set of LANL2DZ for Ru and 6-31G(d) for other atoms were used in geometry optimizations. Single point energy calculations were performed with the M06 functional and a mixed basis set of SDD for Ru and 6-311+G(d,p) for other atoms. The SMD solvation model was used in M06 single point energy calculations. THF was used as solvent. The reported free energies and enthalpies include zero-point energies and thermal corrections calculated at 298K by B3LYP. All calculations were performed with Gaussian 09. The 3D structures of molecules were generated using CYLView (http://www.cylview.org).

The Gibbs free energies in Gaussian were calculated under p = 1 atm. The standard free energies in solution were calculated under the standard state in solution, *i.e.* M = 1 mol/L. The correction was made by adding $RT \ln(c_{0s}/c_{0g})$ (i.e., about 1.84 kcal/mol) to energies of all structures, where c_{0s} is the standard molar concentration in aqueous solution (1 mol/L), c_{0g} the standard molar concentration in gas phase (0.0446 mol/L), and R the gas constant.

Complete Reference of Gaussian 09 (Ref. 23)

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2010**.

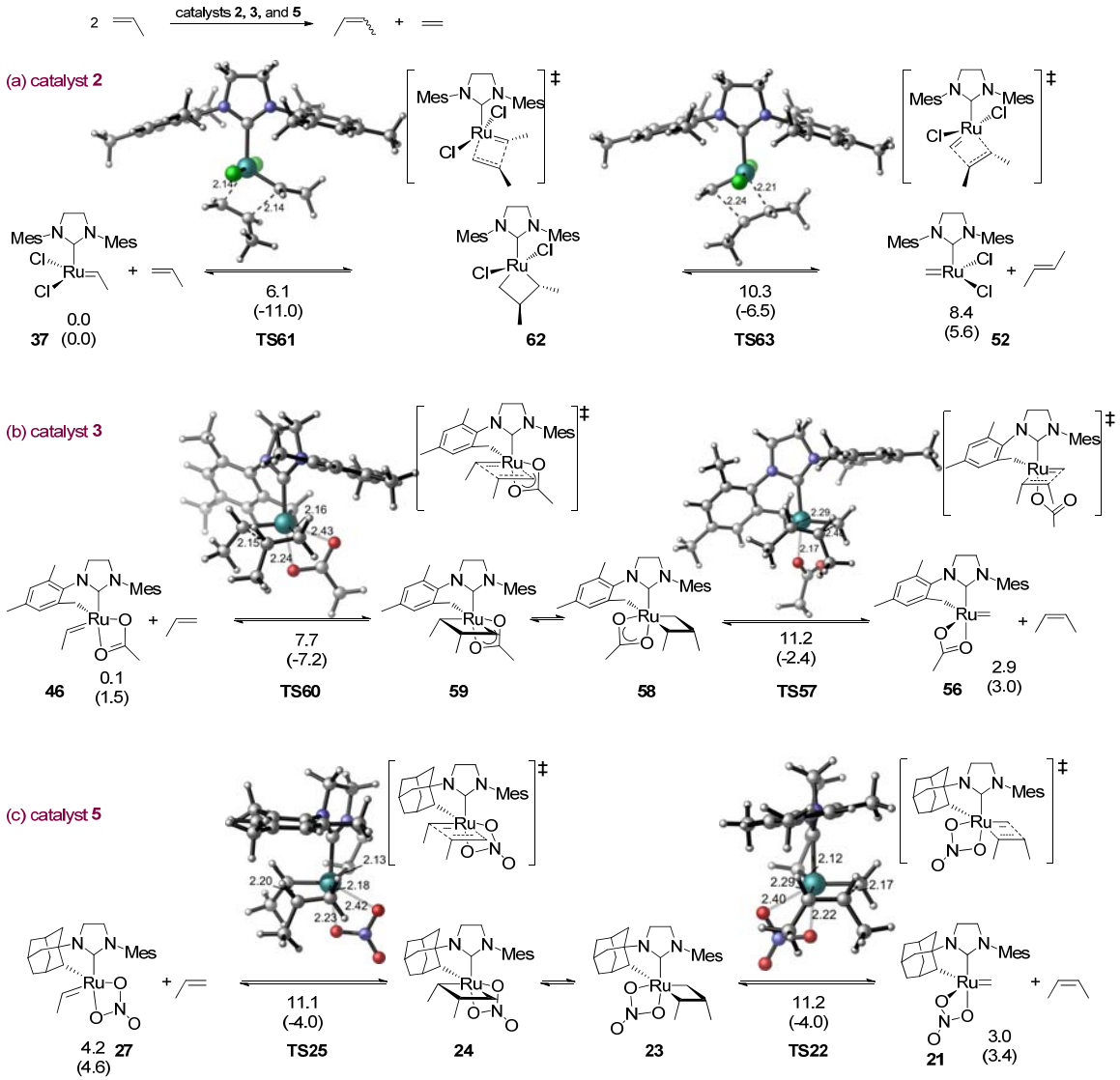


Figure S1. Free energies and enthalpies (in parenthesis) of the reaction of propene with ruthenium ethylidene complexes from (a) catalyst **2**; (b) catalyst **3**; and (c) catalyst **5** All energies are with respect to the most stable isomer of ruthenium alkylidene complexes (**37**, **41**, and **47**, respectively) and are given in kcal/mol. For clarity, the chelating adamantyl group is not shown in the 3D structures of **TS22** and **TS25**.

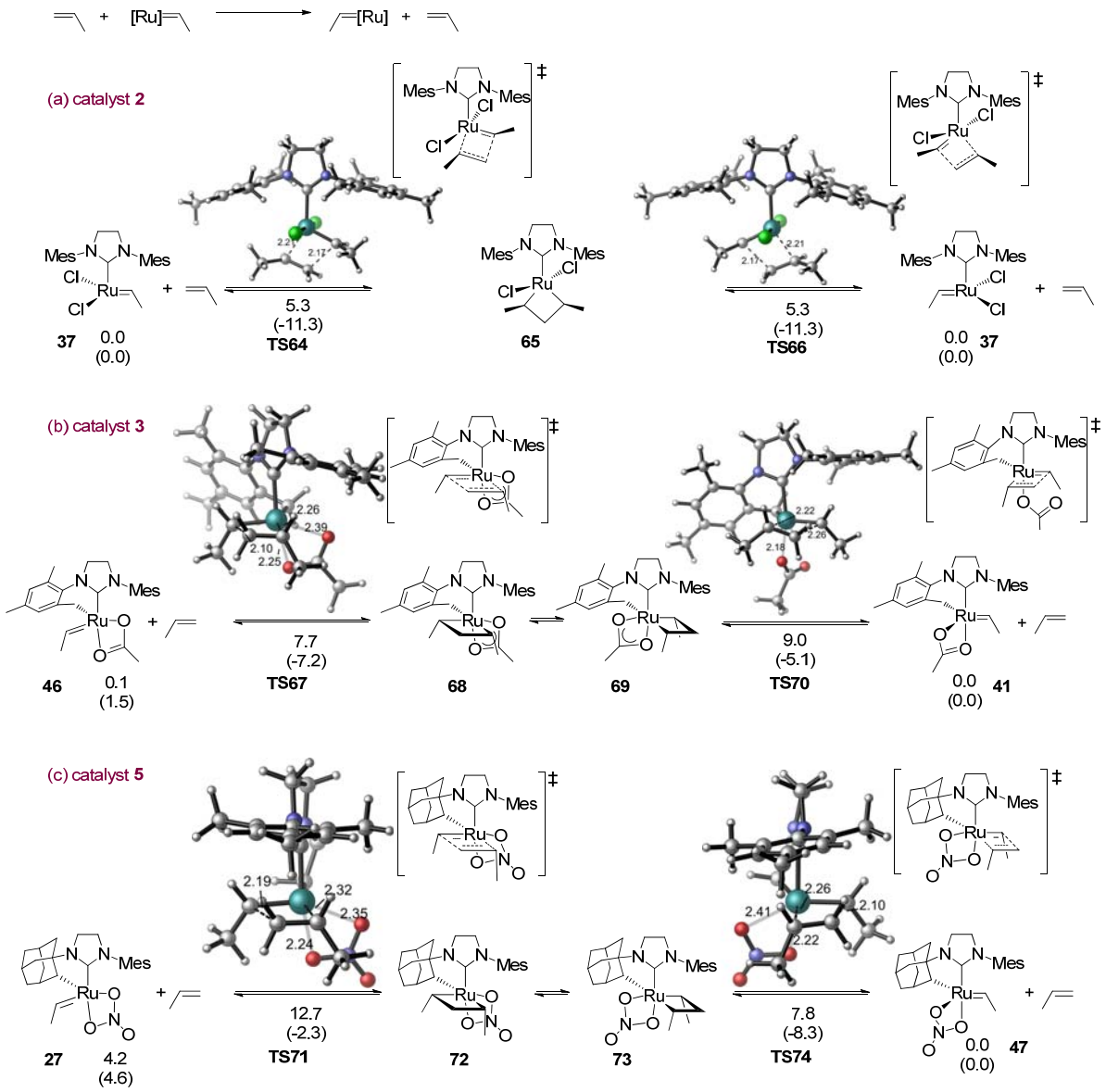
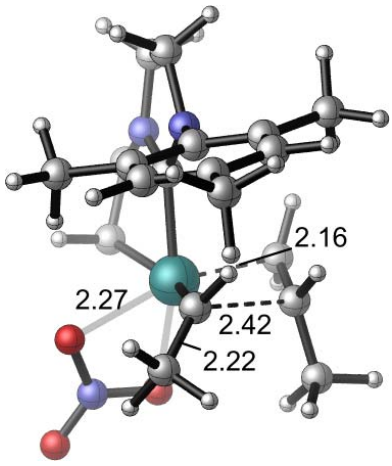


Figure S2. Free energies and enthalpies (in parenthesis) of the transition states and ruthenacyclobutane intermediates in the non-productive metathesis pathways of the reaction of propene and ruthenium ethylidene complexes from (a) catalyst **2**; (b) catalyst **3**; and (c) catalyst **5**. All energies are with respect to the most stable isomer of ruthenium alkylidene complexes (**37**, **41**, and **47**, respectively) and are given in kcal/mol. For clarity, the chelating adamantyl group is not shown in the 3D structures of **TS71** and **TS74**.

Direct productive cleavage of ruthenacyclobutane 23

In the ethenolysis of *Z*-2-butene with catalyst **5** (Figure 2 in the manuscript), the first metathesis transition state **TS22** leads to a ruthenacyclobutane intermediate **23**, in which the nitrate is syn to the α-H atom on the chelating adamantyl group. Direct productive cleavage of 23 via metathesis transition state **TS25'** would lead to a propene-ruthenium ethylidene complex, an isomer of **26**. This direct cleavage pathway is highly unfavorable due to the high activation energy of **TS25'** ($\Delta G^{\ddagger}$ = 20.9 kcal/mol). Thus, **23** undergoes isomerization (see next page for more details) to form another ruthenacyclobutane intermediate **24**, in which the nitrate is anti to the α-H atom on the adamantyl. Subsequent productive cleavage of **24** (via **TS23**, $\Delta G^{\ddagger}$ = 8.6 kcal/mol) is much more favorable than the direct cleavage of **23** via **TS25'**. The 3D structure of **TS25'** is shown below. In **TS25'**, the forming alkylidene is trans to the chelating adamantyl group. Both alkylidene and adamantyl are strongly electron-donating ligands and thus prefer to not be *trans* to each other due to trans influences.

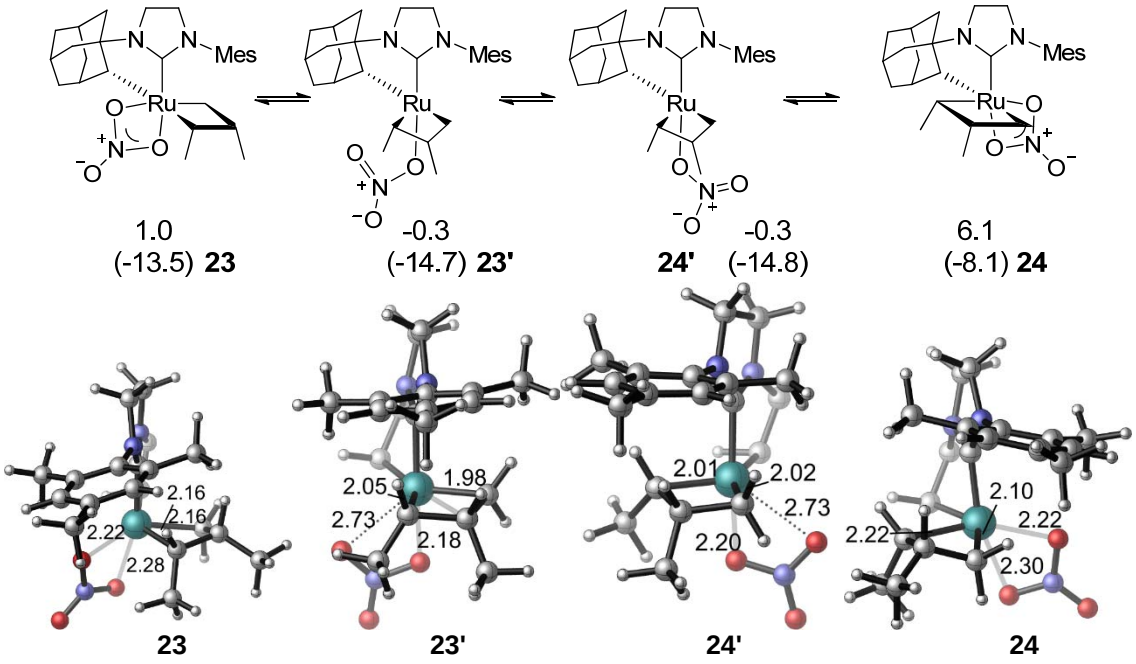


TS25'

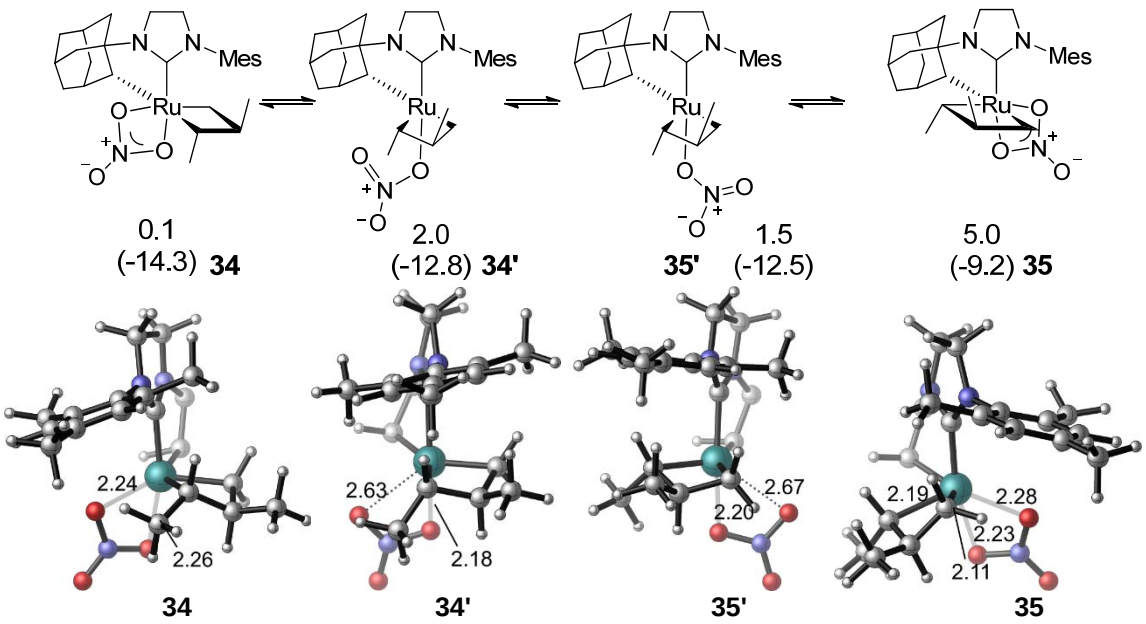
$\Delta G^{\ddagger}$ = 20.9 kcal/mol

Interconversion of Ruthenacyclopropane Intermediates 23 and 24

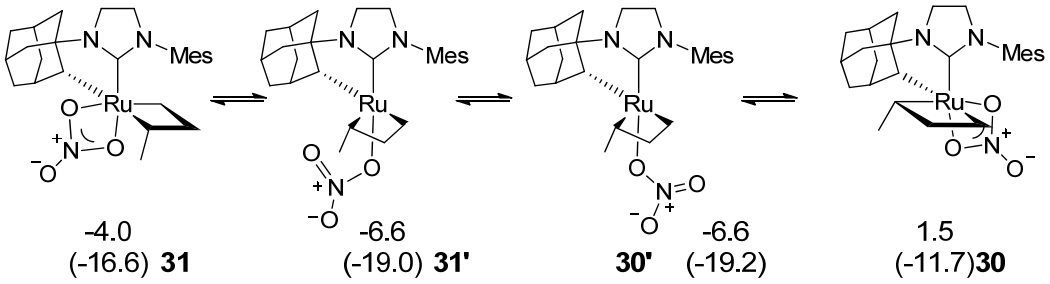
The interconversion of the ruthenacyclopropane intermediates **23** and **24** occurs via monodentate nitrato complexes **23'** and **24'**, which are five-coordinated trigonal bipyramidal geometry. Both **23'** and **24'** are lower in energy than corresponding bidentate nitrato complexes. The interconversion between **23'** and **24'** involves rotation of the Ru–O dative single bond. This rotation step is expected to have low barrier. Thus, the interconversion between **23** and **24** should be facile.



The interconversion between the metallacycle intermediates **34** and **35** from the ethenolysis of *E*-2-butene proceeds via a similar mechanism involving mono-dentate nitrato complexes **34'** and **35'**.

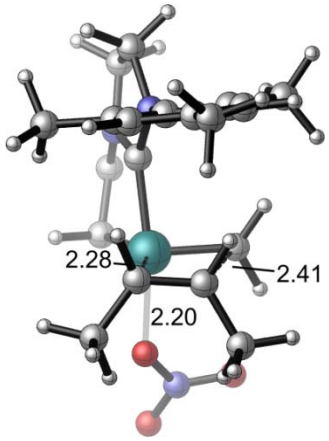


Similarly, the interconversion between the mono-substituted ruthenacyclopentane intermediates **31** and **30** also readily occurs via stable monodentate intermediates **31'** and **30'**.

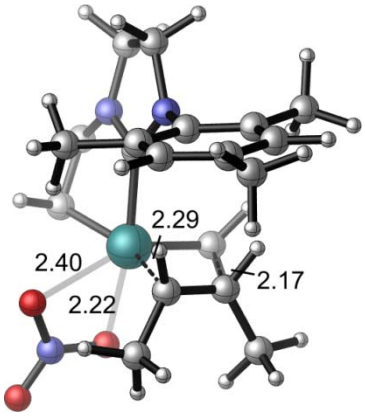


Monodentate Transition State Structures

In the ethenolysis reaction of *Z*-2-butene with catalyst **5**, the nitrate binds to the ruthenium in a bidentate fashion in all four metathesis transition states in the catalytic cycle (Figure 2 in the manuscript). The monodentate TS structures are 1~4 kcal/mol less stable than corresponding bidentate TSs. The 3D structures of the rate-determining transition state **TS22** and the monodentate nitrato isomer (**TS22-mono**) are shown below. The chelating adamantyl groups are not shown for clarity.



TS22-mono
$\Delta G^{\ddagger}$ = 9.4 kcal/mol
$\Delta H^{\ddagger}$ = -2.9 kcal/mol



TS22
$\Delta G^{\ddagger}$ = 8.8 kcal/mol
$\Delta H^{\ddagger}$ = -5.8 kcal/mol

The Cartesian coordinates (Å), SCF energies, enthalpies at 298K, and Gibbs free energies at 298K for the optimized structures.

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B3LYP SCF energy: -1378.80943708 a.u.
B3LYP enthalpy: -1378.265763 a.u.
B3LYP free energy: -1378.354118 a.u.
M06 SCF energy in solution: -1379.29385334 a.u.
M06 enthalpy in solution: -1378.750179 a.u.
M06 free energy in solution: -1378.838534 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.221418	1.045699	0.243937
O	1.352359	2.324036	-0.558184
O	-0.297726	3.317514	0.459632
N	-0.964268	-1.605015	-0.626983
N	1.209359	-1.639479	-0.285630
C	0.103342	-0.857736	-0.238986
C	-0.628955	-3.025515	-0.772929
H	-1.081353	-3.459521	-1.669284
H	-0.973574	-3.598781	0.098740
C	0.908273	-2.973131	-0.848922
H	1.395351	-3.763558	-0.271661
H	1.271207	-3.032358	-1.883623
C	-2.299978	-1.060345	-0.353653
C	-2.811052	-1.536223	1.029452
H	-2.059455	-1.296431	1.788749
H	-2.942951	-2.627595	1.021662
C	-4.146559	-0.845916	1.366419
H	-4.495606	-1.195140	2.347247
C	-5.188073	-1.202974	0.287028
H	-5.364972	-2.287919	0.275121
H	-6.150209	-0.725176	0.516083
C	-4.681976	-0.727697	-1.090604
H	-5.420086	-0.980600	-1.862935
C	-3.346595	-1.439324	-1.425774
H	-2.984694	-1.135476	-2.417004
H	-3.505234	-2.527734	-1.454619
C	-4.481277	0.803561	-1.046853
H	-4.159731	1.175224	-2.029193
H	-5.437886	1.293826	-0.817999
C	-3.422948	1.164754	0.030301
H	-3.272824	2.251021	0.048468
C	-2.112089	0.471115	-0.364329
H	-1.882899	0.761426	-1.416989
C	-3.922354	0.679703	1.405035
H	-3.190265	0.933413	2.181311
H	-4.859681	1.191777	1.662043
C	2.569791	-1.196367	-0.148358
C	3.264708	-1.513879	1.034303
C	4.600969	-1.121890	1.146629
H	5.142644	-1.361405	2.059284
C	5.256611	-0.430354	0.122587
C	4.541980	-0.145244	-1.043254
H	5.036735	0.384207	-1.854850
C	3.202172	-0.514957	-1.204319
C	2.593690	-2.249893	2.170345
H	3.295208	-2.406695	2.995123
H	2.218278	-3.234268	1.864158
H	1.737099	-1.688086	2.558674
C	6.691343	0.016130	0.281250
H	6.742784	1.044401	0.662781
H	7.225092	-0.001118	-0.675145
H	7.235187	-0.621390	0.986354
C	2.478040	-0.150627	-2.479327
H	1.726716	-0.893901	-2.763664
H	3.186240	-0.051666	-3.308237
H	1.965875	0.811699	-2.363930
C	-0.261883	0.694957	2.031838
H	0.029991	-0.230924	2.539756
O	1.325983	4.517681	-0.402945
N	0.806457	3.449497	-0.168269
H	-0.533445	1.524256	2.701229

23

B3LYP SCF energy: -1536.03762970 a.u.
B3LYP enthalpy: -1535.374117 a.u.
B3LYP free energy: -1535.472050 a.u.
M06 SCF energy in solution: -1536.45146189 a.u.
M06 enthalpy in solution: -1535.787949 a.u.
M06 free energy in solution: -1535.885882 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.278681	0.951366	-0.094649
O	1.099384	1.939049	-1.528488
O	-0.556305	3.113991	-0.747766
N	-0.989926	-1.842127	-0.218439
N	1.193625	-1.803733	0.010867
C	0.079712	-1.012280	-0.051054
C	-0.656005	-3.262560	-0.111839
H	-1.127747	-3.852557	-0.904004
H	-0.980858	-3.668723	0.855868
C	0.874947	-3.227319	-0.232585
H	1.374886	-3.871021	0.496349
H	1.217531	-3.518747	-1.234312
C	-2.342501	-1.297370	-0.224589
C	-3.128535	-1.694188	1.051329
H	-2.554749	-1.422300	1.942791
H	-3.254641	-2.785933	1.072526
C	-4.513810	-1.014027	1.054664
H	-5.051187	-1.299792	1.968226
C	-5.309046	-1.477064	-0.182354
H	-5.461386	-2.565136	-0.152180
H	-6.305176	-1.015011	-0.184896
C	-4.539826	-1.082115	-1.459105
H	-5.100318	-1.407243	-2.345203
C	-3.159862	-1.780901	-1.456679
H	-2.603129	-1.551377	-2.374326
H	-3.296402	-2.871489	-1.421153
C	-4.363481	0.452100	-1.494333
H	-3.856170	0.758905	-2.418593
H	-5.347342	0.941010	-1.493855
C	-3.546643	0.917671	-0.253111
H	-3.410668	2.004240	-0.291311
C	-2.182372	0.224514	-0.357769
H	-1.801206	0.432766	-1.404672
C	-4.337852	0.517299	1.011262
H	-3.837781	0.874935	1.915494
H	-5.323662	1.001766	0.985035
C	2.563261	-1.396707	-0.151354
C	3.441334	-1.530015	0.943834
C	4.784201	-1.188079	0.769064
H	5.462567	-1.280026	1.614835
C	5.277265	-0.732600	-0.458773
C	4.390076	-0.649843	-1.533422
H	4.758500	-0.322232	-2.503373
C	3.034996	-0.981990	-1.410992

