Supporting Information

Z-Selectivity in Olefin Metathesis with Chelated Ru Catalysts: Computational Studies of Mechanism and Selectivity

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Computational Details

The geometries of all intermediates and transition states were optimized with B3LYP[1] 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[2] functional and a mixed basis set of SDD for Ru and 6-311+G(d,p) for other atoms. The SMD[3] 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. Under this theoretical level, the bottom-bound pathway is favored by 8.6 kcal/mol in the metathesis of ethylene using the second generation Grubbs catalyst with the SIMes NHC ligand. This qualitatively agrees with previous calculations on the same catalyst using different functional and basis set.[4] All calculations were performed with Gaussian 09.[5] The 3D structures of molecules were generated using CYLView.[6]

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.

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1 (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

2 (a) Zhao,Y.; Truhlar, D. G. *Theor. Chem. Acc.*, **2008**, *120*, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.*, **2008**, *41*, 157.

3 Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., *J. Phys. Chem. B* **2009,** *113*, 6378.

4 Cavallo, L.; Correa, A. *J. Am. Chem. Soc.* **2006**, *128*, 13352.

5 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**.

6 CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, **2009** (http://www.cylview.org).

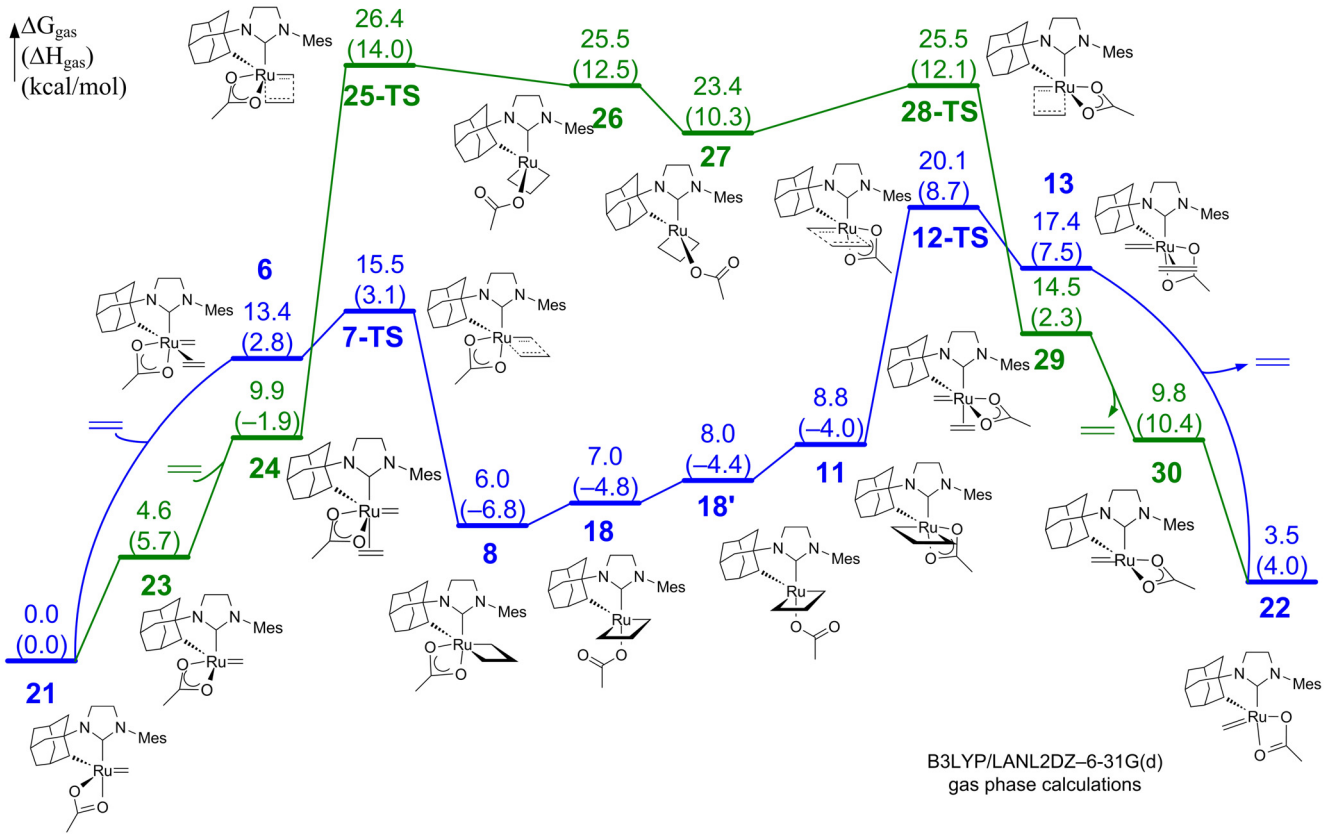


Figure S1. Free energy profiles of the side-(in blue) and bottom-(in green) bound pathways of olefin metathesis with chelated Ru catalyst **1**. Energies were calculated using B3LYP/LANL2DZ–6-31G(d) in gas phase.

B3LYP predicted much higher energies of the Ru-olefin π complexes (**6** and **24**) than M06. This is in agreement with previous calculations with the unchelated catalysts. Both B3LYP and M06 predicted the side-bound pathway is much more favorable than the bottom-bound pathway.

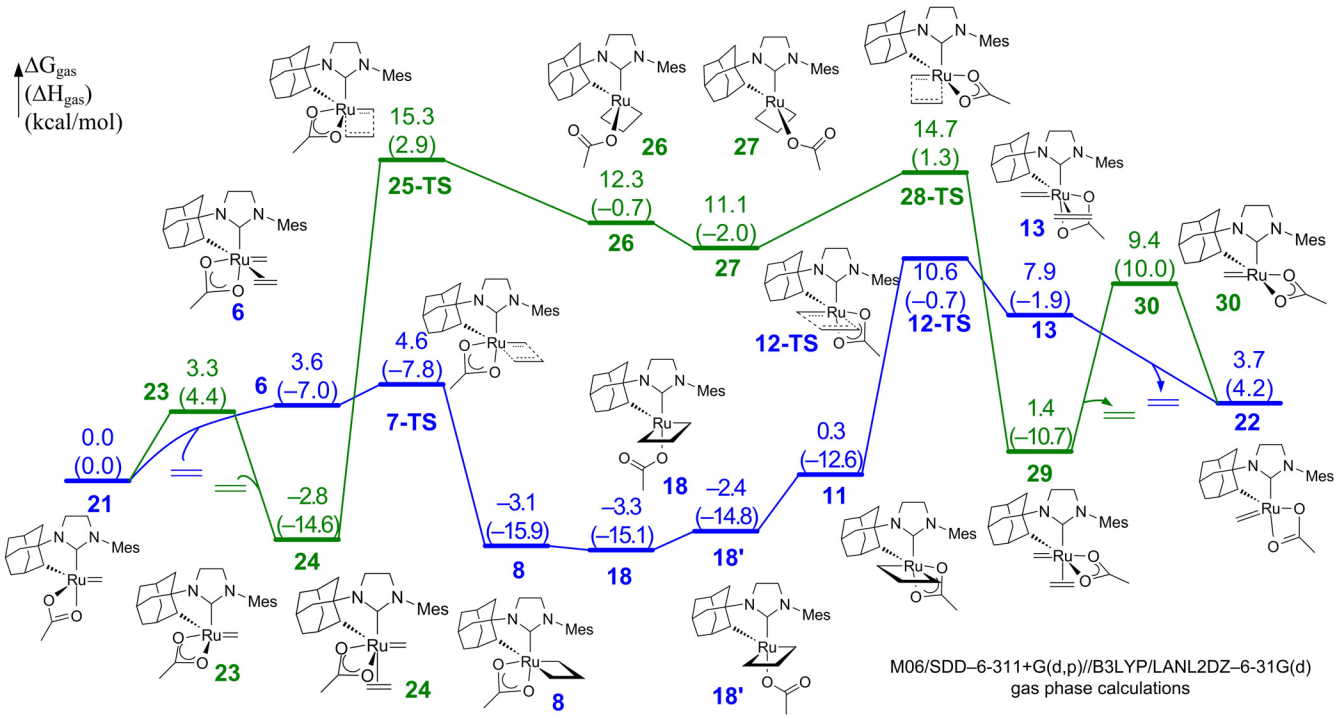