C	2.961613	-2.039262	2.283262
H	3.725597	-1.883740	3.050914
H	2.743667	-3.115523	2.255546
H	2.046172	-1.534183	2.604226
C	6.725921	-0.331403	-0.612090
H	6.871870	0.725394	-0.352076
H	7.071346	-0.462460	-1.642982
H	7.377546	-0.919874	0.043023
C	2.141935	-0.887458	-2.626661
H	1.318521	-1.607384	-2.597426
H	2.720699	-1.072629	-3.537722
H	1.703490	0.112780	-2.707152
C	-1.089136	1.108761	1.896867
C	1.137457	1.366942	1.476790
C	0.233377	0.945504	2.627711
H	-1.463244	2.140962	1.909947
H	-1.874242	0.437962	2.236703
H	0.383143	-0.127165	2.812293
H	1.985989	0.702530	1.299904
C	1.597186	2.818366	1.466081
H	2.250672	3.008125	2.332144
H	2.181783	3.042355	0.568995
H	0.766971	3.530150	1.519260
C	0.354969	1.676760	3.974012
H	-0.391355	1.297256	4.683586
H	1.346432	1.532298	4.423041
H	0.189754	2.754294	3.864711
N	0.450288	3.068326	-1.535900
O	0.788558	3.994837	-2.242538

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B3LYP SCF energy: -1536.03033809 a.u.
B3LYP enthalpy: -1535.366408 a.u.
B3LYP free energy: -1535.464862 a.u.
M06 SCF energy in solution: -1536.44322417 a.u.
M06 enthalpy in solution: -1535.779294 a.u.
M06 free energy in solution: -1535.877748 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.412524	0.823417	0.007527
O	0.065171	1.658132	-2.020255
O	1.259606	2.860394	-0.656685
N	0.771300	-1.962358	0.102984
N	-1.399606	-1.745059	-0.164076
C	-0.244230	-1.052741	0.022711
C	0.359108	-3.301202	-0.327614
H	0.793524	-4.081761	0.302843
H	0.658552	-3.491327	-1.368713
C	-1.169529	-3.205923	-0.181571
H	-1.711907	-3.668094	-1.011191
H	-1.516864	-3.661038	0.754027
C	2.139210	-1.426428	0.019764
C	2.554471	-1.149450	-1.452823
H	1.820161	-0.491666	-1.939740
H	2.556813	-2.092703	-2.018004
C	3.952449	-0.499083	-1.495829
H	4.230741	-0.315074	-2.541447
C	4.977182	-1.448492	-0.843151
H	5.030439	-2.394564	-1.400292
H	5.979094	-1.000171	-0.877899
C	4.570860	-1.714009	0.621144
H	5.297528	-2.390034	1.090492
C	3.177213	-2.383007	0.649363
H	2.878984	-2.619238	1.679021
H	3.213076	-3.330546	0.090583
C	4.535866	-0.375032	1.390262
H	4.284233	-0.548058	2.445285
H	5.531763	0.089227	1.369206
C	3.494052	0.577422	0.740312
H	3.478542	1.528045	1.284479
C	2.123244	-0.114475	0.859341
H	1.976979	-0.416216	1.897482
C	3.910299	0.833186	-0.723026
H	3.216929	1.535867	-1.194943
H	4.901458	1.306644	-0.743472
C	-2.728199	-1.218261	-0.285661
C	-3.152422	-0.694363	-1.524176
C	-4.461804	-0.213708	-1.625452
H	-4.794233	0.193498	-2.578125
C	-5.354897	-0.252249	-0.549807
C	-4.914214	-0.813369	0.651333
H	-5.598515	-0.869940	1.495550
C	-3.614403	-1.307675	0.805643
C	-2.243908	-0.653133	-2.730244
H	-2.834650	-0.575853	-3.648474
H	-1.622641	-1.552485	-2.801084
H	-1.565605	0.206169	-2.697768
C	-6.752394	0.306433	-0.683845
H	-6.757951	1.395107	-0.541105
H	-7.430376	-0.124566	0.060093
H	-7.168608	0.109564	-1.677989
C	-3.213332	-1.943010	2.118640
H	-3.403979	-3.025068	2.112417
H	-3.793856	-1.521360	2.945147
H	-2.152702	-1.796567	2.341670
C	-1.231525	1.946327	0.676008
C	0.069960	0.953594	2.200299
H	0.182321	-0.021498	2.686922
C	-1.398013	1.385143	2.059662
H	-2.015964	0.485507	1.999248
H	-2.001829	1.735277	-0.074052
C	-2.004928	2.313678	3.122046
H	-3.048921	2.543076	2.874276
H	-1.992219	1.846111	4.115164
H	-1.464456	3.264140	3.190682
C	0.980338	1.987558	2.850147
H	0.654001	2.199602	3.879807
H	2.016096	1.642245	2.912672
H	0.982973	2.939865	2.306607
H	-0.915999	2.994266	0.646801
N	0.723268	2.764977	-1.812824
O	0.816296	3.620721	-2.668163

26

B3LYP SCF energy: -1536.02641534 a.u.
B3LYP enthalpy: -1535.364599 a.u.
B3LYP free energy: -1535.470096 a.u.
M06 SCF energy in solution: -1536.43822690 a.u.
M06 enthalpy in solution: -1535.776411 a.u.
M06 free energy in solution: -1535.881908 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.296125	0.866820	0.281549
O	1.071631	1.704964	-1.771191
O	1.194432	2.911060	0.033813
N	0.764258	-1.984588	0.226704
N	-1.412955	-1.792024	0.091567
C	-0.249087	-1.080477	0.177775
C	0.333194	-3.358999	-0.041014
H	0.797609	-4.067077	0.650753
H	0.594290	-3.660358	-1.065232
C	-1.185984	-3.250626	0.157079
H	-1.760343	-3.766766	-0.617806
H	-1.502801	-3.640761	1.133456
C	2.145258	-1.506249	0.080735
C	2.550286	-1.469847	-1.416003
H	1.836083	-0.850045	-1.970287
H	2.510678	-2.484617	-1.838907
C	3.972792	-0.895117	-1.565889
H	4.248522	-0.890333	-2.628671

C	4.968837	-1.764278	-0.774147
H	4.982441	-2.790579	-1.169329
H	5.986396	-1.365813	-0.885603
C	4.564994	-1.772972	0.714307
H	5.275767	-2.383292	1.287567
C	3.153770	-2.392819	0.846897
H	2.855234	-2.458148	1.901916
H	3.168457	-3.417665	0.445624
C	4.574511	-0.323092	1.251655
H	4.332204	-0.314668	2.323282
H	5.584891	0.098211	1.149620
C	3.550878	0.541315	0.463265
H	3.560532	1.565482	0.854306
C	2.162520	-0.093228	0.705260
H	2.092913	-0.246609	1.787816
C	3.982900	0.545769	-1.019607
H	3.323033	1.168933	-1.625518
H	4.994224	0.968256	-1.101753
C	-2.745061	-1.303838	-0.096965
C	-3.190766	-1.052820	-1.413022
C	-4.509903	-0.636377	-1.603498
H	-4.854557	-0.432592	-2.615193
C	-5.399099	-0.479400	-0.532657
C	-4.939387	-0.772352	0.752461
H	-5.620955	-0.677494	1.595700
C	-3.625202	-1.196431	0.994129
C	-2.272238	-1.247250	-2.598407
H	-2.774838	-0.961311	-3.527093
H	-1.962741	-2.295504	-2.698713
H	-1.355995	-0.653423	-2.510829
C	-6.810903	0.005518	-0.766406
H	-6.838809	1.096009	-0.891479
H	-7.465720	-0.245059	0.074379
H	-7.240238	-0.433419	-1.673961
C	-3.212595	-1.570110	2.399582
H	-2.131263	-1.508231	2.540765
H	-3.518463	-2.598266	2.636739
H	-3.692836	-0.917524	3.136477
C	-1.740369	2.115360	-0.911239
H	-2.067238	1.231601	-1.441388
C	-0.219031	0.969259	2.061333
H	-1.040248	0.388313	2.509993
C	-2.168448	2.381188	0.342340
H	-2.805167	1.651592	0.840063
C	-1.962271	3.694382	1.045050
H	-2.884856	4.289736	0.988961
H	-1.735587	3.561616	2.107886
H	-1.151160	4.267589	0.587943
H	-1.187608	2.853331	-1.483167
C	0.439803	1.876479	3.057687
H	-0.292604	2.419694	3.673567
H	1.019500	1.247608	3.756377
H	1.128404	2.590669	2.597644
O	1.984760	3.699584	-1.854870
N	1.440180	2.807761	-1.225456

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B3LYP SCF energy: -1418.12464492 a.u.
B3LYP enthalpy: -1417.550645 a.u.
B3LYP free energy: -1417.643262 a.u.
M06 SCF energy in solution: -1418.58692432 a.u.
M06 enthalpy in solution: -1418.012924 a.u.
M06 free energy in solution: -1418.105541 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.309338	0.900446	-0.522082
O	0.487957	2.429573	0.835372
O	-0.897750	3.130949	-0.687820
N	-0.784329	-1.741242	0.440211
N	1.396130	-1.486276	0.524969
C	0.235095	-0.888600	0.154146
C	-0.360481	-2.859461	1.285423
H	-0.823146	-3.800725	0.975854
H	-0.618155	-2.679042	2.339351
C	1.164874	-2.845468	1.059721
H	1.737358	-2.999635	1.978760
H	1.474503	-3.603926	0.329794
C	-2.145785	-1.211769	0.276675
C	-2.595958	-0.420799	1.533613
H	-1.845587	0.346550	1.778500
H	-2.653051	-1.093356	2.401866
C	-3.964845	0.240755	1.277177
H	-4.274893	0.791076	2.175025
C	-5.001608	-0.855573	0.954539
H	-5.112114	-1.537034	1.810039
H	-5.985901	-0.400969	0.779458
C	-4.553094	-1.637411	-0.297389
H	-5.291036	-2.416588	-0.529218
C	-3.186796	-2.310329	-0.018493
H	-2.862574	-2.899490	-0.886493
H	-3.284108	-3.002347	0.831963
C	-4.438527	-0.659303	-1.488801
H	-4.151355	-1.202984	-2.399074
H	-5.419293	-0.202742	-1.684205
C	-3.387739	0.436620	-1.170824
H	-3.308783	1.126892	-2.019871
C	-2.036361	-0.264432	-0.947590
H	-1.831778	-0.897963	-1.816691
C	-3.840194	1.211293	0.084361
H	-3.124752	2.011922	0.310616
H	-4.807985	1.696290	-0.103590
C	2.722844	-0.991486	0.292092
C	3.304048	-0.110938	1.224032
C	4.607184	0.339364	0.985540
H	5.060754	1.022505	1.700561
C	5.339204	-0.061003	-0.135469
C	4.741453	-0.956291	-1.027755
H	5.299005	-1.291692	-1.900218
C	3.443100	-1.437069	-0.834021
C	2.561629	0.358025	2.452812
H	3.266332	0.694956	3.219773
H	1.941843	-0.435261	2.883804
H	1.899569	1.197944	2.215203
C	6.730435	0.472382	-0.387360
H	6.699322	1.379472	-1.005492
H	7.351993	-0.259060	-0.915153
H	7.234620	0.735135	0.548591
C	2.863406	-2.431849	-1.815122
H	3.026728	-3.466015	-1.481812
H	3.342560	-2.333369	-2.794255
H	1.785691	-2.300509	-1.950344
C	0.502647	0.715441	-2.148157
H	1.185949	-0.114118	-2.369857
O	-0.032898	4.563348	0.733592
N	-0.151011	3.437116	0.301248
C	0.360019	1.702140	-3.271811
H	1.344308	2.100371	-3.562942
H	-0.045254	1.190314	-4.159748
H	-0.293869	2.541897	-3.022839

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B3LYP SCF energy: -1496.70937437 a.u.
B3LYP enthalpy: -1496.077119 a.u.
B3LYP free energy: -1496.177201 a.u.
M06 SCF energy in solution: -1497.14232971 a.u.
M06 enthalpy in solution: -1496.510074 a.u.
M06 free energy in solution: -1496.610156 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.269356	0.967328	0.331471

O	1.211557	1.863815	-1.638205
O	1.268850	2.971326	0.231838
N	0.612882	-1.900801	0.135854
N	-1.552820	-1.602800	0.015801
C	-0.356078	-0.948303	0.134593
C	0.119115	-3.239650	-0.196314
H	0.549461	-4.000382	0.460736
H	0.369094	-3.503202	-1.233442
C	-1.393203	-3.071668	0.005377
H	-1.987927	-3.520871	-0.795481
H	-1.733266	-3.496324	0.959583
C	2.018613	-1.490648	0.021373
C	2.447379	-1.427207	-1.467397
H	1.776940	-0.749371	-2.008258
H	2.358330	-2.422955	-1.926599
C	3.902604	-0.928870	-1.577378
H	4.195011	-0.906047	-2.635552
C	4.836373	-1.877637	-0.801048
H	4.798356	-2.890492	-1.228261
H	5.876160	-1.533979	-0.886694
C	4.409727	-1.909528	0.680720
H	5.077212	-2.575389	1.244248
C	2.965626	-2.456419	0.771183
H	2.645986	-2.540403	1.818728
H	2.933315	-3.466970	0.335916
C	4.488802	-0.480039	1.265026
H	4.229462	-0.493127	2.332707
H	5.522521	-0.112586	1.192298
C	3.526799	0.463762	0.490451
H	3.586576	1.472827	0.915562
C	2.101111	-0.102181	0.689613
H	2.009407	-0.287167	1.766465
C	3.986461	0.490520	-0.984298
H	3.376736	1.172249	-1.578936
H	5.023021	0.852823	-1.034407
C	-2.868850	-1.054353	-0.115176
C	-3.349642	-0.763666	-1.411941
C	-4.652475	-0.282712	-1.550400
H	-5.022323	-0.048445	-2.546506
C	-5.495976	-0.099636	-0.446089
C	-5.007153	-0.436000	0.816359
H	-5.655088	-0.325692	1.684066
C	-3.706403	-0.925677	1.006130
C	-2.483944	-0.983811	-2.632091
H	-2.999139	-0.647680	-3.536775
H	-2.241278	-2.045778	-2.766163
H	-1.531160	-0.448079	-2.563694
C	-6.890545	0.453800	-0.624328
H	-6.868827	1.542678	-0.763255
H	-7.519060	0.246316	0.247581
H	-7.381113	0.026756	-1.506245
C	-3.272250	-1.336640	2.395199
H	-2.206072	-1.565639	2.441865
H	-3.822677	-2.227447	2.724849
H	-3.481892	-0.546357	3.125336
C	-1.591706	2.185331	-0.780161
H	-2.119695	1.432914	-1.349563
C	-0.290853	1.020341	2.111376
H	-1.051832	0.361131	2.553546
C	-1.881999	2.396858	0.533377
H	-2.635903	1.805351	1.042521
O	2.245823	3.797399	-1.551028
N	1.601883	2.913471	-1.011128
H	-0.993147	2.891625	-1.341945
C	0.257220	1.992757	3.113823
H	0.837864	1.420083	3.857046
H	0.917308	2.742730	2.670018
H	-0.544129	2.495747	3.676457
H	-1.495837	3.266955	1.055106

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B3LYP SCF energy: -1496.71777081 a.u.
B3LYP enthalpy: -1496.083214 a.u.
B3LYP free energy: -1496.178109 a.u.
M06 SCF energy in solution: -1497.15197226 a.u.
M06 enthalpy in solution: -1496.517415 a.u.
M06 free energy in solution: -1496.612310 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.351748	0.906896	0.224345
O	-0.722724	2.104326	-1.391838
O	1.008873	2.951152	-0.389685
N	0.724081	-1.995267	0.297015
N	-1.444760	-1.682551	0.174337
C	-0.246879	-1.035116	0.273303
C	0.221854	-3.326549	-0.050126
H	0.668440	-4.101597	0.578851
H	0.437826	-3.568942	-1.100603
C	-1.282199	-3.153348	0.197751
H	-1.905872	-3.617220	-0.571139
H	-1.581199	-3.554504	1.173786
C	2.065186	-1.510433	-0.032260
C	2.215955	-1.350249	-1.570524
H	1.391412	-0.732979	-1.954802
H	2.137015	-2.331804	-2.059245
C	3.566303	-0.697856	-1.909732
H	3.660939	-0.597839	-2.998942
C	4.705826	-1.584563	-1.367310
H	4.682816	-2.569502	-1.855010
H	5.679475	-1.134541	-1.603712
C	4.555961	-1.740166	0.160493
H	5.368693	-2.367664	0.549021
C	3.201237	-2.419459	0.480476
H	3.090353	-2.573754	1.561651
H	3.163283	-3.409335	0.001027
C	4.625080	-0.340011	0.810169
H	4.567750	-0.422186	1.903803
H	5.591774	0.126971	0.573444
C	3.463506	0.546729	0.282455
H	3.525926	1.537688	0.738126
C	2.148929	-0.153928	0.696056
H	2.202665	-0.380187	1.764318
C	3.611308	0.691179	-1.247298
H	2.817930	1.334365	-1.649715
H	4.562593	1.190262	-1.477471
C	-2.754577	-1.138913	-0.049349
C	-3.092953	-0.659538	-1.330858
C	-4.389614	-0.177089	-1.536610
H	-4.653698	0.199794	-2.522436
C	-5.353548	-0.176213	-0.524393
C	-4.998588	-0.701693	0.720968
H	-5.738857	-0.729106	1.518143
C	-3.715541	-1.193648	0.979003
C	-2.113538	-0.674627	-2.480759
H	-2.648008	-0.622428	-3.434494
H	-1.502891	-1.584258	-2.484384
H	-1.433538	0.182467	-2.436969
C	-6.734469	0.386080	-0.768582
H	-6.752660	1.471908	-0.606315
H	-7.474058	-0.057341	-0.093581
H	-7.063499	0.208009	-1.798181
C	-3.404843	-1.778219	2.338631
H	-3.584658	-2.861869	2.359267
H	-4.045030	-1.332973	3.106643
H	-2.362709	-1.615165	2.629293
C	-1.361071	1.282435	1.403701
C	0.695076	1.429364	2.328036
C	-0.633384	2.165571	2.385642
H	-1.780611	0.398463	1.876009
H	-1.078827	2.222883	3.395127
H	0.648653	0.503532	2.910414
C	1.913224	2.258233	2.691535
H	2.832336	1.669577	2.761396

H	2.072815	3.077914	1.982047
H	1.747878	2.713188	3.681732
H	-2.071738	1.738172	0.709326
N	0.110024	3.088769	-1.304308
O	0.051450	4.061093	-2.025826
H	-0.525262	3.189506	2.009364

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B3LYP SCF energy: -1496.72453047 a.u.
B3LYP enthalpy: -1496.090787 a.u.
B3LYP free energy: -1496.186569 a.u.
M06 SCF energy in solution: -1497.15895055 a.u.
M06 enthalpy in solution: -1496.525207 a.u.
M06 free energy in solution: -1496.620989 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.275328	0.985587	0.128628
O	1.037735	2.152996	-1.242456
O	-0.451372	3.235119	-0.083003
N	-1.023961	-1.757051	-0.426659
N	1.154841	-1.769600	-0.175745
C	0.049081	-0.968589	-0.134332
C	-0.699139	-3.181817	-0.511408
H	-1.177665	-3.658314	-1.372647
H	-1.022386	-3.710618	0.395601
C	0.830653	-3.138256	-0.631204
H	1.329794	-3.886710	-0.010073
H	1.168370	-3.274940	-1.667160
C	-2.369340	-1.213547	-0.300335
C	-3.105573	-1.793900	0.935517
H	-2.501458	-1.632042	1.834598
H	-3.221167	-2.879712	0.811778
C	-4.490830	-1.136569	1.090033
H	-4.994534	-1.564751	1.966400
C	-5.333842	-1.397740	-0.173322
H	-5.490452	-2.476796	-0.312147
H	-6.326740	-0.941669	-0.063556
C	-4.609787	-0.803057	-1.397879
H	-5.205043	-0.979717	-2.303088
C	-3.237969	-1.497658	-1.558323
H	-2.714785	-1.130862	-2.450581
H	-3.383608	-2.580277	-1.686621
C	-4.422731	0.717152	-1.192447
H	-3.949647	1.167703	-2.074883
H	-5.402330	1.200071	-1.073964
C	-3.554310	0.975514	0.073988
H	-3.412389	2.054544	0.205757
C	-2.199353	0.308540	-0.195273
H	-1.851643	0.685191	-1.204323
C	-4.303825	0.378967	1.287039
H	-3.765243	0.571168	2.218765
H	-5.283218	0.868239	1.378557
C	2.531615	-1.361495	-0.203312
C	3.350408	-1.674892	0.900847
C	4.699120	-1.314124	0.854703
H	5.332196	-1.541887	1.709894
C	5.255209	-0.672252	-0.257338
C	4.427441	-0.419908	-1.353374
H	4.847284	0.051278	-2.239723
C	3.068882	-0.760214	-1.357081
C	2.810349	-2.408808	2.107258
H	3.495849	-2.315713	2.955030
H	2.690262	-3.482369	1.905548
H	1.831812	-2.028723	2.415499
C	6.707212	-0.254570	-0.265808
H	6.833723	0.738341	0.185736
H	7.103134	-0.200304	-1.285340
H	7.329994	-0.952108	0.304928
C	2.240233	-0.478722	-2.589311
H	1.429504	-1.201855	-2.721196
H	2.869947	-0.511236	-3.484579
H	1.787531	0.516520	-2.535987
C	-1.069631	0.944487	2.138797
C	1.168078	1.112895	1.719556
C	0.161107	1.606259	2.736417
H	1.482308	0.094409	1.951529
H	0.376827	1.334741	3.784991
H	-1.241984	-0.061191	2.528332
H	-1.981869	1.538880	2.201318
C	2.370025	1.999719	1.438563
H	2.075586	3.033933	1.229391
H	3.007679	2.024672	2.338267
H	2.983944	1.639484	0.609303
N	0.472012	3.291574	-0.969884
O	0.805242	4.320610	-1.519245
H	0.073252	2.698041	2.686812

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B3LYP SCF energy: -1536.04068799 a.u.
B3LYP enthalpy: -1535.377028 a.u.
B3LYP free energy: -1535.474688 a.u.
M06 SCF energy in solution: -1536.45461758 a.u.
M06 enthalpy in solution: -1535.790958 a.u.
M06 free energy in solution: -1535.888618 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.290743	0.952299	-0.101232
O	0.984821	1.971680	-1.629344
O	-0.487492	3.160801	-0.556390
N	-1.041191	-1.832796	-0.360926
N	1.139806	-1.819906	-0.130569
C	0.034192	-1.018852	-0.159322
C	-0.715955	-3.259257	-0.311622
H	-1.195985	-3.814290	-1.123665
H	-1.037505	-3.701396	0.641175
C	0.814059	-3.228433	-0.438265
H	1.314353	-3.907648	0.257427
H	1.150319	-3.474235	-1.454324
C	-2.385953	-1.280600	-0.264555
C	-3.094481	-1.734794	1.038265
H	-2.470573	-1.483504	1.902704
H	-3.209678	-2.827600	1.026669
C	-4.478381	-1.066579	1.154584
H	-4.963456	-1.404628	2.079458
C	-5.344313	-1.456288	-0.059589
H	-5.498653	-2.544252	-0.085050
H	-6.337174	-0.994502	0.023193
C	-4.647787	-0.987588	-1.352995
H	-5.260987	-1.256439	-2.222888
C	-3.276472	-1.691560	-1.470688
H	-2.771767	-1.413686	-2.404843
H	-3.419296	-2.781848	-1.487464
C	-4.461490	0.545558	-1.307533
H	-4.005406	0.903295	-2.240076
H	-5.439792	1.037994	-1.221659
C	-3.570528	0.932887	-0.090639
H	-3.430740	2.020017	-0.071731
C	-2.218579	0.244569	-0.317095
H	-1.892743	0.516889	-1.365901
C	-4.293559	0.461429	1.191986
H	-3.737645	0.750551	2.088020
H	-5.272857	0.955775	1.252312
C	2.518195	-1.421718	-0.194269
C	3.330427	-1.621358	0.940434
C	4.682329	-1.277445	0.862579
H	5.309881	-1.416772	1.740562
C	5.248463	-0.764647	-0.309250
C	4.426078	-0.622101	-1.429297
H	4.852825	-0.250827	-2.358843
C	3.064636	-0.948746	-1.402620

C	2.781920	-2.219373	2.215964
H	3.417913	-1.962766	3.068696
H	2.744953	-3.316488	2.160716
H	1.766969	-1.871905	2.428085
C	6.704785	-0.364758	-0.357623
H	6.835150	0.685146	-0.063477
H	7.116776	-0.471988	-1.366654
H	7.311028	-0.970917	0.324196
C	2.243997	-0.790378	-2.661889
H	1.411264	-1.498578	-2.709354
H	2.871941	-0.947981	-3.545190
H	1.821469	0.217318	-2.728983
C	-1.048780	1.133623	1.910264
C	1.173649	1.250124	1.442319
C	0.191992	1.841466	2.436599
H	1.504918	0.264927	1.777391
H	-1.226011	0.176236	2.407884
H	-1.956082	1.739762	1.918061
C	2.360741	2.104601	1.025763
H	2.052770	3.109516	0.716508
H	3.035189	2.226093	1.889647
H	2.941480	1.656176	0.215830
N	0.413403	3.127334	-1.468172
O	0.720053	4.093582	-2.134860
H	0.096299	2.917960	2.240306
C	0.507165	1.634535	3.925384
H	1.442985	2.132747	4.209400
H	-0.292397	2.037638	4.560154
H	0.611635	0.566189	4.156974

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B3LYP SCF energy: -1536.03280947 a.u.
B3LYP enthalpy: -1535.368807 a.u.
B3LYP free energy: -1535.465833 a.u.
M06 SCF energy in solution: -1536.45265636 a.u.
M06 enthalpy in solution: -1535.788654 a.u.
M06 free energy in solution: -1535.885680 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.495200	0.846753	0.283596
O	-1.426959	2.481998	-1.551765
O	-1.580199	2.710965	0.612706
N	-0.655476	-2.002349	-0.187672
N	1.496181	-1.695198	0.032225
C	0.288377	-1.043509	-0.007164
C	-0.154824	-3.369193	-0.049122
H	-0.579588	-4.035692	-0.804579
H	-0.397795	-3.774483	0.943458
C	1.348321	-3.148083	-0.227588
H	1.957087	-3.732289	0.466963
H	1.680833	-3.376382	-1.249132
C	-2.063670	-1.618345	-0.128200
C	-2.612979	-1.707113	1.320819
H	-1.971849	-1.119741	1.990003
H	-2.577834	-2.750565	1.666279
C	-4.060522	-1.180092	1.366406
H	-4.437243	-1.247745	2.395471
C	-4.941078	-2.036341	0.433358
H	-4.953661	-3.080963	0.776108
H	-5.978992	-1.678710	0.461061
C	-4.396327	-1.954385	-1.007736
H	-5.020420	-2.563812	-1.674561
C	-2.949764	-2.496841	-1.043270
H	-2.554221	-2.475667	-2.067462
H	-2.938700	-3.544032	-0.706246
C	-4.414151	-0.484579	-1.473851
H	-4.057804	-0.405747	-2.509449
H	-5.444297	-0.102030	-1.460012
C	-3.524155	0.381767	-0.540547
H	-3.559888	1.413818	-0.893070
C	-2.091408	-0.168437	-0.641671
H	-1.763912	-0.154098	-1.690110
C	-4.072462	0.289514	0.898451
H	-3.471586	0.914763	1.569700
H	-5.097202	0.683967	0.929254
C	2.811725	-1.164052	-0.184796
C	3.769665	-1.282908	0.838639
C	5.075295	-0.843163	0.586600
H	5.815772	-0.922556	1.379863
C	5.451838	-0.311347	-0.648505
C	4.483873	-0.239181	-1.657374
H	4.761932	0.152604	-2.633677
C	3.168297	-0.665001	-1.456530
C	3.428011	-1.889504	2.180408
H	4.128961	-1.551478	2.949826
H	3.487913	-2.986312	2.151169
H	2.414231	-1.629698	2.497413
C	6.858461	0.184391	-0.890108
H	6.915044	1.276740	-0.794661
H	7.204929	-0.068973	-1.898263
H	7.563909	-0.244106	-0.170946
C	2.164814	-0.576443	-2.583119
H	1.630402	-1.521723	-2.732807
H	2.663915	-0.321500	-3.522592
H	1.403645	0.186959	-2.385616
C	0.171759	0.918857	2.169811
C	1.263931	1.882272	0.000340
C	1.137120	2.016927	1.558170
H	0.709868	0.080407	2.619854
H	-0.544463	1.361451	2.869322
H	2.091068	1.229944	-0.271649
C	1.335965	3.188526	-0.762970
H	2.334934	3.632574	-0.623923
H	1.193865	3.032983	-1.836377
H	0.599994	3.921076	-0.423817
N	-1.841770	3.169281	-0.578136
O	-2.462296	4.216734	-0.706396
C	2.528479	1.944922	2.215635
H	3.017442	0.987856	2.017921
H	3.175504	2.741220	1.829106
H	2.438378	2.072448	3.300665
H	0.684147	2.990715	1.759477

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B3LYP SCF energy: -1536.03334049 a.u.
B3LYP enthalpy: -1535.369113 a.u.
B3LYP free energy: -1535.467126 a.u.
M06 SCF energy in solution: -1536.44702106 a.u.
M06 enthalpy in solution: -1535.782794 a.u.
M06 free energy in solution: -1535.880807 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.363797	0.858989	-0.058322
O	-0.723012	1.619373	-1.912742
O	0.951778	2.742980	-1.104987
N	0.810631	-1.942361	0.664726
N	-1.361173	-1.727873	0.424405
C	-0.182541	-1.040287	0.408907
C	0.350251	-3.331899	0.607397
H	0.791505	-3.934822	1.405913
H	0.610390	-3.794044	-0.355677
C	-1.165811	-3.155111	0.765565
H	-1.749568	-3.789864	0.093330
H	-1.494058	-3.348598	1.793975
C	2.145240	-1.503793	0.251286
C	2.318281	-1.686938	-1.282687
H	1.486392	-1.192605	-1.804147
H	2.270417	-2.754315	-1.541020
C	3.657754	-1.090449	-1.744845
H	3.767552	-1.232971	-2.827899

C	4.809112	-1.803035	-1.006326
H	4.817008	-2.872157	-1.262033
H	5.775369	-1.390551	-1.326343
C	4.637408	-1.618074	0.516131
H	5.458611	-2.120503	1.043804
C	3.294267	-2.245133	0.965352
H	3.169936	-2.157740	2.052526
H	3.286382	-3.317590	0.718559
C	4.660935	-0.107368	0.837719
H	4.587551	0.053864	1.921435
H	5.619960	0.321599	0.513569
C	3.487856	0.608847	0.113068
H	3.523328	1.677957	0.336416
C	2.182455	-0.017284	0.658041
H	2.223586	0.002383	1.750482
C	3.657999	0.411703	-1.408903
H	2.856560	0.927445	-1.953911
H	4.600779	0.872509	-1.734234
C	-2.674491	-1.281662	0.053681
C	-2.984780	-1.103301	-1.309186
C	-4.283612	-0.707151	-1.646493
H	-4.525724	-0.560708	-2.696965
C	-5.275352	-0.506866	-0.682902
C	-4.947433	-0.740838	0.655767
H	-5.710012	-0.612080	1.421432
C	-3.664136	-1.134169	1.045830
C	-1.975186	-1.346654	-2.406358
H	-2.486103	-1.559054	-3.350861
H	-1.320015	-2.193984	-2.177917
H	-1.341023	-0.468159	-2.565125
C	-6.658007	-0.041051	-1.075471
H	-6.720489	1.055267	-1.071914
H	-7.419777	-0.412364	-0.381494
H	-6.922819	-0.377081	-2.083631
C	-3.382989	-1.402247	2.507402
H	-3.556343	-2.456984	2.761779
H	-4.045261	-0.807145	3.143971
H	-2.349852	-1.166309	2.779392
C	-1.372864	1.434974	0.995198
C	0.654543	1.842390	1.880945
C	-0.701313	2.531050	1.787666
H	-1.778181	0.658252	1.640142
H	0.631754	1.065878	2.653896
C	1.846356	2.766545	2.053592
H	2.779327	2.233523	2.255817
H	1.991871	3.410590	1.179203
H	1.664723	3.427047	2.916521
H	-2.084941	1.709165	0.211438
N	0.067901	2.634223	-2.037433
O	-0.014643	3.418128	-2.958462
C	-1.360454	2.911532	3.123798
H	-0.758397	3.646663	3.672097
H	-2.354587	3.346841	2.962527
H	-1.478805	2.028051	3.764280
H	-0.599546	3.432915	1.169413

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B3LYP SCF energy: -1536.03343169 a.u.
B3LYP enthalpy: -1535.369701 a.u.
B3LYP free energy: -1535.467990 a.u.
M06 SCF energy in solution: -1536.45179671 a.u.
M06 enthalpy in solution: -1535.788066 a.u.
M06 free energy in solution: -1535.886355 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.407143	0.932897	0.173487
O	1.856719	2.082517	-1.748053
O	1.414396	2.889499	0.232232
N	0.672980	-1.964602	0.173489
N	-1.480486	-1.671701	-0.013917
C	-0.290731	-1.005249	0.087005
C	0.185751	-3.327267	-0.051625
H	0.597301	-4.027557	0.680544
H	0.462369	-3.679030	-1.054766
C	-1.325991	-3.138353	0.095451
H	-1.903286	-3.644317	-0.683689
H	-1.693019	-3.484320	1.070294
C	2.084518	-1.598486	0.104640
C	2.651361	-1.797104	-1.327043
H	2.043734	-1.222205	-2.036654
H	2.580319	-2.857191	-1.608732
C	4.121474	-1.332727	-1.383582
H	4.508552	-1.499006	-2.397285
C	4.959897	-2.135481	-0.369031
H	4.942329	-3.206806	-0.616017
H	6.009131	-1.814566	-0.414108
C	4.399246	-1.909700	1.050204
H	4.998281	-2.470329	1.779911
C	2.942472	-2.419068	1.101689
H	2.525374	-2.312743	2.112036
H	2.915814	-3.488706	0.847088
C	4.442674	-0.404537	1.390466
H	4.071283	-0.235369	2.410666
H	5.480453	-0.045125	1.364900
C	3.589924	0.397946	0.365018
H	3.624122	1.460900	0.622872
C	2.152504	-0.122659	0.492238
H	1.835314	-0.015446	1.560025
C	4.180780	0.166716	-1.042034
H	3.629977	0.754012	-1.779877
H	5.223352	0.513025	-1.057543
C	-2.818578	-1.173741	-0.137912
C	-3.337847	-0.949534	-1.430951
C	-4.672424	-0.556870	-1.553968
H	-5.074324	-0.371049	-2.547794
C	-5.509129	-0.414511	-0.439608
C	-4.977914	-0.691180	0.821483
H	-5.616340	-0.603528	1.698431
C	-3.643019	-1.079624	0.997840
C	-2.494881	-1.180153	-2.664786
H	-3.025977	-0.850410	-3.562583
H	-2.264738	-2.246478	-2.792151
H	-1.538330	-0.651421	-2.619872
C	-6.941265	0.038891	-0.601444
H	-7.000182	1.130039	-0.708212
H	-7.550204	-0.238484	0.265034
H	-7.401455	-0.397810	-1.494707
C	-3.147584	-1.420822	2.385465
H	-3.404062	-2.455761	2.650517
H	-3.615024	-0.774683	3.135772
H	-2.063874	-1.314926	2.474793
C	-0.902202	1.542659	1.579677
C	-1.456787	2.409521	0.359715
C	-1.005427	1.808124	-1.006078
H	-1.652643	0.819572	1.905637
H	-1.758226	1.181116	-1.479243
H	-0.591983	2.544072	-1.694429
C	-0.371826	2.363491	2.743743
H	-1.170383	2.983965	3.180659
H	0.001675	1.710470	3.542395
H	0.438597	3.030096	2.433859
O	2.644653	4.039449	-1.162981
N	1.997514	3.028013	-0.924763
H	-0.992812	3.394433	0.451673
C	-2.986798	2.549599	0.449554
H	-3.489930	1.588413	0.330132
H	-3.273441	2.970613	1.421114
H	-3.347439	3.226106	-0.334089

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B3LYP SCF energy: -2175.59729155 a.u.

B3LYP enthalpy: -2174.962966 a.u.
B3LYP free energy: -2175.072060 a.u.
M06 SCF energy in solution: -2176.04627634 a.u.
M06 enthalpy in solution: -2175.411951 a.u.
M06 free energy in solution: -2175.521045 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	1.102364	-1.815533	0.179168
C	0.768609	-3.247730	0.343988
H	1.106723	-3.814027	-0.530290
C	-0.761953	-3.227464	0.483953
N	-1.094943	-1.804999	0.250029
H	-1.099023	-3.531908	1.480396
C	2.481965	-1.408321	0.067962
C	-2.476424	-1.392213	0.194759
C	-5.192330	-0.693315	0.087755
C	-3.151188	-1.063783	1.388688
C	-3.156209	-1.453069	-1.038802
C	-4.506993	-1.088089	-1.064628
C	-4.500769	-0.704861	1.302710
C	-2.476293	-1.119062	2.737786
C	-2.481379	-1.914745	-2.307456
H	-5.037215	-1.124721	-2.013738
H	-5.027132	-0.441246	2.217532
C	-6.641610	-0.270474	0.023890
C	5.193788	-0.714913	-0.131662
C	3.098758	-1.397246	-1.199499
C	3.217952	-1.156610	1.244407
C	4.564268	-0.799971	1.114242
C	4.448676	-1.033980	-1.269866
C	2.363355	-1.787854	-2.458543
C	2.606273	-1.294681	2.617358
H	5.137133	-0.595041	2.016051
H	4.930562	-1.014138	-2.244851
C	6.640731	-0.293761	-0.241887
H	-2.078432	-2.119697	2.950760
H	-1.643138	-0.412190	2.805518
H	-2.004855	-2.895211	-2.183371
H	-1.707020	-1.209402	-2.626348
H	-7.156546	-0.730593	-0.826003
H	-6.730826	0.817935	-0.091560
H	-7.180301	-0.543726	0.937713
H	2.266251	-2.321747	2.805878
H	1.747422	-0.628838	2.744826
H	3.055476	-1.822125	-3.305387
H	1.565910	-1.076719	-2.697936
H	7.106831	-0.693100	-1.148739
H	7.224611	-0.634230	0.620188
H	6.731611	0.799823	-0.283046
C	0.004246	-1.037099	0.111153
Ru	-0.000563	1.004845	-0.124222
Cl	0.146294	1.274552	2.323083
Cl	-0.127209	0.762497	-2.574398
C	-1.368999	2.442913	-0.101742
H	3.343984	-1.050882	3.387802
H	1.904090	-2.780420	-2.370224
H	-3.214261	-2.006299	-3.114826
H	-3.192818	-0.879025	3.529221
H	-1.265505	-3.858808	-0.253975
H	1.270635	-3.652258	1.227413
C	-0.036085	3.285229	-0.430888
C	1.328108	2.457775	-0.493869
H	-0.190428	3.614596	-1.461750
H	1.656593	2.381021	-1.531471
C	0.037016	4.459516	0.557363
H	0.895115	5.102437	0.335099
H	-0.871626	5.065922	0.477208
H	0.122149	4.101336	1.586184
H	-1.681738	2.635812	0.927367
C	2.468334	2.794481	0.439483
H	2.165328	2.878250	1.482572
H	3.231100	2.011022	0.367013
H	2.943862	3.735304	0.121282
C	-2.510030	2.561020	-1.084945
H	-3.282565	1.822419	-0.844078
H	-2.972281	3.556860	-0.992860
H	-2.192191	2.404173	-2.116079

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B3LYP SCF energy: -1483.00601958 a.u.
B3LYP enthalpy: -1482.333900 a.u.
B3LYP free energy: -1482.443620 a.u.
M06 SCF energy in solution: -1483.39668026 a.u.
M06 enthalpy in solution: -1482.724561 a.u.
M06 free energy in solution: -1482.834281 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	3.365962	2.361564	-0.430098
O	1.137929	2.736487	-0.475820
C	0.713210	0.612029	1.911919
C	2.380601	3.072249	-0.654429
H	0.410234	-0.336115	2.366277
C	-1.315128	1.677604	0.569846
C	-0.493012	1.650860	1.954783
H	-2.175228	1.019104	0.659701
H	-1.206548	1.188081	2.647813
C	2.557065	4.505196	-1.166901
H	3.609501	4.712958	-1.373077
H	2.189197	5.216215	-0.417261
H	1.962570	4.661082	-2.074015
Ru	0.370613	0.761678	-0.071316
C	-0.390725	-1.136401	-0.103457
C	1.335925	-0.009644	-1.757747
N	0.514605	-2.169668	-0.136203
N	-1.617216	-1.698436	-0.293297
C	2.346767	-0.843729	-1.050022
H	0.662101	-0.596470	-2.392137
H	1.784241	0.808518	-2.324762
C	-0.075551	-3.424873	-0.637089
C	1.919960	-1.924038	-0.239765
C	-1.566846	-3.170701	-0.416729
C	-2.906824	-1.069564	-0.282885
C	3.715621	-0.555351	-1.109629
H	0.288732	-4.295924	-0.090301
H	0.173085	-3.554867	-1.699574
C	2.839340	-2.707608	0.474577
H	-2.192038	-3.507361	-1.248562
H	-1.934391	-3.643939	0.502573
C	-3.392266	-0.476541	-1.464333
C	-3.695969	-1.120238	0.881394
C	4.658500	-1.338062	-0.437373
H	4.035768	0.316378	-1.668639
C	4.201650	-2.404969	0.341556
C	2.409091	-3.817778	1.406063
C	-4.674718	0.078322	-1.450271
C	-2.548317	-0.410197	-2.714339
C	-4.974404	-0.551666	0.844369
C	-3.189476	-1.745181	2.161522
C	6.130888	-1.014446	-0.538780
H	4.922066	-3.004277	0.895152
H	1.475707	-3.568319	1.922590
H	3.176212	-3.997503	2.165795
H	2.252806	-4.770251	0.880557
C	-5.484097	0.049673	-0.309027
H	-5.050970	0.546763	-2.357400
H	-1.688757	0.255537	-2.574728
H	-3.134828	-0.034459	-3.558038
H	-2.148744	-1.393008	-2.991150
H	-5.582550	-0.574063	1.746347
H	-2.121008	-1.559667	2.309802
H	-3.336121	-2.833801	2.169854
H	-3.727929	-1.344122	3.025662

H	6.521299	-1.237474	-1.540445
H	6.719855	-1.591487	0.181809
H	6.309879	0.050380	-0.352099
C	-6.876919	0.635147	-0.333224
H	-7.239297	0.848647	0.677488
H	-7.590613	-0.058027	-0.798211
H	-6.909897	1.566628	-0.908937
C	-1.742438	3.022345	0.010961
H	-2.296616	2.862542	-0.922313
H	-2.429727	3.534049	0.702792
H	-0.893316	3.671797	-0.199670
C	-0.094082	3.038985	2.462051
H	0.394278	2.966366	3.439768
H	0.589656	3.528778	1.765877
H	-0.978584	3.674231	2.578047
C	2.081472	1.030002	2.413875
H	2.054803	1.248095	3.493506
H	2.783497	0.201607	2.266700
H	2.485955	1.893314	1.883486

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B3LYP SCF energy: -1483.01097092 a.u.
B3LYP enthalpy: -1482.338670 a.u.
B3LYP free energy: -1482.447516 a.u.
M06 SCF energy in solution: -1483.40010746 a.u.
M06 enthalpy in solution: -1482.727807 a.u.
M06 free energy in solution: -1482.836653 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	-0.343761	2.584655	-1.722469
O	1.076465	2.895899	-0.032886
C	1.024597	0.497412	1.988919
C	0.445751	3.309700	-1.072969
H	0.986337	-0.529734	2.365125
C	-1.316612	1.333275	1.075132
C	-0.349427	1.252424	2.335603
H	-2.035547	0.518629	1.111348
H	-0.862780	0.557794	3.012411
C	0.675962	4.757587	-1.484438
H	0.249741	4.952116	-2.471058
H	1.746235	4.988071	-1.485101
H	0.201504	5.424905	-0.754407
Ru	0.404345	0.799050	0.102812
C	-0.086584	-1.158157	-0.117243
C	1.413438	0.336078	-1.683550
N	0.944065	-2.061159	-0.270012
N	-1.235571	-1.842667	-0.362423
C	2.542679	-0.407993	-1.073035
H	0.791445	-0.268488	-2.349643
H	1.722874	1.249214	-2.190581
C	0.503706	-3.318339	-0.903446
C	2.298073	-1.618052	-0.376934
C	-1.007641	-3.270794	-0.667969
C	-2.588825	-1.362897	-0.321194
C	3.855418	0.083406	-1.110940
H	0.972471	-4.192692	-0.448137
H	0.759780	-3.306783	-1.971910
C	3.341187	-2.329684	0.233611
H	-1.590768	-3.571224	-1.543153
H	-1.312047	-3.897679	0.179011
C	-3.104579	-0.645547	-1.418312
C	-3.399832	-1.686194	0.783883
C	4.921699	-0.618609	-0.540021
H	4.039377	1.028089	-1.617112
C	4.642743	-1.819048	0.120436
C	3.097790	-3.583754	1.040926
C	-4.444929	-0.248077	-1.373962
C	-2.251543	-0.282461	-2.609440
C	-4.733778	-1.265463	0.778004
C	-2.860532	-2.447661	1.973806
C	6.336061	-0.096058	-0.643713
H	5.456657	-2.364444	0.594184
H	2.164215	-3.515152	1.609963
H	3.915149	-3.748626	1.749769
H	3.035412	-4.481078	0.409943
C	-5.275532	-0.542747	-0.288325
H	-4.849430	0.308129	-2.217083
H	-1.596484	0.567367	-2.381618
H	-2.881767	-0.001838	-3.459179
H	-1.612483	-1.115986	-2.922309
H	-5.361345	-1.502863	1.634726
H	-1.822894	-2.175670	2.192269
H	-2.887372	-3.533940	1.812411
H	-3.460536	-2.242987	2.865876
H	6.768087	-0.309644	-1.630575
H	6.989045	-0.555020	0.105932
H	6.371456	0.990160	-0.504502
C	-6.710099	-0.068772	-0.259959
H	-6.773813	0.978850	0.062680
H	-7.315560	-0.662104	0.433075
H	-7.171935	-0.128850	-1.251722
C	-2.041571	2.636075	0.807638
H	-2.535200	2.590803	-0.167019
H	-2.821031	2.798130	1.569554
H	-1.381541	3.504355	0.812308
C	-0.139386	2.598678	3.037048
H	0.464538	2.469269	3.941533
H	0.369909	3.311122	2.383535
H	-1.099595	3.031979	3.337527
C	2.331684	1.164844	2.383235
H	2.442327	1.229655	3.477021
H	3.168966	0.564540	2.008173
H	2.424853	2.170742	1.966144

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B3LYP SCF energy: -1575.34547253 a.u.
B3LYP enthalpy: -1574.651561 a.u.
B3LYP free energy: -1574.752804 a.u.
M06 SCF energy in solution: -1575.74732225 a.u.
M06 enthalpy in solution: -1575.053411 a.u.
M06 free energy in solution: -1575.154654 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.424055	0.769475	0.071953
O	-1.471569	2.672835	0.285245
O	-1.590038	2.390106	-1.881212
N	-0.621910	-2.111373	-0.204175
N	1.526994	-1.798137	0.041083
C	0.324935	-1.148613	-0.069790
C	-0.127999	-3.470924	0.021278
H	-0.521033	-4.171546	-0.720721
H	-0.417932	-3.830422	1.018392
C	1.386302	-3.266266	-0.095983
H	1.954620	-3.781495	0.683974
H	1.774256	-3.592964	-1.069166
C	-2.028888	-1.719085	-0.125008
C	-2.528529	-1.749754	1.344763
H	-1.864346	-1.132280	1.963462
H	-2.479096	-2.776589	1.735138
C	-3.974566	-1.224046	1.421140
H	-4.315610	-1.254540	2.464500
C	-4.883032	-2.117704	0.551706
H	-4.880338	-3.148375	0.934852
H	-5.920568	-1.761391	0.601480
C	-4.388402	-2.090120	-0.909747
H	-5.034069	-2.725332	-1.530394
C	-2.942289	-2.632004	-0.975250
H	-2.582467	-2.647176	-2.012638
H	-2.917193	-3.666735	-0.601838
C	-4.426610	-0.638514	-1.428989

H	-4.105397	-0.597545	-2.478174
H	-5.457471	-0.258777	-1.395513
C	-3.508075	0.262595	-0.560089
H	-3.554293	1.280096	-0.949961
C	-2.075648	-0.285397	-0.681926
H	-1.784860	-0.306947	-1.743262
C	-4.006843	0.226256	0.898677
H	-3.382642	0.876142	1.524009
H	-5.030691	0.620877	0.951595
C	2.854866	-1.268498	-0.097559
C	3.682599	-1.160738	1.032821
C	4.998124	-0.705319	0.857168
H	5.638631	-0.612296	1.732207
C	5.508430	-0.378958	-0.398222
C	4.669756	-0.532982	-1.511286
H	5.053759	-0.300192	-2.502347
C	3.354032	-0.980293	-1.389817
C	3.219693	-1.537169	2.422597
H	3.845971	-2.337635	2.835752
H	2.182166	-1.875865	2.431453
H	3.298438	-0.685175	3.108517
C	6.920695	0.132038	-0.562901
H	6.930103	1.211348	-0.763006
H	7.426970	-0.355062	-1.404169
H	7.517380	-0.041196	0.338182
C	2.491137	-1.134273	-2.622041
H	3.054543	-0.866440	-3.520520
H	1.602098	-0.495605	-2.577986
H	2.136875	-2.164287	-2.750103
C	0.375809	0.984814	1.894628
H	0.885642	0.110824	2.305882
C	1.293326	1.690752	-0.517332
H	2.044043	0.992647	-0.874961
C	1.433097	1.872861	1.055815
H	2.389916	1.389801	1.279131
C	1.465789	3.339989	1.499175
H	1.672416	3.410458	2.572115
H	2.259091	3.881692	0.973205
H	0.516687	3.842241	1.299526
C	1.292594	2.927634	-1.393012
H	2.313970	3.337013	-1.445845
H	0.990498	2.666624	-2.411403
H	0.633748	3.721750	-1.041730
O	-2.465461	4.169248	-0.955476
N	-1.861580	3.103466	-0.886144
C	-0.439424	1.678324	2.976044
H	-1.126439	0.956402	3.434715
H	0.207569	2.055360	3.782729
H	-1.029791	2.512850	2.592006

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B3LYP SCF energy: -1575.34328511 a.u.
B3LYP enthalpy: -1574.649435 a.u.
B3LYP free energy: -1574.749969 a.u.
M06 SCF energy in solution: -1575.74246821 a.u.
M06 enthalpy in solution: -1575.048618 a.u.
M06 free energy in solution: -1575.149152 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.361041	0.824832	0.244176
O	1.305411	2.804172	0.444289
O	1.831111	2.099713	-1.550797
N	0.719018	-2.063962	0.113555
N	-1.444054	-1.822863	-0.056983
C	-0.267925	-1.130026	0.065700
C	0.265899	-3.430885	-0.156850
H	0.693902	-4.143775	0.553399
H	0.553300	-3.743819	-1.169737
C	-1.252065	-3.287377	-0.008560
H	-1.812526	-3.776707	-0.810499
H	-1.614388	-3.683665	0.949049
C	2.120426	-1.654135	0.052251
C	2.677874	-1.785304	-1.389794
H	2.052441	-1.195857	-2.071636
H	2.626874	-2.834704	-1.713222
C	4.137262	-1.288980	-1.440850
H	4.518641	-1.406654	-2.463646
C	5.001678	-2.112725	-0.465901
H	5.003312	-3.174042	-0.753725
H	6.043731	-1.768800	-0.508115
C	4.450046	-1.952835	0.965488
H	5.067135	-2.528923	1.667697
C	3.004563	-2.494088	1.008859
H	2.595147	-2.434959	2.026312
H	2.999236	-3.554008	0.714606
C	4.466174	-0.460877	1.363051
H	4.104695	-0.338762	2.393494
H	5.496607	-0.080166	1.339325
C	3.583961	0.360921	0.379763
H	3.604164	1.413816	0.677701
C	2.154607	-0.190365	0.501665
H	1.864849	-0.148279	1.579367
C	4.167838	0.196611	-1.039744
H	3.600318	0.800907	-1.750092
H	5.203069	0.564862	-1.049154
C	-2.792366	-1.339502	-0.133548
C	-3.350710	-1.095472	-1.408514
C	-4.675042	-0.661747	-1.486076
H	-5.103174	-0.457836	-2.465286
C	-5.468502	-0.494235	-0.343271
C	-4.909149	-0.808773	0.895571
H	-5.519347	-0.720136	1.792440
C	-3.584073	-1.248730	1.025710
C	-2.557552	-1.338470	-2.673341
H	-2.371889	-2.410343	-2.823901
H	-1.580888	-0.845814	-2.655708
H	-3.105934	-0.976251	-3.547875
C	-6.887641	0.011733	-0.455382
H	-6.909608	1.102073	-0.582175
H	-7.470140	-0.225695	0.440558
H	-7.401032	-0.423387	-1.320106
C	-3.084713	-1.666051	2.391907
H	-3.390383	-0.947102	3.159691
H	-1.997557	-1.758077	2.429885
H	-3.513563	-2.636677	2.675458
C	-1.154731	1.607615	-0.885440
H	-1.767959	0.828180	-1.328166
C	-0.921804	1.197775	1.734834
H	-1.526856	0.366056	2.091850
C	-1.711907	1.966295	0.560580
H	-2.699879	1.494335	0.579700
C	-1.845410	3.472659	0.810829
H	-2.477965	3.933123	0.044529
H	-2.315031	3.659332	1.782445
H	-0.874234	3.972654	0.798149
C	-0.400731	2.015746	2.907312
H	-1.224879	2.468601	3.479361
H	0.140592	1.356916	3.598213
H	0.278556	2.814117	2.598854
O	2.572393	4.035307	-0.846606
N	1.931973	3.004352	-0.679421
C	-0.983986	2.735793	-1.883337
H	-0.461089	2.373684	-2.772964
H	-1.974016	3.096133	-2.205774
H	-0.432043	3.593364	-1.496692

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B3LYP SCF energy: -2136.28292495 a.u.
B3LYP enthalpy: -2135.678284 a.u.
B3LYP free energy: -2135.783485 a.u.
M06 SCF energy in solution: -2136.75108305 a.u.

M06 enthalpy in solution: -2136.146442 a.u.
M06 free energy in solution: -2136.251643 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.938782	-1.788931	0.239317
C	0.538734	-3.201436	0.421638
H	0.830893	-3.789405	-0.455380
C	-0.986208	-3.101364	0.587307
N	-1.257206	-1.679282	0.278571
H	-1.315727	-3.330611	1.606543
C	2.333076	-1.434213	0.138175
C	-2.616800	-1.200333	0.206631
C	-5.285291	-0.349769	0.064292
C	-3.259519	-0.754178	1.378388
C	-3.309460	-1.306037	-1.016808
C	-4.634765	-0.862934	-1.061944
C	-4.587135	-0.323082	1.274298
C	-2.576482	-0.758313	2.724474
C	-2.674320	-1.905854	-2.247828
H	-5.173720	-0.929937	-2.004498
H	-5.089535	0.032084	2.171397
C	-6.705097	0.158855	-0.025964
C	5.070008	-0.841168	-0.030257
C	2.968739	-1.469042	-1.119780
C	3.057511	-1.179821	1.320990
C	4.418204	-0.876091	1.206394
C	4.331537	-1.155177	-1.174803
C	2.237767	-1.854825	-2.383194
C	2.413937	-1.246676	2.684631
H	4.983391	-0.670914	2.112897
H	4.829307	-1.171591	-2.141871
C	6.533054	-0.475737	-0.125914
H	-2.201618	-1.756156	2.985974
H	-1.725361	-0.070285	2.751708
H	-2.362672	-2.944889	-2.077185
H	-1.794121	-1.336841	-2.560983
H	-7.286354	-0.402140	-0.765832
H	-6.726644	1.214016	-0.329446
H	-7.219773	0.086927	0.938012
H	1.942229	-2.220998	2.865388
H	1.642139	-0.478572	2.798977
H	2.938729	-1.918241	-3.221018
H	1.461329	-1.127382	-2.642922
H	7.007086	-0.942439	-0.995831
H	7.083263	-0.784717	0.769322
H	6.662870	0.609919	-0.227919
C	-0.123932	-0.968149	0.127144
Ru	-0.001319	1.051672	-0.207089
Cl	0.150909	1.499029	2.203353
Cl	-0.278351	0.705734	-2.627471
C	-1.278987	2.544838	-0.381560
H	3.164696	-1.096350	3.466275
H	1.751402	-2.833812	-2.288536
H	-3.387256	-1.912647	-3.077710
H	-3.280780	-0.459558	3.506822
H	-1.533348	-3.748863	-0.103205
H	1.035896	-3.625392	1.298444
C	0.080954	3.309060	-0.682048
C	1.400187	2.381628	-0.706526
H	-0.016687	3.601305	-1.731019
H	1.705225	2.221607	-1.741726
C	0.221105	4.508718	0.263367
H	1.130211	5.078551	0.044973
H	-0.636880	5.177437	0.136300
H	0.252010	4.181666	1.305851
H	-1.745816	2.855397	0.553414
C	2.569035	2.717414	0.190797
H	2.282853	2.891959	1.227402
H	3.284130	1.887718	0.167852
H	3.093091	3.604715	-0.196858
H	-1.946073	2.493478	-1.240311

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B3LYP SCF energy: -1443.69596605 a.u.
B3LYP enthalpy: -1443.053723 a.u.
B3LYP free energy: -1443.161233 a.u.
M06 SCF energy in solution: -1444.10703255 a.u.
M06 enthalpy in solution: -1443.464790 a.u.
M06 free energy in solution: -1443.572300 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.342297	0.807919	-0.119605
O	1.070168	2.799877	-0.484544
O	3.305931	2.467198	-0.519799
N	0.453916	-2.121195	-0.186508
N	-1.669662	-1.613030	-0.340936
C	-0.434926	-1.073971	-0.150861
C	-0.157801	-3.364554	-0.690439
C	-1.645691	-3.085039	-0.465847
C	1.863588	-1.890862	-0.245535
C	2.751693	-2.688899	0.493822
C	4.118257	-2.386711	0.425542
C	4.611176	-1.303517	-0.308850
C	3.700075	-0.505639	-1.005034
C	2.329172	-0.797963	-1.017985
C	2.281272	-3.810069	1.392107
C	6.087974	-0.985443	-0.341140
C	1.362924	0.048014	-1.770126
C	-2.938833	-0.946878	-0.288914
C	-3.459789	-0.376545	-1.466036
C	-4.720020	0.224159	-1.411626
C	-5.469406	0.269951	-0.230409
C	-4.928245	-0.316511	0.916471
C	-3.671075	-0.932395	0.912121
C	-2.673093	-0.382672	-2.754696
C	-6.814618	0.957198	-0.194334
C	-3.135402	-1.555241	2.181526
C	-1.287953	1.831180	0.422232
C	2.300370	3.166527	-0.683795
H	0.191709	-4.244168	-0.147858
H	0.085222	-3.495533	-1.754103
H	-2.277756	-3.411873	-1.296438
H	-2.019122	-3.552693	0.454323
H	4.812576	-2.997868	0.999240
H	4.041196	0.380342	-1.527844
H	1.340185	-3.554475	1.891719
H	3.027096	-4.017119	2.165772
H	2.121034	-4.749378	0.844647
H	6.630396	-1.513203	0.450422
H	6.259292	0.089224	-0.215927
H	6.538206	-1.276025	-1.299710
H	0.698116	-0.528750	-2.423090
H	1.845880	0.858685	-2.317891
H	-5.125963	0.670980	-2.316821
H	-5.495730	-0.293158	1.844584
H	-1.786288	0.257141	-2.676580
H	-3.284418	-0.013311	-3.583439
H	-2.320364	-1.387224	-3.016444
H	-7.380058	0.779973	-1.115901
H	-6.700154	2.044132	-0.089357
H	-7.420787	0.609047	0.648256
H	-2.058642	-1.394727	2.292498
H	-3.307427	-2.639942	2.205824
H	-3.634633	-1.132934	3.058977
H	-2.281300	1.395278	0.362860
H	-1.242423	2.857193	0.051531
C	0.632594	0.722308	1.877788
C	-0.632659	1.689658	1.868310
H	0.370763	-0.233591	2.340916
H	-1.385349	1.160533	2.462928
C	2.433824	4.621010	-1.146642
H	1.857166	4.779000	-2.065176

H	2.017266	5.295235	-0.389090
H	3.481973	4.874158	-1.321693
C	-0.345515	3.076226	2.456268
H	0.354010	3.618231	1.814910
H	-1.273315	3.656183	2.516667
H	0.078228	3.007121	3.464613
C	1.964696	1.223987	2.401487
H	2.720946	0.443681	2.262027
H	2.319447	2.113868	1.880939
H	1.907852	1.436681	3.480768

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B3LYP SCF energy: -1443.70214267 a.u.
B3LYP enthalpy: -1443.059677 a.u.
B3LYP free energy: -1443.166106 a.u.
M06 SCF energy in solution: -1444.10944424 a.u.
M06 enthalpy in solution: -1443.466979 a.u.
M06 free energy in solution: -1443.573408 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	-0.381242	2.660277	-1.656390
O	1.018827	2.955734	0.051511
C	0.909699	0.538642	2.018794
C	0.367910	3.392027	-0.966512
H	0.886373	-0.493341	2.382380
C	-1.307376	1.514682	0.982737
C	-0.510071	1.238570	2.305906
H	-1.472096	2.575710	0.791564
H	-2.220817	0.934485	0.886688
H	-1.083132	0.478965	2.849254
C	0.548023	4.862187	-1.319613
H	1.594224	5.053891	-1.584927
H	0.317291	5.486924	-0.449792
H	-0.095365	5.141496	-2.156644
Ru	0.380972	0.843919	0.099416
C	-0.140575	-1.089808	-0.172550
C	1.425008	0.448860	-1.673215
N	0.875246	-2.003228	-0.358363
N	-1.300449	-1.744502	-0.434371
C	2.517443	-0.339070	-1.053637
H	0.800265	-0.117645	-2.369532
H	1.767400	1.373047	-2.136965
C	0.411079	-3.230329	-1.032277
C	2.236338	-1.575599	-0.419076
C	-1.099242	-3.165542	-0.784205
C	-2.639078	-1.236676	-0.327532
C	3.836374	0.140021	-1.024157
H	0.867410	-4.128203	-0.611345
H	0.659157	-3.186038	-2.101768
C	3.254967	-2.325638	0.190203
H	-1.692653	-3.431156	-1.663751
H	-1.407902	-3.812195	0.046589
C	-3.183156	-0.494319	-1.393796
C	-3.403491	-1.543220	0.813728
C	4.876188	-0.598259	-0.453684
H	4.044828	1.105274	-1.479357
C	4.563313	-1.825462	0.140823
C	2.974345	-3.610190	0.934747
C	-4.507127	-0.058597	-1.284413
C	-2.368674	-0.134380	-2.612537
C	-4.723215	-1.082117	0.874145
C	-2.833008	-2.335219	1.968612
C	6.298819	-0.089366	-0.488098
H	5.356110	-2.400506	0.615315
H	2.028170	-3.552139	1.483738
H	3.771618	-3.818524	1.654824
H	2.914751	-4.477475	0.262973
C	-5.293165	-0.336824	-0.161334
H	-4.933528	0.518629	-2.102212
H	-1.694316	0.703875	-2.397547
H	-3.024225	0.165068	-3.436312
H	-1.753592	-0.973648	-2.956292
H	-5.316503	-1.306784	1.758283
H	-1.782136	-2.088865	2.150176
H	-2.889458	-3.417836	1.790457
H	-3.392760	-2.133685	2.887182
H	6.780019	-0.317392	-1.448709
H	6.907842	-0.546836	0.298687
H	6.336919	0.997577	-0.357489
C	-6.710492	0.178105	-0.063224
H	-7.287261	-0.373716	0.686165
H	-7.233721	0.096190	-1.022566
H	-6.726895	1.237776	0.223584
C	-0.394690	2.524111	3.136421
H	0.145895	2.352730	4.074025
H	0.129359	3.297338	2.567396
H	-1.393754	2.900761	3.384787
C	2.173290	1.247325	2.480388
H	2.228516	1.308783	3.578316
H	3.049104	0.679217	2.144210
H	2.251237	2.258328	2.072591

TS22-monodentateNO3

B3LYP SCF energy: -1536.00941184 a.u.
B3LYP enthalpy: -1535.348797 a.u.
B3LYP free energy: -1535.450126 a.u.
M06 SCF energy in solution: -1536.43168049 a.u.
M06 enthalpy in solution: -1535.771066 a.u.
M06 free energy in solution: -1535.872395 a.u.
Imaginary frequency: -174.2899 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.334003	0.765807	-0.139498
O	-1.380717	2.663318	-0.515874
O	-2.130808	3.299327	1.455746
N	-0.559532	-2.121634	-0.120138
N	1.580222	-1.765486	0.184198
C	0.379240	-1.144566	-0.031938
C	-0.054902	-3.453478	0.224424
H	-0.413274	-4.214574	-0.474356
H	-0.375946	-3.739763	1.235236
C	1.462223	-3.240045	0.145983
H	2.006993	-3.692115	0.980100
H	1.885254	-3.630413	-0.788353
C	-1.978484	-1.747779	-0.091518
C	-2.520534	-1.785611	1.361312
H	-1.883200	-1.155282	1.992638
H	-2.472400	-2.811935	1.753306
C	-3.975935	-1.280112	1.393413
H	-4.345916	-1.317072	2.426652
C	-4.844516	-2.187995	0.498630
H	-4.836894	-3.219218	0.880942
H	-5.888580	-1.848252	0.517729
C	-4.307641	-2.151217	-0.947589
H	-4.924458	-2.796483	-1.587225
C	-2.851361	-2.674294	-0.969373
H	-2.459894	-2.683267	-1.995709
H	-2.825529	-3.710130	-0.598745
C	-4.356480	-0.698489	-1.466746
H	-4.007186	-0.654257	-2.507767
H	-5.395055	-0.339475	-1.464460
C	-3.477594	0.215635	-0.572439
H	-3.517611	1.240396	-0.950759
C	-2.035275	-0.311410	-0.635305
H	-1.728047	-0.345526	-1.708678
C	-4.017067	0.170432	0.872120
H	-3.422406	0.828785	1.515784
H	-5.048034	0.548107	0.894498
C	2.896593	-1.199238	0.116804
C	3.585437	-0.894816	1.304545

C	4.895804	-0.403522	1.211214
H	5.428859	-0.163335	2.129209
C	5.534802	-0.221451	-0.014979
C	4.834322	-0.563206	-1.179300
H	5.319476	-0.443970	-2.146027
C	3.530542	-1.059962	-1.139617
C	2.974979	-1.090753	2.674185
H	2.826164	-0.129662	3.182106
H	3.638417	-1.687046	3.311581
H	2.005531	-1.589767	2.623867
C	6.937268	0.334957	-0.093663
H	6.929570	1.380462	-0.428203
H	7.551566	-0.226461	-0.806824
H	7.435673	0.304574	0.880290
C	2.837665	-1.450547	-2.426780
H	1.789583	-1.136663	-2.444748
H	2.851802	-2.538333	-2.576398
H	3.342125	-1.001701	-3.287672
C	-0.000840	1.099669	1.652541
H	0.605949	0.490491	2.330220
C	1.492886	1.817007	-1.011851
H	2.102336	0.977384	-1.329072
C	1.674400	2.214270	0.322212
H	2.366944	1.614559	0.905854
C	1.416368	3.618405	0.814726
H	1.545216	3.692584	1.897878
H	2.131991	4.306860	0.341972
H	0.407441	3.952344	0.565734
C	1.098113	2.771314	-2.121162
H	1.979854	3.348318	-2.439389
H	0.737969	2.224068	-2.999420
H	0.315093	3.465323	-1.814982
H	-0.506905	1.971012	2.079229
O	-3.275214	3.721131	-0.353089
N	-2.298193	3.239197	0.222873

TS22

B3LYP SCF energy: -1536.01999353 a.u.
B3LYP enthalpy: -1535.358479 a.u.
B3LYP free energy: -1535.456292 a.u.
M06 SCF energy in solution: -1536.43716588 a.u.
M06 enthalpy in solution: -1535.775651 a.u.
M06 free energy in solution: -1535.873464 a.u.
Imaginary frequency: -227.5934 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.372163	0.812326	0.282362
O	-1.323965	2.813707	0.395697
O	-0.800941	2.207690	-1.627150
N	-0.770994	-2.006466	-0.241107
N	1.397826	-1.822589	0.000776
C	0.225556	-1.110646	-0.033489
C	-0.337604	-3.402380	-0.163458
H	-0.778991	-4.007952	-0.960085
H	-0.623778	-3.845040	0.800808
C	1.182741	-3.257052	-0.299838
H	1.741150	-3.889176	0.396171
H	1.530074	-3.481854	-1.317096
C	-2.162763	-1.554770	-0.152171
C	-2.727031	-1.762372	1.275503
H	-2.057475	-1.289078	2.001699
H	-2.764560	-2.836516	1.509531
C	-4.139652	-1.154159	1.371575
H	-4.525280	-1.296132	2.390229
C	-5.063894	-1.866757	0.363586
H	-5.137082	-2.936506	0.607417
H	-6.080348	-1.454927	0.424467
C	-4.506289	-1.679070	-1.062652
H	-5.157619	-2.190442	-1.783935
C	-3.088782	-2.295092	-1.147626
H	-2.686559	-2.197042	-2.164602
H	-3.142178	-3.369811	-0.916216
C	-4.453907	-0.170099	-1.384808
H	-4.096839	-0.010128	-2.410874
H	-5.466620	0.254233	-1.329076
C	-3.513182	0.549892	-0.382189
H	-3.491731	1.618067	-0.619009
C	-2.111346	-0.064433	-0.542730
H	-1.845221	-0.023653	-1.608659
C	-4.062629	0.352264	1.044985
H	-3.418661	0.865607	1.769271
H	-5.061651	0.802604	1.126171
C	2.728136	-1.317993	-0.177569
C	3.645680	-1.421354	0.883864
C	4.962081	-0.992334	0.674345
H	5.672463	-1.062461	1.495552
C	5.387674	-0.485047	-0.555590
C	4.457316	-0.419075	-1.599571
H	4.772537	-0.039384	-2.569369
C	3.131054	-0.829920	-1.439632
C	3.246814	-2.003729	2.220587
H	3.951668	-1.702882	3.001884
H	3.243279	-3.102091	2.195162
H	2.242115	-1.689807	2.518715
C	6.806820	-0.005881	-0.754716
H	7.188049	-0.284118	-1.743574
H	7.481275	-0.424533	-0.000864
H	6.869774	1.087782	-0.680972
C	2.161154	-0.720137	-2.593942
H	1.423054	0.073214	-2.424125
H	1.596576	-1.646120	-2.750056
H	2.693136	-0.491381	-3.522084
C	-0.246954	0.568433	2.142707
H	0.208544	-0.250387	2.714120
C	1.647922	1.891745	0.207658
H	2.252012	1.172657	-0.332665
C	1.549258	1.670655	1.606762
H	2.116374	0.820636	1.977139
C	1.399151	2.831005	2.572676
H	1.267886	2.486138	3.602270
H	2.304067	3.454200	2.539944
H	0.548851	3.465614	2.309484
C	1.672191	3.282519	-0.384779
H	2.673488	3.717356	-0.240447
H	1.474108	3.253722	-1.458119
H	0.950771	3.958229	0.078796
H	-0.740729	1.306014	2.788194
O	-1.852301	4.104816	-1.296277
N	-1.344604	3.080121	-0.868878

TS23

B3LYP SCF energy: -1536.02191790 a.u.
B3LYP enthalpy: -1535.360412 a.u.
B3LYP free energy: -1535.458405 a.u.
M06 SCF energy in solution: -1536.43716343 a.u.
M06 enthalpy in solution: -1535.775658 a.u.
M06 free energy in solution: -1535.873651 a.u.
Imaginary frequency: -218.1681 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.302514	0.893695	0.186298
O	1.498859	1.720932	-1.750936
O	1.310328	2.881479	0.078414
N	0.677042	-1.987571	0.158841
N	-1.488121	-1.737485	-0.011640
C	-0.304739	-1.052760	0.091253
C	0.212210	-3.354911	-0.088818
H	0.642375	-4.060078	0.627463
H	0.489277	-3.683386	-1.099888
C	-1.304762	-3.200929	0.071439

H	-1.875318	-3.707798	-0.712337
H	-1.657860	-3.572053	1.042935
C	2.084897	-1.581907	0.098869
C	2.623073	-1.669165	-1.352752
H	1.995747	-1.053646	-2.008198
H	2.565673	-2.707314	-1.711812
C	4.085366	-1.178617	-1.403498
H	4.455254	-1.262813	-2.433940
C	4.955761	-2.039528	-0.467217
H	4.947079	-3.090851	-0.790226
H	5.999770	-1.700948	-0.509867
C	4.420361	-1.923481	0.974392
H	5.041605	-2.526605	1.650204
C	2.971979	-2.462770	1.012042
H	2.574258	-2.439955	2.035782
H	2.966911	-3.512515	0.681085
C	4.455788	-0.443223	1.418445
H	4.112286	-0.351993	2.458319
H	5.491990	-0.076832	1.391241
C	3.561031	0.412955	0.478829
H	3.591675	1.459141	0.804761
C	2.123368	-0.133223	0.612485
H	1.914954	-0.182502	1.694240
C	4.132453	0.293211	-0.951235
H	3.569755	0.914240	-1.649992
H	5.172019	0.650235	-0.957959
C	-2.823218	-1.230025	-0.120034
C	-3.362753	-1.016433	-1.407814
C	-4.677129	-0.557852	-1.514747
H	-5.090653	-0.378118	-2.504963
C	-5.478321	-0.334772	-0.387585
C	-4.937188	-0.614014	0.868354
H	-5.554144	-0.479731	1.754936
C	-3.623063	-1.075992	1.027285
C	-2.562522	-1.320780	-2.654963
H	-3.060418	-0.918474	-3.542181
H	-2.460014	-2.404576	-2.801460
H	-1.549981	-0.909174	-2.614611
C	-6.885784	0.195226	-0.532603
H	-6.885401	1.283230	-0.680149
H	-7.487207	-0.014453	0.357798
H	-7.392988	-0.246752	-1.397397
C	-3.138646	-1.450286	2.410777
H	-2.051067	-1.529287	2.463360
H	-3.558519	-2.418302	2.715834
H	-3.463843	-0.715346	3.155310
C	-1.286237	1.763876	-1.027170
H	-1.792114	0.984177	-1.580647
C	-0.616343	1.199989	1.816581
H	-1.422055	0.570210	2.204277
C	-1.808521	2.155054	0.237128
H	-2.652199	1.571403	0.597449
C	-1.800245	3.617602	0.628995
H	-2.575596	4.139529	0.051413
H	-2.023666	3.775297	1.687600
H	-0.836940	4.080097	0.398998
H	-0.822159	2.530361	-1.643093
C	-0.125722	2.201105	2.827322
H	-0.942088	2.737694	3.331217
H	0.405210	1.635751	3.610281
H	0.576369	2.923845	2.404068
O	2.470334	3.681416	-1.603316
N	1.786986	2.791744	-1.121004

TS25′

B3LYP SCF energy:	-1535.99618155 a.u.
B3LYP enthalpy:	-1535.335006 a.u.
B3LYP free energy:	-1535.433988 a.u.
M06 SCF energy in solution:	-1536.41625131 a.u.
M06 enthalpy in solution:	-1535.755076 a.u.
M06 free energy in solution:	-1535.854058 a.u.

Imaginary frequency: -109.1007 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.240243	0.943001	0.275833
O	-1.223888	2.936997	0.194898
O	-0.561975	2.059316	-1.672216
N	-0.753217	-1.922879	-0.168064
N	1.420095	-1.750965	0.041572
C	0.249150	-1.035661	0.017060
C	-0.322161	-3.322546	-0.118696
H	-0.763877	-3.905312	-0.931514
H	-0.621464	-3.783216	0.832303
C	1.199301	-3.187053	-0.242006
H	1.747158	-3.812500	0.468379
H	1.558039	-3.427434	-1.251318
C	-2.157802	-1.491295	-0.160637
C	-2.820841	-1.774301	1.210100
H	-2.223040	-1.340198	2.013118
H	-2.866643	-2.859554	1.386872
C	-4.244107	-1.183824	1.229361
H	-4.700285	-1.371302	2.211049
C	-5.083817	-1.863523	0.129408
H	-5.159816	-2.942932	0.325347
H	-6.107454	-1.464987	0.132393
C	-4.426736	-1.611562	-1.243114
H	-5.016510	-2.101397	-2.029558
C	-2.997949	-2.213629	-1.245358
H	-2.524664	-2.076120	-2.226565
H	-3.063186	-3.297166	-1.058532
C	-4.380573	-0.088131	-1.496965
H	-3.961102	0.122546	-2.489478
H	-5.404965	0.313132	-1.490545
C	-3.514805	0.597686	-0.406120
H	-3.491940	1.677500	-0.592662
C	-2.094018	0.003566	-0.498218
H	-1.816613	0.047893	-1.561346
C	-4.163460	0.335428	0.968698
H	-3.585556	0.826104	1.762020
H	-5.172792	0.769822	0.995924
C	2.753882	-1.259445	-0.143200
C	3.660123	-1.337399	0.930358
C	4.976387	-0.908641	0.725408
H	5.679426	-0.959489	1.554264
C	5.411238	-0.422312	-0.511063
C	4.491459	-0.382723	-1.565065
H	4.816183	-0.025243	-2.540249
C	3.164731	-0.797528	-1.410841
C	3.236464	-1.867302	2.280951
H	4.002298	-1.662095	3.034996
H	3.082189	-2.954253	2.261217
H	2.295038	-1.420250	2.615934
C	6.830176	0.060545	-0.703567
H	7.505878	-0.373062	0.040771
H	6.894208	1.152509	-0.607163
H	7.209651	-0.197805	-1.698272
C	2.210124	-0.727676	-2.581151
H	1.667894	-1.668553	-2.728380
H	2.752705	-0.508494	-3.505587
H	1.454377	0.053500	-2.440240
C	-0.493538	0.456318	2.364226
H	-0.314776	-0.585316	2.617561
H	-1.473523	0.833962	2.655075
C	1.591015	1.619419	0.178898
H	2.443047	1.067157	0.584751
C	0.593525	1.368517	2.371924
H	1.581007	0.941332	2.530146
C	2.101940	2.813341	-0.563171
H	2.720450	3.412773	0.124874
H	2.789218	2.483520	-1.358580
H	1.338256	3.453092	-1.004964
C	0.433292	2.794575	2.846612
H	0.488454	2.814173	3.945296

H	1.219476	3.452708	2.462677
H	-0.531525	3.211794	2.548032
N	-1.172480	3.029347	-1.087709
O	-1.658299	3.962876	-1.698715

TS24

B3LYP SCF energy: -1496.70896418 a.u.
B3LYP enthalpy: -1496.077210 a.u.
B3LYP free energy: -1496.172693 a.u.
M06 SCF energy in solution: -1497.14366531 a.u.
M06 enthalpy in solution: -1496.511911 a.u.
M06 free energy in solution: -1496.607394 a.u.
Imaginary frequency: -123.8859 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.265473	0.987159	0.291664
O	1.345493	1.833163	-1.648188
O	1.280941	2.974636	0.201298
N	0.604989	-1.888786	0.128945
N	-1.559135	-1.593949	-0.004757
C	-0.362867	-0.936813	0.115982
C	0.112929	-3.233224	-0.183639
H	0.539630	-3.982469	0.488664
H	0.370449	-3.513129	-1.214414
C	-1.399900	-3.062656	0.005393
H	-1.989212	-3.521926	-0.793713
H	-1.746325	-3.474776	0.962737
C	2.016264	-1.493428	0.044266
C	2.498742	-1.494116	-1.429647
H	1.855092	-0.832675	-2.021003
H	2.417085	-2.506772	-1.851523
C	3.963068	-1.013836	-1.505492
H	4.293317	-1.036417	-2.552487
C	4.858217	-1.939434	-0.658670
H	4.825660	-2.968214	-1.046394
H	5.903664	-1.608103	-0.719814
C	4.378224	-1.909399	0.806747
H	5.017691	-2.559059	1.419539
C	2.926164	-2.438013	0.865515
H	2.567747	-2.476766	1.903192
H	2.897865	-3.464707	0.469534
C	4.448606	-0.459633	1.339367
H	4.146233	-0.429886	2.395409
H	5.487805	-0.103396	1.294690
C	3.528026	0.461697	0.490715
H	3.583033	1.485772	0.878702
C	2.089521	-0.079851	0.650167
H	1.939155	-0.207580	1.731841
C	4.043938	0.426388	-0.965005
H	3.465200	1.093829	-1.605061
H	5.086817	0.773061	-0.989038
C	-2.878218	-1.050393	-0.127568
C	-3.370550	-0.760163	-1.419670
C	-4.672370	-0.272061	-1.545229
H	-5.050570	-0.035952	-2.537711
C	-5.504575	-0.085983	-0.433392
C	-5.007642	-0.431161	0.824047
H	-5.648450	-0.322514	1.697162
C	-3.708048	-0.927465	1.000944
C	-2.525578	-1.000791	-2.650727
H	-3.037766	-0.639088	-3.547185
H	-2.326879	-2.070835	-2.794503
H	-1.551926	-0.504045	-2.590989
C	-6.896887	0.477475	-0.597168
H	-6.870038	1.568520	-0.716908
H	-7.523570	0.258081	0.273180
H	-7.392459	0.068443	-1.484710
C	-3.267754	-1.359969	2.381755
H	-2.187208	-1.502576	2.445171
H	-3.746436	-2.308336	2.660017
H	-3.560325	-0.623678	3.138725
C	-1.410184	2.051275	-0.801655
H	-1.945810	1.337775	-1.412313
C	-0.488215	1.172272	2.013769
H	-1.268721	0.524822	2.430707
C	-1.806182	2.264869	0.520289
H	-2.643132	1.707765	0.927988
O	2.373367	3.767496	-1.529498
N	1.693807	2.892174	-1.019018
H	-0.892398	2.839758	-1.335713
C	-0.009535	2.196598	3.004914
H	0.527248	1.659018	3.803390
H	0.677698	2.924046	2.565068
H	-0.840945	2.726705	3.493085
H	-1.567208	3.208772	1.000321

TS26

B3LYP SCF energy: -1496.70717925 a.u.
B3LYP enthalpy: -1496.075711 a.u.
B3LYP free energy: -1496.170197 a.u.
M06 SCF energy in solution: -1497.14310145 a.u.
M06 enthalpy in solution: -1496.511633 a.u.
M06 free energy in solution: -1496.606119 a.u.
Imaginary frequency: -200.2683 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.338312	0.861051	0.440990
O	-1.310578	2.849098	0.633724
O	-0.630007	2.369175	-1.376799
N	-0.725128	-1.896099	-0.341229
N	1.443886	-1.722097	-0.084730
C	0.265291	-1.021495	-0.039148
C	-0.279251	-3.287636	-0.417396
H	-0.724187	-3.810529	-1.268615
H	-0.548313	-3.832516	0.498458
C	1.238035	-3.111663	-0.555188
H	1.810821	-3.819284	0.050099
H	1.571080	-3.206176	-1.597571
C	-2.120584	-1.458139	-0.235609
C	-2.717150	-1.806430	1.150772
H	-2.068133	-1.405253	1.936292
H	-2.753998	-2.898626	1.276986
C	-4.133784	-1.212240	1.271827
H	-4.543216	-1.454167	2.261910
C	-5.032279	-1.822031	0.176649
H	-5.109150	-2.910525	0.312451
H	-6.050821	-1.417938	0.253975
C	-4.441837	-1.494759	-1.210585
H	-5.073887	-1.934115	-1.993823
C	-3.021080	-2.099276	-1.320120
H	-2.594255	-1.903861	-2.312563
H	-3.078479	-3.191218	-1.194438
C	-4.389102	0.038781	-1.381226
H	-4.009593	0.300066	-2.377913
H	-5.405031	0.452127	-1.306620
C	-3.473938	0.657486	-0.291469
H	-3.450078	1.744247	-0.418051
C	-2.067305	0.063550	-0.482350
H	-1.785550	0.202659	-1.536131
C	-4.052074	0.318703	1.097335
H	-3.422858	0.756715	1.881827
H	-5.052742	0.760089	1.203816
C	2.766456	-1.180159	-0.201098
C	3.691174	-1.418002	0.834077
C	4.998317	-0.942559	0.686425
H	5.712921	-1.117503	1.488192
C	5.410174	-0.255793	-0.459691
C	4.476097	-0.060469	-1.482038
H	4.781752	0.456974	-2.388982
C	3.156187	-0.514519	-1.382027

C	3.303228	-2.185706	2.077329
H	4.035235	-2.028111	2.875266
H	3.260416	-3.266435	1.886163
H	2.316528	-1.891209	2.448613
C	6.819396	0.275420	-0.582687
H	6.904667	1.276502	-0.139456
H	7.126610	0.357003	-1.630513
H	7.538356	-0.369793	-0.066458
C	2.187341	-0.271304	-2.516994
H	1.443506	0.491505	-2.257609
H	1.630056	-1.175730	-2.785187
H	2.720482	0.070504	-3.409114
C	-0.330051	0.453074	2.276323
H	0.077562	-0.416346	2.807700
C	1.682580	2.010326	0.578884
H	2.276428	1.456226	-0.140395
C	1.566593	1.444149	1.858848
H	2.113525	0.537046	2.084794
O	-1.730366	4.233409	-1.014254
N	-1.242476	3.191594	-0.608080
H	-0.816916	1.165519	2.957071
C	1.631022	3.503077	0.362305
H	2.638567	3.920424	0.504614
H	1.318296	3.748701	-0.655481
H	0.956181	3.997094	1.066257
H	1.372878	2.108144	2.698871

TS33

B3LYP SCF energy: -1536.01451892 a.u.
B3LYP enthalpy: -1535.353048 a.u.
B3LYP free energy: -1535.449742 a.u.
M06 SCF energy in solution: -1536.43121933 a.u.
M06 enthalpy in solution: -1535.769748 a.u.
M06 free energy in solution: -1535.866442 a.u.
Imaginary frequency: -214.5273 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.410854	0.833347	0.420212
O	-1.383470	2.822801	0.575248
O	-0.726288	2.304254	-1.433152
N	-0.779884	-1.942129	-0.312518
N	1.394887	-1.759827	-0.144588
C	0.214997	-1.060104	-0.045166
C	-0.334018	-3.330904	-0.412187
H	-0.817001	-3.854401	-1.241676
H	-0.555937	-3.878642	0.514937
C	1.170847	-3.144623	-0.623362
H	1.777048	-3.857641	-0.059196
H	1.451440	-3.219295	-1.682964
C	-2.175580	-1.505440	-0.227022
C	-2.783138	-1.816170	1.162613
H	-2.138960	-1.396717	1.942493
H	-2.821935	-2.904782	1.316274
C	-4.199894	-1.216788	1.256163
H	-4.617787	-1.429583	2.249384
C	-5.090530	-1.856042	0.171436
H	-5.169411	-2.940296	0.336480
H	-6.109241	-1.449220	0.229476
C	-4.489220	-1.568123	-1.219797
H	-5.115327	-2.029359	-1.995196
C	-3.068381	-2.176898	-1.300560
H	-2.633468	-2.010266	-2.294927
H	-3.129308	-3.264627	-1.144710
C	-4.433200	-0.040412	-1.434211
H	-4.045601	0.191950	-2.434989
H	-5.448959	0.376541	-1.379541
C	-3.525685	0.608153	-0.355371
H	-3.501414	1.690702	-0.513036
C	-2.118342	0.006830	-0.518965
H	-1.827632	0.113546	-1.573504
C	-4.116290	0.308743	1.037772
H	-3.495930	0.769916	1.815858
H	-5.118192	0.752273	1.121161
C	2.713310	-1.229612	-0.332323
C	3.718386	-1.570425	0.593401
C	5.018117	-1.097511	0.377371
H	5.792931	-1.350346	1.098490
C	5.346370	-0.319055	-0.734758
C	4.334929	-0.033357	-1.658852
H	4.575660	0.548647	-2.546187
C	3.021262	-0.481237	-1.489829
C	3.435167	-2.454445	1.787253
H	4.125732	-2.235424	2.607923
H	3.565842	-3.515939	1.534979
H	2.411673	-2.331485	2.152321
C	6.748428	0.208412	-0.932641
H	7.018584	0.239113	-1.993807
H	7.487120	-0.409458	-0.411557
H	6.845622	1.231214	-0.544842
C	1.979155	-0.152615	-2.533511
H	1.299703	0.638675	-2.196481
H	1.354499	-1.018681	-2.778572
H	2.458250	0.187837	-3.456493
C	-0.448551	0.459291	2.256704
H	0.004915	-0.376558	2.801947
C	1.627579	1.940443	0.613112
H	2.377586	1.255990	0.227173
C	1.299916	1.779694	1.977846
C	1.650335	3.313838	-0.022641
H	2.636996	3.767114	0.157127
H	1.497067	3.272624	-1.102880
H	0.898661	3.978025	0.412158
H	-1.025530	1.126000	2.913753
H	0.797697	2.631762	2.435893
C	2.200165	0.984744	2.905355
H	1.727212	0.748729	3.862907
H	2.534266	0.058228	2.434602
H	3.094137	1.587368	3.119096
O	-1.824042	4.173746	-1.094916
N	-1.329749	3.139964	-0.675756

TS36

B3LYP SCF energy: -1536.01855539 a.u.
B3LYP enthalpy: -1535.356806 a.u.
B3LYP free energy: -1535.454163 a.u.
M06 SCF energy in solution: -1536.43422044 a.u.
M06 enthalpy in solution: -1535.772471 a.u.
M06 free energy in solution: -1535.869828 a.u.
Imaginary frequency: -241.2579 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.352682	0.940273	0.246824
O	1.539691	1.810687	-1.694387
O	1.436404	2.887791	0.192597
N	0.657408	-1.950992	0.146528
N	-1.502787	-1.660435	0.008443
C	-0.308058	-0.995417	0.105248
C	0.168229	-3.307476	-0.109364
H	0.592552	-4.025250	0.597811
H	0.432708	-3.631964	-1.125123
C	-1.342770	-3.129165	0.065426
H	-1.928946	-3.609825	-0.723286
H	-1.694631	-3.511797	1.032245
C	2.072226	-1.578734	0.076749
C	2.591377	-1.652430	-1.383263
H	1.969046	-1.012865	-2.020265
H	2.507469	-2.682747	-1.758946
C	4.062647	-1.190954	-1.444027
H	4.418197	-1.265437	-2.480244
C	4.926648	-2.084677	-0.532960

H	4.893509	-3.129866	-0.873735
H	5.976567	-1.765911	-0.582416
C	4.410555	-1.983143	0.916842
H	5.027487	-2.610070	1.574674
C	2.952107	-2.494331	0.962987
H	2.567315	-2.482491	1.991833
H	2.921889	-3.537317	0.612905
C	4.480965	-0.511874	1.385382
H	4.150686	-0.431341	2.430385
H	5.523835	-0.165608	1.352430
C	3.593311	0.378209	0.470641
H	3.648749	1.417465	0.814115
C	2.148007	-0.143817	0.614000
H	1.950287	-0.206063	1.696817
C	4.144085	0.271702	-0.968427
H	3.584429	0.914886	-1.649510
H	5.189903	0.609603	-0.983294
C	-2.829384	-1.155101	-0.172136
C	-3.270078	-0.860746	-1.481143
C	-4.592541	-0.450787	-1.663554
H	-4.932859	-0.210941	-2.668803
C	-5.494213	-0.358065	-0.595042
C	-5.040976	-0.702491	0.679465
H	-5.730299	-0.654422	1.520240
C	-3.720037	-1.109630	0.914816
C	-2.349271	-1.023892	-2.669164
H	-2.839088	-0.685710	-3.587109
H	-2.070103	-2.076045	-2.812094
H	-1.417737	-0.461723	-2.550880
C	-6.912896	0.110546	-0.820473
H	-7.559873	-0.149638	0.023328
H	-7.342018	-0.332308	-1.726389
H	-6.955064	1.200664	-0.944015
C	-3.304759	-1.515811	2.310575
H	-2.231716	-1.387464	2.472461
H	-3.542892	-2.571133	2.501666
H	-3.838841	-0.927336	3.063854
C	-1.268686	1.968191	-0.864406
H	-2.029560	1.323384	-1.289663
C	-0.532575	1.263019	1.886083
H	-1.403996	0.694274	2.228954
C	-1.517482	2.526820	0.417290
H	-0.684159	2.532772	-1.582680
C	-0.000912	2.210068	2.929835
H	-0.788038	2.856562	3.347121
H	0.388110	1.609948	3.767099
H	0.812764	2.836487	2.554614
H	-0.942033	3.417625	0.660094
C	-2.895874	2.475120	1.045451
H	-2.873651	2.661537	2.124356
H	-3.507669	3.267731	0.592599
H	-3.397836	1.523701	0.861065
O	2.612342	3.709833	-1.465985
N	1.890725	2.833415	-1.017463

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B3LYP SCF energy: -2018.36200465 a.u.
B3LYP enthalpy: -2017.847508 a.u.
B3LYP free energy: -2017.950265 a.u.
M06 SCF energy in solution: -2018.88886134 a.u.
M06 enthalpy in solution: -2018.374365 a.u.
M06 free energy in solution: -2018.477122 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.156203	1.362190	-0.037302
Cl	0.763925	1.596019	-2.333214
C	-0.010011	-0.602653	0.070587
N	-1.103664	-1.403088	0.161847
N	1.092312	-1.401064	0.136759
C	-0.758503	-2.837952	0.223207
H	-1.283379	-3.319199	1.053567
H	-1.060431	-3.337404	-0.705417
C	0.763138	-2.810504	0.410096
H	1.291650	-3.469877	-0.284467
H	1.064597	-3.075275	1.430746
C	-1.554229	1.962070	-0.159869
H	-2.453252	1.346725	-0.201058
Cl	0.487714	1.732272	2.296982
C	-2.488372	-1.045149	0.059492
C	-5.221551	-0.456632	-0.122162
C	-3.092222	-0.977771	-1.210375
C	-3.222690	-0.827793	1.239485
C	-4.584976	-0.531140	1.121309
C	-4.457186	-0.678157	-1.273340
H	-5.161372	-0.351212	2.026236
H	-4.933130	-0.612475	-2.249452
C	2.471994	-0.990516	0.072708
C	5.170717	-0.240031	-0.086964
C	3.181312	-0.713193	1.257725
C	3.121358	-1.003482	-1.181507
C	4.460687	-0.613149	-1.233945
C	4.520684	-0.319590	1.145590
H	4.964020	-0.605350	-2.198170
H	5.069214	-0.080695	2.054250
C	2.421810	-1.469104	-2.435869
H	1.611062	-0.791319	-2.715968
H	1.996603	-2.473304	-2.311538
H	3.128575	-1.511557	-3.270022
C	2.587103	-0.916157	2.631645
H	3.020499	-0.212948	3.348299
H	2.809902	-1.930901	2.992458
H	1.507637	-0.767382	2.649835
C	6.602513	0.231303	-0.184165
H	6.646632	1.300803	-0.428604
H	7.148811	-0.302505	-0.969691
H	7.137722	0.089787	0.760585
C	-2.292065	-1.172184	-2.477311
H	-2.937153	-1.080648	-3.356149
H	-1.820035	-2.161743	-2.518207
H	-1.491237	-0.428613	-2.565165
C	-2.559953	-0.872234	2.596132
H	-2.097535	-1.847760	2.793053
H	-3.292529	-0.689125	3.387857
H	-1.768231	-0.118492	2.680515
C	-6.701859	-0.168888	-0.219561
H	-7.285369	-1.099330	-0.222594
H	-6.946279	0.369770	-1.141227
H	-7.050516	0.430565	0.627835
C	-1.757208	3.444616	-0.212871
H	-2.285214	3.714470	-1.139678
H	-2.383942	3.761521	0.634218
H	-0.821626	4.014974	-0.175277

TS38

B3LYP SCF energy: -2175.58915930 a.u.
B3LYP enthalpy: -2174.956822 a.u.
B3LYP free energy: -2175.065025 a.u.
M06 SCF energy in solution: -2176.03783512 a.u.
M06 enthalpy in solution: -2175.405498 a.u.
M06 free energy in solution: -2175.513701 a.u.
Imaginary frequency: -206.5483 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	1.024691	-1.853182	0.194846
C	0.646978	-3.273066	0.357891
H	0.961890	-3.849836	-0.518647
C	-0.880738	-3.198775	0.501440
N	-1.166219	-1.769505	0.244692
H	-1.224749	-3.474425	1.504468
C	2.413245	-1.479036	0.087511

C	-2.536689	-1.330466	0.199118
C	-5.247927	-0.611309	0.122149
C	-3.179813	-0.942188	1.390712
C	-3.235046	-1.406306	-1.021874
C	-4.584082	-1.033972	-1.033717
C	-4.528635	-0.574756	1.320666
C	-2.460048	-0.922167	2.717385
C	-2.569243	-1.868166	-2.295585
H	-5.128976	-1.080669	-1.974248
H	-5.030932	-0.262957	2.234027
C	-6.714653	-0.248009	0.085852
C	5.132691	-0.807905	-0.106405
C	3.033817	-1.470527	-1.179243
C	3.154946	-1.251012	1.266494
C	4.503324	-0.902205	1.139046
C	4.386622	-1.116631	-1.246649
C	2.302920	-1.865960	-2.439665
C	2.550297	-1.419620	2.639268
H	5.078598	-0.712307	2.042576
H	4.870054	-1.097751	-2.220909
C	6.581477	-0.392407	-0.213278
H	-2.047556	-1.907529	2.969620
H	-1.625429	-0.212408	2.718029
H	-2.109918	-2.858069	-2.181843
H	-1.779824	-1.174667	-2.605768
H	-7.002425	0.162584	-0.887814
H	-6.963885	0.491464	0.854221
H	-7.345268	-1.129101	0.265989
H	2.245613	-2.459926	2.816625
H	1.674541	-0.779652	2.775864
H	3.001378	-1.915607	-3.280597
H	1.514705	-1.150244	-2.694194
H	7.046828	-0.789195	-1.121665
H	7.163121	-0.739241	0.647773
H	6.676703	0.701000	-0.249081
C	-0.044890	-1.031440	0.110677
Ru	0.105312	1.027202	-0.151280
Cl	0.370952	1.326914	2.288807
Cl	-0.052989	0.772379	-2.608980
C	-1.445872	2.077700	-0.032046
H	3.281973	-1.160512	3.410441
H	1.835062	-2.853631	-2.343175
H	-3.302322	-1.937992	-3.105053
H	-3.149287	-0.641902	3.519925
H	-1.407893	-3.826670	-0.222894
H	1.136424	-3.697842	1.238991
C	0.167989	3.386912	-0.497466
C	1.422465	2.696628	-0.599023
H	-0.298047	3.580862	-1.461340
H	1.711770	2.444258	-1.618132
C	-0.064551	4.433504	0.576522
H	0.619078	5.277153	0.411692
H	-1.086454	4.823569	0.541336
H	0.121823	4.031893	1.575522
H	-1.673308	2.424641	0.982067
C	2.582275	2.922075	0.341947
H	2.268487	3.118329	1.366714
H	3.246735	2.051501	0.352504
H	3.172593	3.777762	-0.022322
C	-2.544907	2.323497	-1.019785
H	-3.389655	1.679216	-0.738591
H	-2.901171	3.362260	-0.945320
H	-2.260394	2.093228	-2.045934

TS40

B3LYP SCF energy:	-2175.58716842 a.u.
B3LYP enthalpy:	-2174.954893 a.u.
B3LYP free energy:	-2175.063588 a.u.
M06 SCF energy in solution:	-2176.03520093 a.u.
M06 enthalpy in solution:	-2175.402926 a.u.
M06 free energy in solution:	-2175.511621 a.u.

Imaginary frequency: -184.9525 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	1.040645	-1.822024	0.242175
C	0.673664	-3.233897	0.482048
H	1.194083	-3.888023	-0.223228
C	-0.847370	-3.222038	0.277355
N	-1.149339	-1.777771	0.157497
H	-1.394097	-3.655202	1.119445
C	2.429510	-1.436591	0.197254
C	-2.522970	-1.364109	0.040972
C	-5.242086	-0.703262	-0.166640
C	-3.273698	-1.160277	1.215285
C	-3.118124	-1.291872	-1.233739
C	-4.472924	-0.948120	-1.308390
C	-4.626239	-0.825837	1.083128
C	-2.658391	-1.299768	2.586617
C	-2.344076	-1.589561	-2.495206
H	-4.939802	-0.884730	-2.288977
H	-5.212602	-0.662122	1.984775
C	-6.696878	-0.309561	-0.279854
C	5.154574	-0.769187	0.097220
C	3.119458	-1.527562	-1.030554
C	3.102596	-1.104953	1.391254
C	4.456940	-0.759203	1.307751
C	4.472648	-1.176574	-1.054017
C	2.448017	-2.017529	-2.290081
C	2.426622	-1.157283	2.740083
H	4.981405	-0.491009	2.222241
H	5.008548	-1.233610	-1.998972
C	6.607545	-0.359795	0.032207
H	-2.284818	-2.316934	2.763664
H	-1.817079	-0.610943	2.717562
H	-1.917979	-2.601024	-2.479671
H	-1.514338	-0.888961	-2.639441
H	-7.154800	-0.722821	-1.184795
H	-6.809884	0.781777	-0.327968
H	-7.274599	-0.656915	0.583390
H	2.045598	-2.163367	2.958716
H	1.583705	-0.462381	2.804387
H	3.170218	-2.067547	-3.110518
H	1.635746	-1.349668	-2.591930
H	7.156559	-0.946144	-0.712752
H	7.104339	-0.486908	0.999751
H	6.707765	0.696671	-0.250098
C	-0.036461	-1.017025	0.102716
Ru	0.099514	1.054829	-0.108809
Cl	-0.107633	1.305938	2.346345
Cl	0.380057	0.837617	-2.559420
C	-1.446746	2.043103	-0.505811
H	3.139122	-0.901038	3.530100
H	2.028667	-3.023587	-2.160424
H	-3.000385	-1.525543	-3.368504
H	-3.401032	-1.086516	3.361490
H	-1.155984	-3.744572	-0.635173
H	0.959992	-3.529358	1.497573
C	0.233522	3.417654	-0.404620
C	1.440413	2.740811	-0.026738
H	-1.647257	2.164269	-1.576097
H	0.147335	3.635011	-1.468646
C	-2.591348	2.426542	0.378544
H	-3.063642	3.356609	0.032875
H	-3.345520	1.633225	0.273129
H	-2.326521	2.499779	1.432922
C	-0.336430	4.455664	0.543833
H	-1.324022	4.812183	0.240910
H	-0.392067	4.066883	1.564021
H	0.338482	5.322099	0.547402
C	2.640573	2.626763	-0.940657
H	3.279005	3.510870	-0.786642
H	3.246014	1.746623	-0.697904
H	2.356212	2.568690	-1.991742

H	1.690605	2.830699	1.031549

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B3LYP SCF energy: -1325.79426306 a.u.
B3LYP enthalpy: -1325.241358 a.u.
B3LYP free energy: -1325.341001 a.u.
M06 SCF energy in solution: -1326.24801714 a.u.
M06 enthalpy in solution: -1325.695112 a.u.
M06 free energy in solution: -1325.794755 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.404764	0.988373	-0.416466
O	0.575464	1.975046	1.529907
O	1.273405	3.151255	-0.208654
N	0.868443	-1.799082	0.085292
N	-1.316559	-1.565928	-0.056917
C	-0.139819	-0.877414	-0.084954
C	0.379041	-3.179444	-0.054929
C	-1.112214	-2.998415	0.238986
C	2.245232	-1.423991	-0.042969
C	3.202233	-1.918117	0.862066
C	4.529516	-1.494601	0.721714
C	4.920406	-0.572152	-0.253366
C	3.940414	-0.067130	-1.111481
C	2.604304	-0.488835	-1.048744
C	2.836993	-2.835906	2.006141
C	6.362511	-0.138486	-0.381078
C	1.555265	0.089822	-1.938924
C	-2.627417	-1.007810	0.118868
C	-3.575489	-1.180015	-0.909613
C	-4.863437	-0.671820	-0.721981
C	-5.231741	-0.010127	0.454301
C	-4.269931	0.134272	1.457327
C	-2.966515	-0.359073	1.321490
C	-3.217983	-1.874972	-2.203330
C	-6.639190	0.507007	0.643382
C	-1.974028	-0.176896	2.445924
C	-1.038638	1.440844	-1.448345
C	1.088541	3.046927	1.033132
C	1.468946	4.163160	1.981008
H	0.862783	-3.865761	0.641376
H	0.556649	-3.540501	-1.078009
H	-1.750754	-3.627499	-0.386096
H	-1.353733	-3.200967	1.291969
H	5.271513	-1.873085	1.422083
H	4.213215	0.665311	-1.868093
H	1.869261	-2.564189	2.441804
H	3.590949	-2.776088	2.796958
H	2.779316	-3.889537	1.699318
H	6.884267	-0.712648	-1.158736
H	6.910005	-0.286470	0.555845
H	6.438995	0.919511	-0.654639
H	1.013761	-0.679252	-2.499453
H	1.966660	0.826161	-2.635784
H	-5.594491	-0.789518	-1.519490
H	-4.538664	0.642328	2.381215
H	-2.242406	-1.549154	-2.578876
H	-3.968700	-1.668406	-2.972211
H	-3.170629	-2.966039	-2.084413
H	-7.311545	-0.287988	0.993312
H	-7.054505	0.890863	-0.295018
H	-6.673688	1.312823	1.383732
H	-1.269470	0.637288	2.239563
H	-1.374970	-1.079257	2.612748
H	-2.496884	0.054627	3.379491
H	-1.906236	0.782652	-1.575082
H	0.600598	4.448373	2.584360
H	2.241978	3.809089	2.672135
H	1.839620	5.028816	1.428777
C	-1.165893	2.750526	-2.175001
H	-2.079268	3.276662	-1.855586
H	-0.309064	3.407558	-2.008924
H	-1.274959	2.566420	-3.256194

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B3LYP SCF energy: -1325.78815128 a.u.
B3LYP enthalpy: -1325.235781 a.u.
B3LYP free energy: -1325.337660 a.u.
M06 SCF energy in solution: -1326.24510729 a.u.
M06 enthalpy in solution: -1325.692737 a.u.
M06 free energy in solution: -1325.794616 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.062284	1.160862	-0.063066
O	-2.062711	1.752807	0.070926
O	-0.589998	3.354944	-0.330253
N	1.370486	-1.550426	-0.078380
N	-0.821168	-1.687783	-0.242492
C	0.208177	-0.816528	-0.051334
C	1.120775	-2.916872	-0.588281
C	-0.375571	-3.086875	-0.330727
C	2.685863	-0.986409	-0.160022
C	3.764886	-1.626146	0.477078
C	5.045057	-1.068389	0.346987
C	5.271457	0.112309	-0.359810
C	4.167029	0.757165	-0.927906
C	2.870553	0.239630	-0.841959
C	3.596878	-2.846553	1.356091
C	6.662790	0.683900	-0.505730
C	1.705255	1.014752	-1.365348
C	-2.221144	-1.397388	-0.100044
C	-3.006267	-1.274891	-1.258605
C	-4.380582	-1.066535	-1.111738
C	-4.982469	-0.979133	0.146567
C	-4.169422	-1.096124	1.277865
C	-2.791139	-1.304729	1.181488
C	-2.387903	-1.340005	-2.635699
C	-6.475095	-0.784828	0.282780
C	-1.945680	-1.389262	2.429976
C	1.045520	1.364964	1.463910
C	-1.786546	2.986235	-0.151962
C	-2.921421	3.986334	-0.186884
H	1.721335	-3.668199	-0.077868
H	1.361471	-2.952007	-1.660049
H	-0.893889	-3.617774	-1.134000
H	-0.578272	-3.612294	0.613249
H	5.879420	-1.564134	0.839453
H	4.309747	1.699745	-1.452822
H	2.638533	-2.832789	1.886501
H	4.393213	-2.880073	2.106371
H	3.653874	-3.788929	0.793777
H	7.075087	0.480110	-1.503206
H	7.352406	0.252673	0.227657
H	6.665779	1.772059	-0.374067
H	1.248797	0.515713	-2.241400
H	2.019975	2.017122	-1.676909
H	-4.993925	-0.963117	-2.004506
H	-4.617939	-1.016531	2.266128
H	-1.608441	-0.579371	-2.761269
H	-3.145700	-1.174761	-3.407423
H	-1.919439	-2.311972	-2.836844
H	-6.993769	-1.745958	0.401433
H	-6.897232	-0.294283	-0.600589
H	-6.720607	-0.174365	1.158548
H	-1.299225	-0.508533	2.521300
H	-1.292311	-2.269826	2.432645
H	-2.577649	-1.439875	3.321901
H	-2.561839	4.969382	-0.497002
H	-3.371511	4.060014	0.809729
H	-3.702617	3.637511	-0.869949

H	1.341594	0.504254	2.081756
C	1.504385	2.692067	1.995057
H	1.158472	2.836849	3.030358
H	2.605597	2.709127	2.027001
H	1.152681	3.527623	1.385237

TS42

B3LYP SCF energy: -1482.99299768 a.u.
B3LYP enthalpy: -1482.323242 a.u.
B3LYP free energy: -1482.433442 a.u.
M06 SCF energy in solution: -1483.38650292 a.u.
M06 enthalpy in solution: -1482.716747 a.u.
M06 free energy in solution: -1482.826947 a.u.
Imaginary frequency: -178.5623 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.412671	-0.691257	0.051125
O	-1.378423	-3.333067	-1.937669
O	-1.740740	-2.418872	0.098002
N	-0.495372	2.183417	-0.232089
N	1.636445	1.694651	-0.361662
C	0.411984	1.153566	-0.126217
C	0.095290	3.393918	-0.831009
C	1.589332	3.152614	-0.597566
C	-1.897935	1.904053	-0.328629
C	-2.830693	2.691965	0.366684
C	-4.185378	2.352208	0.267969
C	-4.624760	1.246697	-0.470547
C	-3.671670	0.469659	-1.132007
C	-2.303686	0.787624	-1.106399
C	-2.410107	3.853213	1.237789
C	-6.095714	0.911100	-0.561926
C	-1.280234	-0.062627	-1.771829
C	2.915063	1.048831	-0.286618
C	3.447722	0.454388	-1.446836
C	4.714261	-0.131550	-1.369085
C	5.458722	-0.135770	-0.183998
C	4.901777	0.467300	0.947222
C	3.638634	1.070125	0.919389
C	2.664132	0.413434	-2.736885
C	6.835555	-0.756913	-0.138687
C	3.078042	1.708564	2.169808
C	1.193951	-1.676146	0.204510
C	-2.005433	-3.234310	-0.876624
H	-0.264103	4.305722	-0.349566
H	-0.155242	3.443902	-1.899623
H	2.210609	3.424902	-1.455581
H	1.962944	3.693843	0.281312
H	-4.913978	2.954340	0.807356
H	-3.985842	-0.401278	-1.701775
H	-1.471775	3.640886	1.761784
H	-3.177102	4.068834	1.988132
H	-2.261750	4.774930	0.658248
H	-6.543720	1.330648	-1.472815
H	-6.652977	1.313555	0.290744
H	-6.256264	-0.171892	-0.592079
H	-0.601375	0.508658	-2.414008
H	-1.692935	-0.918135	-2.304528
H	5.128051	-0.601308	-2.259015
H	5.462063	0.469087	1.879879
H	1.767843	-0.208472	-2.633081
H	3.273172	0.000777	-3.546564
H	2.327979	1.410994	-3.044140
H	7.588244	-0.084364	-0.571194
H	6.872211	-1.691219	-0.709707
H	7.143276	-0.975426	0.888901
H	2.038664	1.413460	2.346895
H	3.095951	2.804874	2.111621
H	3.666862	1.422686	3.046546
H	2.131191	-1.180004	0.466920
C	-0.707432	-0.428885	2.191805
C	0.298849	-1.447558	2.243015
H	-0.364336	0.574642	2.445671
H	1.290529	-1.097667	2.523427
C	-3.214510	-4.138005	-0.606102
H	-4.109625	-3.527931	-0.436308
H	-3.386001	-4.812063	-1.448384
H	-3.051280	-4.725502	0.305149
C	-0.030382	-2.860975	2.665264
H	-0.822773	-3.278038	2.039691
H	0.845705	-3.513101	2.608702
H	-0.374921	-2.862487	3.709602
C	-2.145596	-0.697781	2.596104
H	-2.787268	0.141721	2.308882
H	-2.533306	-1.600744	2.122899
H	-2.214387	-0.808388	3.689746
C	1.401554	-3.104421	-0.208771
H	0.505023	-3.577727	-0.606961
H	2.163443	-3.099210	-1.003554
H	1.822458	-3.705089	0.611912

TS45

B3LYP SCF energy: -1482.99960790 a.u.
B3LYP enthalpy: -1482.329438 a.u.
B3LYP free energy: -1482.437286 a.u.
M06 SCF energy in solution: -1483.38857176 a.u.
M06 enthalpy in solution: -1482.718402 a.u.
M06 free energy in solution: -1482.826250 a.u.
Imaginary frequency: -240.8078 cm-1

Cartesian coordinates

ATOM	X	Y	Z
O	-0.749536	2.163225	-1.611841
O	0.647076	3.093254	-0.168459
C	1.312564	0.685576	1.753213
C	-0.094326	3.164542	-1.205126
H	1.337679	-0.241951	2.340476
C	-1.540528	1.313101	1.294544
C	-0.565804	1.398294	2.354956
H	-2.105701	0.389109	1.274608
H	-0.585438	0.550442	3.038426
C	-0.157425	4.473510	-1.971213
H	-1.123157	4.578544	-2.472432
H	0.625288	4.479410	-2.739874
H	0.019554	5.321094	-1.303725
Ru	0.302214	0.895986	0.153362
C	0.043803	-1.104010	-0.041831
C	1.531192	0.498165	-1.545720
N	1.130630	-1.944317	-0.166569
N	-1.058494	-1.864891	-0.303138
C	2.693543	-0.272385	-1.020730
H	0.945200	-0.070472	-2.277738
H	1.846094	1.438935	-2.004650
C	0.768696	-3.228694	-0.798998
C	2.477344	-1.471681	-0.300769
C	-0.739701	-3.279897	-0.572137
C	-2.443153	-1.485711	-0.285974
C	4.007828	0.192231	-1.139207
H	1.292142	-4.070384	-0.343276
H	1.028639	-3.198590	-1.866217
C	3.536653	-2.166541	0.298759
H	-1.297107	-3.640149	-1.441542
H	-1.007591	-3.904316	0.290135
C	-3.019396	-0.918361	-1.439073
C	-3.226451	-1.786988	0.845885
C	5.095020	-0.498589	-0.585822
H	4.181616	1.118681	-1.682813
C	4.839175	-1.668270	0.129990
C	3.322335	-3.395585	1.153315
C	-4.388542	-0.629047	-1.417099
C	-2.206974	-0.615307	-2.674747

C	-4.590008	-1.477917	0.816672
C	-2.625973	-2.417086	2.082625
C	6.505676	0.013362	-0.767308
H	5.666111	-2.203700	0.592424
H	2.379952	-3.338690	1.708939
H	4.136063	-3.503169	1.877735
H	3.301278	-4.320647	0.560284
C	-5.189683	-0.892660	-0.302318
H	-4.840199	-0.188814	-2.303789
H	-1.657951	0.325992	-2.559176
H	-2.861876	-0.521943	-3.547175
H	-1.473517	-1.401685	-2.883758
H	-5.196250	-1.697696	1.693275
H	-1.620180	-2.035304	2.284624
H	-2.546272	-3.508460	1.987002
H	-3.249685	-2.217314	2.959436
H	6.863462	-0.158478	-1.791346
H	7.204027	-0.485747	-0.087306
H	6.567855	1.092454	-0.583811
C	-6.658196	-0.536031	-0.301619
H	-6.809736	0.515560	-0.023965
H	-7.219710	-1.146516	0.413388
H	-7.104935	-0.675463	-1.292144
C	-2.374926	2.508998	0.891537
H	-2.836476	2.342706	-0.084205
H	-3.180911	2.656278	1.627923
H	-1.795414	3.432472	0.843076
C	-0.285141	2.738590	3.007806
H	0.469852	2.659815	3.794556
H	0.053558	3.472733	2.272539
H	-1.206079	3.120529	3.469653
C	2.412817	1.636030	2.137287
H	2.508524	1.771942	3.223799
H	3.351131	1.177695	1.788489
H	2.314923	2.608513	1.649171

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B3LYP SCF energy: -1418.13051205 a.u.
B3LYP enthalpy: -1417.556611 a.u.
B3LYP free energy: -1417.648604 a.u.
M06 SCF energy in solution: -1418.59410000 a.u.
M06 enthalpy in solution: -1418.020199 a.u.
M06 free energy in solution: -1418.112192 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.231927	1.041275	0.260103
O	1.396355	2.326795	-0.471499
O	-0.317540	3.329972	0.420464
N	-0.975475	-1.593198	-0.661092
N	1.196050	-1.637910	-0.308484
C	0.090133	-0.854024	-0.251443
C	-0.640014	-3.009845	-0.839176
H	-1.088123	-3.422339	-1.747790
H	-0.989027	-3.603982	0.016739
C	0.897295	-2.956827	-0.906173
H	1.380941	-3.762106	-0.346686
H	1.265226	-2.990515	-1.940316
C	-2.313032	-1.057517	-0.379728
C	-2.827487	-1.569396	0.989158
H	-2.081053	-1.340865	1.757526
H	-2.950630	-2.661367	0.957648
C	-4.170308	-0.897543	1.334925
H	-4.523406	-1.273750	2.304382
C	-5.203290	-1.232932	0.240593
H	-5.373038	-2.318293	0.199030
H	-6.169645	-0.767398	0.477066
C	-4.692800	-0.718561	-1.121305
H	-5.425668	-0.955393	-1.903717
C	-3.352318	-1.415141	-1.466196
H	-2.985903	-1.085028	-2.447308
H	-3.506025	-2.503244	-1.523464
C	-4.499830	0.812020	-1.037312
H	-4.175416	1.210144	-2.008192
H	-5.460268	1.291477	-0.800946
C	-3.448343	1.149890	0.054025
H	-3.304920	2.236332	0.101754
C	-2.129627	0.474307	-0.349190
H	-1.903362	0.790823	-1.395321
C	-3.957631	0.627811	1.412119
H	-3.236813	0.868455	2.202208
H	-4.901841	1.126112	1.671751
C	2.556854	-1.199672	-0.160694
C	3.252701	-1.549323	1.012512
C	4.589205	-1.161151	1.135102
H	5.131077	-1.425830	2.040713
C	5.245101	-0.443101	0.129719
C	4.530650	-0.128114	-1.028408
H	5.025841	0.421301	-1.826355
C	3.190626	-0.492877	-1.199167
C	2.584059	-2.318892	2.127666
H	3.284747	-2.491758	2.950011
H	2.217246	-3.298032	1.795275
H	1.721700	-1.774597	2.527969
C	6.680088	-0.001640	0.300025
H	6.732288	1.017920	0.704205
H	7.215065	0.001709	-0.655849
H	7.222428	-0.655269	0.991447
C	2.468855	-0.098158	-2.466361
H	1.714286	-0.831607	-2.766997
H	3.178100	0.015253	-3.292571
H	1.961408	0.863841	-2.330020
C	-0.246522	0.638564	2.048045
H	0.020467	-0.355705	2.433201
O	1.349556	4.522392	-0.366078
N	0.824119	3.453280	-0.141964
C	-0.520952	1.646367	3.130997
H	-1.326302	1.288653	3.791720
H	0.370895	1.768873	3.765202
H	-0.796917	2.627706	2.736772

TS48

B3LYP SCF energy: -1575.33621703 a.u.
B3LYP enthalpy: -1574.644401 a.u.
B3LYP free energy: -1574.744989 a.u.
M06 SCF energy in solution: -1575.73592476 a.u.
M06 enthalpy in solution: -1575.044109 a.u.
M06 free energy in solution: -1575.144697 a.u.
Imaginary frequency: -230.6816 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.370126	0.817258	0.126153
O	-1.385690	2.790533	0.129317
O	-0.968640	2.096414	-1.888411
N	-0.689752	-2.051467	-0.186845
N	1.469255	-1.805858	0.072307
C	0.284819	-1.119917	-0.039799
C	-0.232750	-3.427913	0.011639
H	-0.646793	-4.103479	-0.742086
H	-0.531762	-3.796838	1.002533
C	1.285916	-3.265055	-0.104826
H	1.839720	-3.821828	0.656197
H	1.660837	-3.572049	-1.090011
C	-2.093885	-1.634255	-0.144454
C	-2.664173	-1.749137	1.290991
H	-2.016874	-1.195681	1.979751
H	-2.666056	-2.801025	1.612680
C	-4.098692	-1.187090	1.328576
H	-4.491572	-1.265336	2.351449
C	-4.986111	-2.005831	0.369024
H	-5.024010	-3.056509	0.691396

H	-6.016888	-1.627245	0.391702
C	-4.420955	-1.905714	-1.062934
H	-5.047987	-2.490993	-1.748664
C	-2.983861	-2.478542	-1.088504
H	-2.573222	-2.443641	-2.106263
H	-3.004746	-3.534041	-0.777001
C	-4.412295	-0.424483	-1.498324
H	-4.048489	-0.330832	-2.530041
H	-5.438837	-0.030822	-1.484054
C	-3.508647	0.400077	-0.543720
H	-3.521022	1.446717	-0.861662
C	-2.083191	-0.176049	-0.638396
H	-1.803309	-0.203179	-1.701575
C	-4.073379	0.291398	0.887146
H	-3.464629	0.886506	1.577428
H	-5.090685	0.705877	0.919095
C	2.803038	-1.309173	-0.110792
C	3.686156	-1.299163	0.984378
C	5.008091	-0.888286	0.773421
H	5.691744	-0.870903	1.619768
C	5.473670	-0.510962	-0.488294
C	4.578549	-0.560503	-1.563354
H	4.925191	-0.284516	-2.557088
C	3.248215	-0.958082	-1.403788
C	3.250485	-1.749918	2.359910
H	3.935144	-1.374819	3.126874
H	3.245784	-2.845703	2.439627
H	2.239616	-1.409416	2.600782
C	6.898067	-0.048241	-0.688346
H	7.296965	-0.385121	-1.651469
H	7.556492	-0.423288	0.101925
H	6.963832	1.047738	-0.676975
C	2.318113	-0.982737	-2.595390
H	1.542792	-0.211252	-2.517685
H	1.798354	-1.942470	-2.694797
H	2.875103	-0.807863	-3.520519
C	-0.126621	0.739911	2.013749
H	0.440536	-0.052095	2.519732
C	1.569268	1.832640	-0.166131
H	2.216268	1.069477	-0.580882
C	1.509359	1.844849	1.274052
H	2.163652	1.113939	1.744287
C	1.416187	3.173895	2.000193
H	1.393747	3.046294	3.085300
H	2.299979	3.779946	1.758220
H	0.531631	3.740584	1.698240
C	1.606658	3.122412	-0.957996
H	2.613120	3.562653	-0.875053
H	1.409397	2.938617	-2.016140
H	0.894345	3.869778	-0.603915
O	-2.058744	3.975447	-1.587492
N	-1.490410	2.986837	-1.146940
C	-0.935183	1.557492	2.991038
H	-1.703638	0.895856	3.417178
H	-0.335942	1.918560	3.838211
H	-1.442398	2.403583	2.521392

TS51

B3LYP SCF energy: -1575.32385084 a.u.
B3LYP enthalpy: -1574.632942 a.u.
B3LYP free energy: -1574.736596 a.u.
M06 SCF energy in solution: -1575.72500829 a.u.
M06 enthalpy in solution: -1575.034099 a.u.
M06 free energy in solution: -1575.137753 a.u.
Imaginary frequency: -132.0763 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.356557	0.712167	-0.006794
O	-2.436106	2.971752	-1.656452
O	-1.538149	2.529159	0.308493
N	-0.463746	-2.170188	0.056308
N	1.674336	-1.749368	0.280005
C	0.444989	-1.168147	0.083309
C	0.081217	-3.472377	0.444971
H	-0.288707	-4.274472	-0.199055
H	-0.189852	-3.713515	1.482495
C	1.587499	-3.227857	0.287764
H	2.181928	-3.645441	1.105560
H	1.972750	-3.634508	-0.656103
C	-1.888641	-1.826636	-0.001877
C	-2.475762	-1.655692	1.424455
H	-1.878778	-0.916746	1.978183
H	-2.405145	-2.604752	1.976561
C	-3.944396	-1.194770	1.338937
H	-4.346546	-1.082128	2.354634
C	-4.760404	-2.255180	0.571788
H	-4.739608	-3.214975	1.108369
H	-5.812215	-1.945749	0.509975
C	-4.178816	-2.424333	-0.847254
H	-4.758758	-3.178524	-1.395888
C	-2.711626	-2.901630	-0.745576
H	-2.287979	-3.060136	-1.746438
H	-2.675856	-3.865857	-0.215310
C	-4.241036	-1.072059	-1.587565
H	-3.857110	-1.182304	-2.611117
H	-5.287082	-0.745158	-1.673257
C	-3.412155	-0.007562	-0.822239
H	-3.464566	0.940863	-1.361060
C	-1.948358	-0.484945	-0.770195
H	-1.614641	-0.684892	-1.799803
C	-4.004610	0.154323	0.593906
H	-3.455354	0.924001	1.148462
H	-5.046466	0.495883	0.527163
C	2.963377	-1.165328	0.032460
C	3.806376	-0.851194	1.113992
C	5.073158	-0.314054	0.843449
H	5.721412	-0.061908	1.680601
C	5.527532	-0.103692	-0.458365
C	4.687266	-0.476376	-1.515419
H	5.033802	-0.349744	-2.539161
C	3.419001	-1.019395	-1.299322
C	3.416347	-1.100790	2.553971
H	3.391729	-0.165993	3.126451
H	4.150153	-1.754191	3.041574
H	2.434236	-1.570086	2.637341
C	6.881523	0.510563	-0.726401
H	7.373495	0.038096	-1.583808
H	7.543571	0.415513	0.140184
H	6.791761	1.580686	-0.955207
C	2.593301	-1.473611	-2.483831
H	1.534317	-1.223905	-2.378427
H	2.661409	-2.561457	-2.618735
H	2.959902	-1.013362	-3.406381
C	0.731475	1.314574	1.850967
H	1.224432	0.399773	2.166432
C	0.879253	1.373480	-1.248289
H	1.843519	0.882863	-1.403797
C	1.466692	2.111496	0.946693
H	2.429241	1.708968	0.642095
C	-0.221581	1.885936	2.885138
H	0.355333	2.298986	3.726652
H	-0.861708	2.668311	2.477401
H	-0.866850	1.100198	3.295482
C	1.320834	3.609441	0.858590
H	1.787351	4.069733	1.742292
H	1.826323	4.014974	-0.022503
H	0.272128	3.910836	0.831138
O	-3.218758	3.894426	0.160466
N	-2.432618	3.148807	-0.424635
C	0.633048	2.499951	-2.203431
H	1.438773	3.247537	-2.137542
H	0.683501	2.088516	-3.224525
H	-0.340030	2.976460	-2.077566

TS51'

B3LYP SCF energy: -1575.33106604 a.u.
B3LYP enthalpy: -1574.639452 a.u.
B3LYP free energy: -1574.739869 a.u.
M06 SCF energy in solution: -1575.72768388 a.u.
M06 enthalpy in solution: -1575.036070 a.u.
M06 free energy in solution: -1575.136487 a.u.
Imaginary frequency: -222.8024 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.302175	0.838066	0.240600
O	1.682970	1.779911	-1.460712
O	1.324859	2.812916	0.415815
N	0.741569	-1.982720	-0.280391
N	-1.420373	-1.738717	-0.526054
C	-0.261742	-1.075249	-0.190977
C	0.336519	-3.255700	-0.881743
H	0.759227	-4.108510	-0.343832
H	0.668912	-3.311599	-1.927162
C	-1.189507	-3.178532	-0.769399
H	-1.706197	-3.505915	-1.676568
H	-1.571431	-3.770638	0.072932
C	2.137775	-1.575457	-0.087754
C	2.859792	-1.379763	-1.445159
H	2.315447	-0.640620	-2.042779
H	2.866952	-2.327181	-2.004328
C	4.309452	-0.904665	-1.205636
H	4.811173	-0.787145	-2.175226
C	5.065878	-1.940352	-0.351494
H	5.116580	-2.908418	-0.871011
H	6.100713	-1.608528	-0.191724
C	4.346539	-2.103123	1.002787
H	4.884847	-2.832238	1.623420
C	2.916400	-2.627260	0.741989
H	2.387614	-2.805936	1.688180
H	2.974995	-3.590402	0.212272
C	4.295567	-0.739690	1.730030
H	3.816256	-0.854351	2.712267
H	5.319202	-0.383149	1.913663
C	3.515809	0.292189	0.866674
H	3.486143	1.254830	1.390623
C	2.080503	-0.258415	0.705682
H	1.745332	-0.523964	1.721169
C	4.280318	0.447156	-0.467491
H	3.826845	1.205563	-1.105239
H	5.308591	0.773856	-0.256651
C	-2.772246	-1.323644	-0.287254
C	-3.568151	-0.904835	-1.371604
C	-4.891489	-0.521386	-1.123512
H	-5.501291	-0.180412	-1.957916
C	-5.450155	-0.568712	0.155727
C	-4.655998	-1.051861	1.201746
H	-5.083549	-1.134377	2.199340
C	-3.330735	-1.451661	1.004186
C	-3.054204	-0.903442	-2.794404
H	-3.405959	-0.021260	-3.339858
H	-3.424702	-1.783696	-3.337249
H	-1.963236	-0.922962	-2.838567
C	-6.867735	-0.109790	0.406681
H	-6.890505	0.929063	0.761649
H	-7.358551	-0.722746	1.170591
H	-7.471180	-0.156050	-0.505613
C	-2.571647	-2.079199	2.154383
H	-1.491139	-1.945482	2.071672
H	-2.768921	-3.159156	2.199544
H	-2.894831	-1.658064	3.111977
C	-1.284116	1.775468	-1.010057
H	-1.711524	0.932112	-1.540501
C	-0.743433	0.978412	1.820862
H	-1.558169	0.307264	2.103264
C	-1.840179	2.016761	0.288665
H	-2.665018	1.360928	0.554511
C	-0.910384	2.918860	-1.929521
H	-1.829770	3.354237	-2.352208
H	-0.375050	3.724135	-1.422151
H	-0.292063	2.571010	-2.759259
C	-1.945974	3.433104	0.818361
H	-2.612445	4.016490	0.167620
H	-2.367630	3.459974	1.826643
H	-0.975135	3.934884	0.835000
O	2.670924	3.698809	-1.073679
N	1.923521	2.796702	-0.727922
C	-0.343550	1.890263	2.952223
H	-1.204246	2.362078	3.446778
H	0.147074	1.261707	3.712628
H	0.368043	2.662959	2.650907

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B3LYP SCF energy: -1979.03579316 a.u.
B3LYP enthalpy: -1978.551488 a.u.
B3LYP free energy: -1978.649665 a.u.
M06 SCF energy in solution: -1979.58117039 a.u.
M06 enthalpy in solution: -1979.096865 a.u.
M06 free energy in solution: -1979.195042 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.163661	1.021805	0.969125
C	2.396457	-0.159366	0.921406
C	2.994960	-1.409336	0.657211
C	4.351840	-1.435114	0.327762
C	5.124464	-0.270579	0.276253
C	4.517098	0.939149	0.620941
N	1.003054	-0.134422	1.291474
C	0.631194	-0.228385	2.715813
C	-0.881452	-0.462876	2.649051
N	-1.194131	-0.160668	1.237663
C	-0.079608	-0.023478	0.473505
C	-2.568769	-0.220780	0.829150
C	-3.357536	0.941938	0.916546
C	-4.707935	0.847519	0.568170
C	-5.284377	-0.358222	0.151148
C	-4.470693	-1.493180	0.084632
C	-3.112381	-1.452686	0.422120
Ru	0.107756	0.426227	-1.444476
Cl	1.083706	-1.555657	-2.303637
C	-2.765520	2.261897	1.349543
C	-6.751169	-0.427011	-0.205915
C	-2.259726	-2.694457	0.299942
C	2.220700	-2.701619	0.762915
C	6.576413	-0.321234	-0.136860
C	2.601995	2.335648	1.458379
Cl	0.207425	2.776786	-1.100361
C	-1.566559	0.251972	-2.101779
H	1.172192	-1.047188	3.197991
H	0.887038	0.704226	3.231927
H	-1.446825	0.197984	3.311954
H	-1.159214	-1.498258	2.881736
H	-2.478035	-0.080486	-1.608494
H	-1.658939	0.513966	-3.169843
H	-5.324713	1.742153	0.622422
H	-4.900238	-2.437965	-0.240898
H	4.816975	-2.393296	0.107809
H	5.112877	1.849120	0.636462
H	3.280874	3.156712	1.209631
H	1.630401	2.565719	1.018108
H	2.491952	2.327859	2.552122
H	2.889371	-3.556804	0.627413
H	1.741887	-2.809219	1.744737
H	1.441925	-2.761377	-0.001905

H	7.157534	0.477801	0.335897
H	7.035570	-1.279975	0.126809
H	6.678097	-0.199545	-1.223317
H	-2.867253	-3.547016	-0.017304
H	-1.456538	-2.560243	-0.433996
H	-1.784821	-2.965062	1.250905
H	-3.528946	3.045471	1.343903
H	-2.354130	2.209571	2.365901
H	-1.950074	2.571899	0.686780
H	-7.014950	-1.400654	-0.630191
H	-7.382586	-0.266623	0.677336
H	-7.020729	0.344044	-0.937288

TS53

B3LYP SCF energy: -2136.26989020 a.u.
B3LYP enthalpy: -2135.667767 a.u.
B3LYP free energy: -2135.774037 a.u.
M06 SCF energy in solution: -2136.73685495 a.u.
M06 enthalpy in solution: -2136.134732 a.u.
M06 free energy in solution: -2136.241002 a.u.
Imaginary frequency: -207.2349 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	0.922005	-1.810967	0.303030
C	0.509894	-3.187878	0.645999
H	0.956748	-3.904591	-0.049333
C	-1.021316	-3.116264	0.530718
N	-1.268610	-1.676166	0.293126
H	-1.531582	-3.442960	1.441374
C	2.316964	-1.459682	0.209008
C	-2.624808	-1.204980	0.178569
C	-5.302273	-0.392433	-0.020376
C	-3.323841	-0.844806	1.347424
C	-3.255776	-1.217451	-1.080452
C	-4.589226	-0.798013	-1.151919
C	-4.655500	-0.436385	1.218487
C	-2.678045	-0.895664	2.710746
C	-2.542541	-1.674603	-2.330126
H	-5.083621	-0.799332	-2.121039
H	-5.201573	-0.151103	2.115231
C	-6.731420	0.085976	-0.132066
C	5.047036	-0.835063	0.020916
C	2.982829	-1.633413	-1.023388
C	3.015101	-1.063097	1.368729
C	4.372156	-0.742358	1.241338
C	4.339519	-1.301926	-1.091237
C	2.282914	-2.190955	-2.238775
C	2.358448	-1.013783	2.727280
H	4.916781	-0.427737	2.128877
H	4.857622	-1.423264	-2.039998
C	6.503146	-0.448920	-0.094200
H	-2.295298	-1.897341	2.945055
H	-1.836695	-0.197644	2.777933
H	-2.128149	-2.684340	-2.217357
H	-1.711449	-1.009340	-2.589406
H	-7.229743	-0.339811	-1.009354
H	-6.776436	1.178930	-0.230155
H	-7.315231	-0.182667	0.755105
H	1.934467	-1.987096	3.005264
H	1.549667	-0.277049	2.762741
H	2.993360	-2.315192	-3.061583
H	1.482851	-1.526097	-2.578349
H	7.030197	-1.082051	-0.816286
H	7.017494	-0.529246	0.869173
H	6.609871	0.589212	-0.435918
C	-0.126819	-0.975116	0.141501
Ru	0.093226	1.044919	-0.242199
Cl	-0.049573	1.551650	2.167294
Cl	0.228979	0.674448	-2.677464
C	-1.481483	1.972292	-0.506050
H	3.093419	-0.748162	3.493252
H	1.840652	-3.174577	-2.035088
H	-3.236355	-1.698775	-3.176083
H	-3.404301	-0.633568	3.486230
H	-1.409877	-3.705526	-0.307117
H	0.844781	-3.440673	1.657985
C	0.169774	3.414985	-0.776080
C	1.426979	2.762710	-0.633067
H	-1.960171	2.019933	-1.487948
H	-0.174192	3.494868	-1.804901
H	1.869112	2.422099	-1.567860
C	2.417781	3.077671	0.463211
H	3.093453	2.232044	0.630007
H	3.037453	3.931025	0.146008
H	1.939544	3.320154	1.411805
C	-0.290413	4.492294	0.183038
H	-1.304911	4.828774	-0.048826
H	-0.263498	4.145674	1.218998
H	0.378100	5.359662	0.094345
H	-2.022558	2.406750	0.338375

TS55

B3LYP SCF energy: -2136.27474827 a.u.
B3LYP enthalpy: -2135.672171 a.u.
B3LYP free energy: -2135.776932 a.u.
M06 SCF energy in solution: -2136.74259784 a.u.
M06 enthalpy in solution: -2136.140021 a.u.
M06 free energy in solution: -2136.244782 a.u.
Imaginary frequency: -201.6078 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	1.190152	-1.700208	0.288075
C	0.883281	-3.110443	0.610847
H	1.424343	-3.781557	-0.061908
C	-0.639320	-3.171916	0.423059
N	-1.001954	-1.748365	0.242847
H	-1.159446	-3.589801	1.289314
C	2.560064	-1.254344	0.210254
C	-2.389357	-1.387878	0.116517
C	-5.128549	-0.824821	-0.104431
C	-3.141172	-1.159284	1.285224
C	-2.989682	-1.382868	-1.157896
C	-4.355323	-1.087962	-1.239742
C	-4.504639	-0.875512	1.146227
C	-2.515010	-1.215948	2.657847
C	-2.207166	-1.695364	-2.410796
H	-4.827288	-1.077787	-2.219907
H	-5.092868	-0.694112	2.043205
C	-6.596440	-0.486379	-0.227006
C	5.245150	-0.455627	0.046090
C	3.243858	-1.376796	-1.017980
C	3.224480	-0.827505	1.378282
C	4.558803	-0.419458	1.262346
C	4.576317	-0.958223	-1.074429
C	2.591128	-1.975798	-2.239964
C	2.562787	-0.841318	2.735229
H	5.076486	-0.077940	2.156034
H	5.106642	-1.036978	-2.020945
C	6.672855	0.027750	-0.056796
H	-2.078852	-2.201252	2.867592
H	-1.716229	-0.473580	2.761620
H	-1.713063	-2.673148	-2.347685
H	-1.426277	-0.950354	-2.600828
H	-6.745239	0.594247	-0.354260
H	-7.153212	-0.787202	0.666768
H	-7.050426	-0.979545	-1.093184
H	2.214961	-1.847523	3.002610
H	1.699441	-0.170263	2.777969
H	3.302674	-2.013003	-3.070250
H	1.728183	-1.385483	-2.560254

H	7.245020	-0.561565	-0.781732
H	7.186308	-0.027403	0.908866
H	6.711233	1.073972	-0.388178
C	0.078968	-0.949896	0.127817
Ru	0.108686	1.108139	-0.194142
Cl	-0.065890	1.500159	2.233963
Cl	0.469225	0.822540	-2.618864
C	-1.467873	2.028804	-0.641328
H	3.274160	-0.528136	3.505458
H	2.251512	-3.003159	-2.053646
H	-2.872990	-1.720351	-3.278876
H	-3.267075	-1.021494	3.428545
H	-0.933837	-3.747138	-0.462233
H	1.189970	-3.334942	1.638495
C	0.132202	3.454668	-0.627830
C	1.376483	2.795639	-0.350736
H	-1.686747	2.067565	-1.713946
H	-0.054031	3.629739	-1.685811
H	2.046748	2.585041	-1.179827
C	-2.612962	2.432430	0.235106
H	-3.101878	3.338137	-0.150837
H	-3.355759	1.624153	0.176664
H	-2.337682	2.563672	1.281141
C	-0.367402	4.510362	0.336484
H	-1.386311	4.837165	0.114093
H	-0.323285	4.149459	1.367360
H	0.285642	5.388831	0.252355
H	1.833997	2.973885	0.620983
H	-1.441268	-2.932519	1.574226
H	5.215934	-1.684599	1.570512
H	4.181623	0.491469	-1.976476
H	1.806355	-2.222346	2.658922
H	3.525646	-2.411201	3.037671
H	2.704002	-3.630056	2.067108
H	6.830031	-0.810761	-1.144904
H	6.878358	-0.249837	0.530244
H	6.412549	0.862458	-0.768850
H	0.970739	-0.888257	-2.459134
H	1.939370	0.582982	-2.765594
H	-5.583235	-0.775862	-1.625610
H	-4.616726	1.036440	2.138007
H	-2.234519	-1.639301	-2.526704
H	-3.952403	-1.859868	-2.912278
H	-3.117995	-3.024834	-1.883599
H	-7.352526	0.027194	0.824872
H	-7.070782	0.987486	-0.629590
H	-6.699100	1.662279	0.966507
H	-1.345947	0.973983	2.082793
H	-1.486176	-0.688088	2.644468
H	-2.609009	0.539235	3.249040
H	-1.006371	2.359838	-2.193945
H	-1.998863	0.866797	-1.721849
H	0.615458	4.748206	2.023307
H	2.270215	4.143832	2.109855
H	1.798785	5.227212	0.767379

56

B3LYP SCF energy: -1286.47272499 a.u.
B3LYP enthalpy: -1285.949811 a.u.
B3LYP free energy: -1286.045471 a.u.
M06 SCF energy in solution: -1286.94855166 a.u.
M06 enthalpy in solution: -1286.425638 a.u.
M06 free energy in solution: -1286.521298 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.376970	1.011158	-0.587893
O	0.604373	2.177692	1.228031
O	1.191128	3.189027	-0.650484
N	0.812205	-1.708100	0.232829
N	-1.367956	-1.465660	0.045576
C	-0.183683	-0.801666	-0.050027
C	0.305157	-3.089594	0.253315
C	-1.186613	-2.856486	0.507762
C	2.193015	-1.364752	0.066110
C	3.145506	-1.767015	1.019762
C	4.477177	-1.376230	0.833395
C	4.877523	-0.570385	-0.236493
C	3.902005	-0.150827	-1.144283
C	2.561963	-0.549791	-1.036239
C	2.771368	-2.550019	2.257148
C	6.324125	-0.169154	-0.410836
C	1.521663	-0.066341	-1.991317
C	-2.673148	-0.872889	0.121024
C	-3.591000	-1.133665	-0.915078
C	-4.874627	-0.589114	-0.821177
C	-5.265505	0.195311	0.269174
C	-4.331315	0.428816	1.281699
C	-3.033985	-0.095515	1.237638
C	-3.201673	-1.955976	-2.122104
C	-6.668087	0.750445	0.361134
C	-2.067422	0.196780	2.361438
C	-1.058325	1.416684	-1.629377
C	1.069184	3.206810	0.601783
C	1.465648	4.416456	1.417906
H	0.772480	-3.693474	1.032347
H	0.487258	-3.573003	-0.717049
H	-1.828033	-3.545095	-0.047736

TS57

B3LYP SCF energy: -1443.67459973 a.u.
B3LYP enthalpy: -1443.035410 a.u.
B3LYP free energy: -1443.143404 a.u.
M06 SCF energy in solution: -1444.08729563 a.u.
M06 enthalpy in solution: -1443.448106 a.u.
M06 free energy in solution: -1443.556100 a.u.
Imaginary frequency: -126.6487 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.421739	0.729941	0.015832
O	1.030305	3.403305	-1.968168
O	1.651058	2.513307	0.020579
N	0.473114	-2.140061	-0.241117
N	-1.654116	-1.632090	-0.375992
C	-0.426565	-1.103040	-0.136966
C	-0.126049	-3.345331	-0.841864
C	-1.619461	-3.090763	-0.607941
C	1.875837	-1.855845	-0.323304
C	2.800245	-2.634662	0.396550
C	4.154202	-2.291741	0.320796
C	4.605096	-1.190429	-0.419260
C	3.662981	-0.423449	-1.105233
C	2.294541	-0.746668	-1.106467
C	2.364774	-3.790498	1.267286
C	6.077022	-0.853153	-0.484116
C	1.287695	0.102240	-1.798280
C	-2.920591	-0.966577	-0.273145
C	-3.484897	-0.395372	-1.430240
C	-4.737370	0.215172	-1.324394
C	-5.436184	0.269451	-0.112569
C	-4.847965	-0.309700	1.015078
C	-3.598179	-0.938467	0.958391
C	-2.742611	-0.398994	-2.745093
C	-6.796915	0.922164	-0.035524
C	-3.008211	-1.563127	2.202266
C	-1.094233	1.787395	-0.088440
C	1.716381	3.387339	-0.943225
H	0.224946	-4.261059	-0.361077
H	0.122889	-3.396975	-1.910782
H	-2.242861	-3.362340	-1.464664
H	-1.996416	-3.626499	0.273216

H	4.874241	-2.886513	0.879639
H	3.984026	0.445312	-1.674327
H	1.422367	-3.570655	1.780864
H	3.123279	-4.009176	2.025282
H	2.215225	-4.712439	0.688547
H	6.234112	0.223346	-0.608166
H	6.562200	-1.353148	-1.333318
H	6.602160	-1.171264	0.423101
H	0.608011	-0.468192	-2.439428
H	1.715603	0.945325	-2.338141
H	-5.174543	0.668131	-2.211819
H	-5.373669	-0.274535	1.967020
H	-1.825477	0.197093	-2.677129
H	-3.363879	0.021265	-3.541380
H	-2.447808	-1.410995	-3.047927
H	-7.569984	0.281425	-0.479862
H	-6.815546	1.873161	-0.579675
H	-7.088881	1.119472	1.000819
H	-1.962289	-1.274195	2.346898
H	-3.035586	-2.659922	2.158761
H	-3.570886	-1.261065	3.090723
H	-2.133251	1.463742	0.019168
C	0.682994	0.604483	2.286841
C	-0.337712	1.560784	2.262031
H	0.377791	-0.419369	2.497365
H	-1.353141	1.194580	2.390159
C	2.763546	4.481385	-0.695625
H	3.740356	4.035146	-0.477003
H	2.842808	5.137154	-1.565678
H	2.481432	5.079024	0.180088
C	-0.112729	3.026984	2.537046
H	0.712875	3.410072	1.932884
H	-1.009229	3.615859	2.322950
H	0.136895	3.168188	3.599168
C	2.123402	0.928824	2.629703
H	2.785254	0.109566	2.330388
H	2.459988	1.837565	2.127680
H	2.231644	1.059268	3.717476
H	-0.949321	2.857954	-0.263755

TS60

B3LYP SCF energy: -1443.68952604 a.u.
B3LYP enthalpy: -1443.049442 a.u.
B3LYP free energy: -1443.155367 a.u.
M06 SCF energy in solution: -1444.09586616 a.u.
M06 enthalpy in solution: -1443.455782 a.u.
M06 free energy in solution: -1443.561707 a.u.
Imaginary frequency: -231.1418 cm-1

Cartesian coordinates

ATOM	X	Y	Z
O	-0.759744	2.648139	-0.879667
O	0.535443	3.190709	0.832189
C	1.146077	0.396829	2.147738
C	-0.173006	3.519454	-0.178825
H	1.114824	-0.637121	2.516458
C	-1.629108	1.244086	1.580581
C	-0.835662	0.977332	2.740458
H	-1.932577	2.274648	1.412645
H	-2.341133	0.500880	1.247346
H	-0.963651	-0.012260	3.176703
C	-0.275161	4.989183	-0.546097
H	0.627624	5.288971	-1.092198
H	-0.334604	5.605252	0.355932
H	-1.142563	5.168378	-1.185721
Ru	0.262632	0.980941	0.566760
C	0.049377	-0.917414	-0.108416
C	1.560280	1.031272	-1.118463
N	1.153930	-1.684464	-0.412535
N	-1.033323	-1.610495	-0.562151
C	2.715505	0.162447	-0.758818
H	1.004962	0.658054	-1.987616
H	1.872856	2.059844	-1.314613
C	0.825709	-2.776406	-1.350481
C	2.495576	-1.182126	-0.375371
C	-0.682783	-2.912419	-1.160324
C	-2.424096	-1.283382	-0.428081
C	4.024234	0.654175	-0.703354
H	1.365357	-3.694717	-1.115210
H	1.089371	-2.473109	-2.373165
C	3.545913	-1.995914	0.071353
H	-1.226242	-3.064167	-2.097281
H	-0.942009	-3.731202	-0.476359
C	-3.038583	-0.470974	-1.400353
C	-3.168954	-1.853111	0.622759
C	5.103705	-0.144862	-0.302375
H	4.199925	1.689797	-0.987240
C	4.844175	-1.460097	0.083262
C	3.324916	-3.401628	0.583020
C	-4.410516	-0.224184	-1.280902
C	-2.256453	0.149005	-2.532506
C	-4.537454	-1.573762	0.698102
C	-2.525208	-2.738296	1.666156
C	6.509667	0.410261	-0.291499
H	5.663925	-2.087896	0.426922
H	2.362952	-3.494443	1.098763
H	4.114685	-3.678873	1.288619
H	3.341953	-4.149704	-0.221909
C	-5.176624	-0.758237	-0.240447
H	-4.892036	0.405373	-2.026282
H	-1.713535	1.036310	-2.186645
H	-2.930252	0.455925	-3.338934
H	-1.520221	-0.546125	-2.950776
H	-5.115843	-2.002453	1.514179
H	-1.519407	-2.394142	1.926629
H	-2.433970	-3.776630	1.319676
H	-3.127200	-2.758050	2.579944
H	6.893880	0.543087	-1.311635
H	7.200100	-0.256210	0.235947
H	6.549413	1.391943	0.195257
C	-6.649609	-0.441903	-0.121606
H	-7.183061	-1.216138	0.439815
H	-7.120382	-0.350735	-1.106573
H	-6.808351	0.510113	0.402135
C	-0.590666	2.102763	3.727197
H	0.160480	1.852124	4.480940
H	-0.276559	3.008308	3.200940
H	-1.528044	2.320499	4.257015
C	2.196238	1.227957	2.830578
H	2.209180	1.099933	3.922231
H	3.167934	0.869792	2.456168
H	2.114765	2.289229	2.583577

E-butene

B3LYP SCF energy: -157.22387052 a.u.
B3LYP enthalpy: -157.108916 a.u.
B3LYP free energy: -157.142690 a.u.
M06 SCF energy in solution: -157.13351694 a.u.
M06 enthalpy in solution: -157.018562 a.u.
M06 free energy in solution: -157.052336 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.538154	-0.395563	0.000045
H	-0.392445	-1.477890	-0.000051
C	0.538151	0.395548	0.000018
H	0.392391	1.477873	-0.000028
C	-1.963802	0.079262	-0.000030
H	-2.508227	-0.289062	-0.880482
H	-2.508226	-0.289044	0.880481
H	-2.022894	1.173244	0.000016
C	1.963808	-0.079246	-0.000013

H	2.022921	-1.173239	-0.000229
H	2.508268	0.289234	-0.880395
H	2.508194	0.288879	0.880568

ethylene

B3LYP SCF energy: -78.58582485 a.u.
B3LYP enthalpy: -78.530604 a.u.
B3LYP free energy: -78.555465 a.u.
M06 SCF energy in solution: -78.53967110 a.u.
M06 enthalpy in solution: -78.484450 a.u.
M06 free energy in solution: -78.509311 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	0.665610
H	0.000000	0.923760	1.239622
H	0.000000	-0.923760	1.239622
C	0.000000	0.000000	-0.665610
H	0.000000	-0.923760	-1.239622
H	0.000000	0.923760	-1.239622

propene

B3LYP SCF energy: -117.90521904 a.u.
B3LYP enthalpy: -117.820087 a.u.
B3LYP free energy: -117.850105 a.u.
M06 SCF energy in solution: -117.83720744 a.u.
M06 enthalpy in solution: -117.752075 a.u.
M06 free energy in solution: -117.782093 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.139458	-0.504279	0.000000
H	0.779347	-1.538748	0.000000
H	1.781316	-0.366166	0.880645
H	1.781316	-0.366166	-0.880645
C	0.000000	0.475026	0.000000
H	0.277926	1.530165	0.000000
C	-1.293406	0.149794	0.000000
H	-1.621773	-0.887951	0.000000
H	-2.074446	0.905621	0.000000

Z-butene

B3LYP SCF energy: -157.22172615 a.u.
B3LYP enthalpy: -157.106612 a.u.
B3LYP free energy: -157.140805 a.u.
M06 SCF energy in solution: -157.13186478 a.u.
M06 enthalpy in solution: -157.016751 a.u.
M06 free energy in solution: -157.050944 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.669341	0.664333	0.000017
H	-1.169678	1.633564	-0.000021
C	0.669331	0.664372	0.000011
H	1.169571	1.633649	-0.000063
C	-1.593233	-0.521956	-0.000003
H	-2.250579	-0.505579	-0.880214
H	-1.060367	-1.476899	0.000055
H	-2.250674	-0.505532	0.880113
C	1.593246	-0.521949	0.000000
H	1.060349	-1.476859	0.000189
H	2.250550	-0.505677	-0.880247
H	2.250810	-0.505469	0.880041

23-mono

B3LYP SCF energy: -1536.03380584 a.u.
B3LYP enthalpy: -1535.369804 a.u.
B3LYP free energy: -1535.467919 a.u.
M06 SCF energy in solution: -1536.45382313 a.u.
M06 enthalpy in solution: -1535.789821 a.u.
M06 free energy in solution: -1535.887936 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.433569	0.803673	0.203201
O	-1.497047	2.507263	-1.643022
O	-1.465675	2.692377	0.535121
N	-0.646777	-2.053470	-0.180673
N	1.506822	-1.764092	0.066336
C	0.308479	-1.103782	-0.019586
C	-0.163013	-3.422013	0.008730
H	-0.568969	-4.102708	-0.744695
H	-0.445125	-3.800904	1.000899
C	1.351539	-3.225791	-0.120687
H	1.923546	-3.776159	0.631339
H	1.722979	-3.518301	-1.111366
C	-2.050880	-1.648581	-0.108192
C	-2.574496	-1.713603	1.351999
H	-1.915671	-1.121824	1.999966
H	-2.542608	-2.752136	1.712201
C	-4.016354	-1.174427	1.418790
H	-4.373490	-1.227230	2.455743
C	-4.920351	-2.036282	0.513572
H	-4.933716	-3.076276	0.870299
H	-5.954985	-1.670763	0.556240
C	-4.402625	-1.976871	-0.938705
H	-5.043817	-2.590335	-1.585335
C	-2.960625	-2.530014	-0.995837
H	-2.584819	-2.522969	-2.027621
H	-2.950080	-3.573736	-0.647823
C	-4.419458	-0.512705	-1.422354
H	-4.082135	-0.449146	-2.465400
H	-5.446820	-0.123432	-1.394494
C	-3.505821	0.357954	-0.517161
H	-3.536751	1.385593	-0.882417
C	-2.077931	-0.200333	-0.632990
H	-1.767710	-0.197599	-1.688789
C	-4.026177	0.289245	0.933084
H	-3.404476	0.916858	1.583082
H	-5.046680	0.692904	0.980711
C	2.830355	-1.233943	-0.106652
C	3.708105	-1.204960	0.992712
C	5.015673	-0.745515	0.791287
H	5.693922	-0.710991	1.641364
C	5.473371	-0.339619	-0.464414
C	4.587683	-0.417479	-1.545347
H	4.930025	-0.123816	-2.535445
C	3.271883	-0.864060	-1.395511
C	3.285620	-1.687245	2.361305
H	3.952337	-1.293821	3.134654
H	3.325421	-2.783277	2.427731
H	2.262337	-1.388988	2.602831
C	6.878796	0.182473	-0.651612
H	6.902837	1.279097	-0.601244
H	7.286251	-0.104933	-1.626946
H	7.553800	-0.194500	0.123620
C	2.354332	-0.925786	-2.595827
H	1.902661	-1.916841	-2.719784
H	2.905523	-0.695333	-3.512107
H	1.528714	-0.210199	-2.510442
C	0.262675	0.942326	2.056745
C	1.309731	1.782392	-0.239509
C	1.408132	1.800359	1.342879
H	0.658615	0.082452	2.599841
H	-0.375417	1.566099	2.691062
H	2.330967	1.251645	1.554219
H	2.059090	1.112102	-0.650044
C	1.456426	3.208879	1.948928

H	1.635603	3.140578	3.027809
H	2.261415	3.808173	1.509443
H	0.508068	3.730794	1.793796
C	1.331789	3.101580	-0.984250
H	2.353711	3.512152	-0.965882
H	1.058503	2.948837	-2.032061
H	0.663615	3.856140	-0.568055
N	-1.811077	3.177678	-0.626137
O	-2.413973	4.243757	-0.676197

24-mono

B3LYP SCF energy: -1536.03471628 a.u.
B3LYP enthalpy: -1535.370905 a.u.
B3LYP free energy: -1535.468727 a.u.
M06 SCF energy in solution: -1536.45385846 a.u.
M06 enthalpy in solution: -1535.790047 a.u.
M06 free energy in solution: -1535.887869 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.332880	0.865344	-0.173476
O	-1.772311	2.154169	1.761104
O	-1.245855	2.867225	-0.237983
N	-0.695674	-2.016420	-0.204171
N	1.467367	-1.778888	-0.013413
C	0.292275	-1.086998	-0.105072
C	-0.239922	-3.394924	-0.004610
H	-0.659347	-4.069237	-0.756601
H	-0.534866	-3.763594	0.987014
C	1.280924	-3.239898	-0.133013
H	1.835432	-3.765172	0.650150
H	1.651734	-3.589862	-1.105200
C	-2.095007	-1.602464	-0.115375
C	-2.646338	-1.792583	1.323122
H	-2.008878	-1.243787	2.027453
H	-2.607154	-2.856484	1.597188
C	-4.098526	-1.279358	1.405904
H	-4.474930	-1.438682	2.424788
C	-4.978540	-2.048633	0.400616
H	-4.992225	-3.121285	0.642146
H	-6.015853	-1.693753	0.463658
C	-4.432997	-1.832939	-1.026084
H	-5.060505	-2.370988	-1.748851
C	-2.993395	-2.387119	-1.104061
H	-2.589852	-2.285463	-2.120444
H	-2.996813	-3.459392	-0.858680
C	-4.436306	-0.324841	-1.357258
H	-4.077840	-0.160817	-2.382971
H	-5.462443	0.065029	-1.311803
C	-3.541026	0.443465	-0.343251
H	-3.545353	1.508989	-0.593043
C	-2.120924	-0.118036	-0.492790
H	-1.821129	-0.019864	-1.565840
C	-4.113565	0.223512	1.073043
H	-3.530391	0.789249	1.803167
H	-5.143700	0.603813	1.110042
C	2.802177	-1.274525	0.123028
C	3.315229	-1.063007	1.421302
C	4.625329	-0.598488	1.552902
H	5.020276	-0.419420	2.550761
C	5.445707	-0.368954	0.440653
C	4.929407	-0.648575	-0.825624
H	5.560713	-0.506430	-1.700642
C	3.620544	-1.115090	-1.009789
C	2.494224	-1.378463	2.651741
H	2.986539	-0.999980	3.552402
H	2.373903	-2.463221	2.776456
H	1.489746	-0.948781	2.605462
C	6.847189	0.168933	0.612193
H	6.836227	1.254291	0.777246
H	7.461195	-0.021784	-0.273795
H	7.346876	-0.283155	1.476208
C	3.159174	-1.479492	-2.403788
H	3.559494	-2.459068	-2.698593
H	3.520866	-0.753551	-3.139775
H	2.071131	-1.528095	-2.483056
C	0.985475	1.393025	-1.590352
C	1.741296	2.045438	-0.323586
C	1.072955	1.645705	1.041835
H	1.602351	0.596459	-2.004773
H	2.716841	1.551261	-0.324997
H	1.688834	0.989741	1.650703
H	0.703104	2.499320	1.610234
C	0.490406	2.315667	-2.693136
H	1.328806	2.822488	-3.194315
H	-0.026601	1.724298	-3.459457
H	-0.200904	3.078468	-2.328137
O	-2.427249	4.133228	1.094943
N	-1.840328	3.074304	0.905863
C	1.901552	3.568194	-0.426720
H	2.506708	3.933932	0.410508
H	2.405375	3.856157	-1.356174
H	0.929215	4.065967	-0.388948

30-mono

B3LYP SCF energy: -1496.72425741 a.u.
B3LYP enthalpy: -1496.090256 a.u.
B3LYP free energy: -1496.185918 a.u.
M06 SCF energy in solution: -1497.16342619 a.u.
M06 enthalpy in solution: -1496.529425 a.u.
M06 free energy in solution: -1496.625087 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.308622	0.947510	-0.204367
O	-1.784914	2.234515	1.690059
O	-1.258102	2.926264	-0.316010
N	-0.582577	-1.943942	-0.150158
N	1.572447	-1.629960	0.027371
C	0.374828	-0.981331	-0.083633
C	-0.081503	-3.299102	0.095489
H	-0.481514	-4.013086	-0.629967
H	-0.360362	-3.641407	1.101127
C	1.433344	-3.099351	-0.045582
H	2.007551	-3.582011	0.750629
H	1.811191	-3.467430	-1.008376
C	-1.994713	-1.569994	-0.078993
C	-2.545960	-1.728840	1.362876
H	-1.928664	-1.137438	2.050528
H	-2.475859	-2.781364	1.672519
C	-4.013673	-1.257296	1.423136
H	-4.390016	-1.394416	2.445260
C	-4.865294	-2.085497	0.440367
H	-4.847523	-3.149638	0.716826
H	-5.913231	-1.760733	0.487958
C	-4.319897	-1.900226	-0.990548
H	-4.927800	-2.480022	-1.697619
C	-2.864170	-2.414083	-1.044206
H	-2.458660	-2.334614	-2.061789
H	-2.837070	-3.477196	-0.762895
C	-4.366517	-0.404374	-1.371172
H	-4.007966	-0.263265	-2.400241
H	-5.404378	-0.045067	-1.342747
C	-3.500132	0.423775	-0.379648
H	-3.535761	1.480128	-0.664278
C	-2.062952	-0.099549	-0.506349
H	-1.763994	-0.030511	-1.581040
C	-4.072310	0.232769	1.040829
H	-3.509955	0.839362	1.754186
H	-5.113604	0.582834	1.061876
C	2.888868	-1.072287	0.132388
C	3.408317	-0.802685	1.417517

C	4.698991	-0.280181	1.518951
H	5.097633	-0.055965	2.506177
C	5.495446	-0.047783	0.389808
C	4.976115	-0.384671	-0.861120
H	5.590475	-0.241437	-1.747944
C	3.686248	-0.911678	-1.014881
C	2.615826	-1.116119	2.667131
H	3.094972	-0.679758	3.548510
H	2.554783	-2.200503	2.832071
H	1.589545	-0.742142	2.615899
C	6.875317	0.551929	0.528454
H	6.820054	1.634016	0.705230
H	7.472612	0.396666	-0.375586
H	7.418698	0.115246	1.373989
C	3.225929	-1.338690	-2.391450
H	3.666663	-2.308178	-2.660757
H	3.546925	-0.620715	-3.153649
H	2.140327	-1.438404	-2.455993
C	0.995004	1.475983	-1.631171
C	1.679855	2.197591	-0.378620
C	1.071101	1.802455	1.002324
H	1.646543	0.695174	-2.020436
H	1.574772	3.275229	-0.520901
H	2.730771	1.896299	-0.388126
H	1.718567	1.175989	1.608493
H	0.668015	2.642986	1.564782
C	0.523983	2.409399	-2.733750
H	1.379177	2.940553	-3.180505
H	0.040437	1.841636	-3.538523
H	-0.184026	3.155192	-2.362701
O	-2.489490	4.181484	0.981460
N	-1.870183	3.137397	0.816677

31-mono

B3LYP SCF energy: -1496.72303339 a.u.
B3LYP enthalpy: -1496.088920 a.u.
B3LYP free energy: -1496.185017 a.u.
M06 SCF energy in solution: -1497.16320049 a.u.
M06 enthalpy in solution: -1496.529087 a.u.
M06 free energy in solution: -1496.625184 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.408766	0.856085	0.343563
O	-1.457067	2.679957	-1.373330
O	-1.485940	2.687787	0.812274
N	-0.554284	-1.965370	-0.239997
N	1.590400	-1.645855	0.056078
C	0.378091	-1.009482	-0.007598
C	-0.042938	-3.332869	-0.133689
H	-0.421605	-3.970664	-0.937240
H	-0.332471	-3.783001	0.826044
C	1.469759	-3.096388	-0.224613
H	2.041428	-3.681327	0.501103
H	1.862985	-3.317987	-1.225287
C	-1.968629	-1.590546	-0.188707
C	-2.544453	-1.761185	1.242728
H	-1.924152	-1.201236	1.953796
H	-2.503286	-2.820582	1.534802
C	-3.999826	-1.254643	1.288067
H	-4.393757	-1.382518	2.304948
C	-4.850771	-2.072078	0.294733
H	-4.855222	-3.133443	0.581822
H	-5.893871	-1.729795	0.321561
C	-4.280835	-1.906228	-1.129308
H	-4.884295	-2.487038	-1.839293
C	-2.826802	-2.428167	-1.165892
H	-2.412133	-2.347701	-2.179458
H	-2.807992	-3.491916	-0.885287
C	-4.309019	-0.413932	-1.516653
H	-3.932779	-0.276659	-2.539185
H	-5.344383	-0.045723	-1.505237
C	-3.449040	0.412354	-0.521760
H	-3.488127	1.460920	-0.820936
C	-2.006129	-0.109922	-0.618421
H	-1.659724	-0.033207	-1.660115
C	-4.023744	0.237418	0.898724
H	-3.444369	0.833074	1.614210
H	-5.054714	0.615159	0.930623
C	2.895632	-1.066956	-0.099250
C	3.789484	-1.083703	0.986761
C	5.078687	-0.569423	0.798374
H	5.769575	-0.570568	1.638866
C	5.502570	-0.064353	-0.432914
C	4.601248	-0.095593	-1.503406
H	4.917264	0.276717	-2.475716
C	3.303113	-0.593882	-1.365620
C	3.402907	-1.667137	2.326274
H	4.088020	-1.328431	3.109354
H	3.445995	-2.764855	2.311857
H	2.385174	-1.391392	2.615093
C	6.888191	0.512495	-0.606653
H	6.870537	1.608617	-0.545492
H	7.310926	0.251071	-1.583032
H	7.573080	0.152329	0.167685
C	2.366550	-0.599063	-2.552560
H	1.931650	-1.589254	-2.731272
H	2.897018	-0.300024	-3.461235
H	1.528911	0.092869	-2.407896
C	0.242464	0.842746	2.223526
C	1.311833	1.915811	0.026418
C	1.350353	1.790064	1.593474
H	0.658965	-0.054743	2.682998
H	-0.422991	1.382595	2.902961
H	2.323296	1.363720	1.851548
H	2.094520	1.320915	-0.436080
C	1.310720	3.329717	-0.517934
H	2.322506	3.753615	-0.418116
H	1.047793	3.345078	-1.579093
H	0.620454	3.985727	0.017577
N	-1.819864	3.254880	-0.313871
O	-2.458366	4.300639	-0.295497
H	1.232207	2.788945	2.018660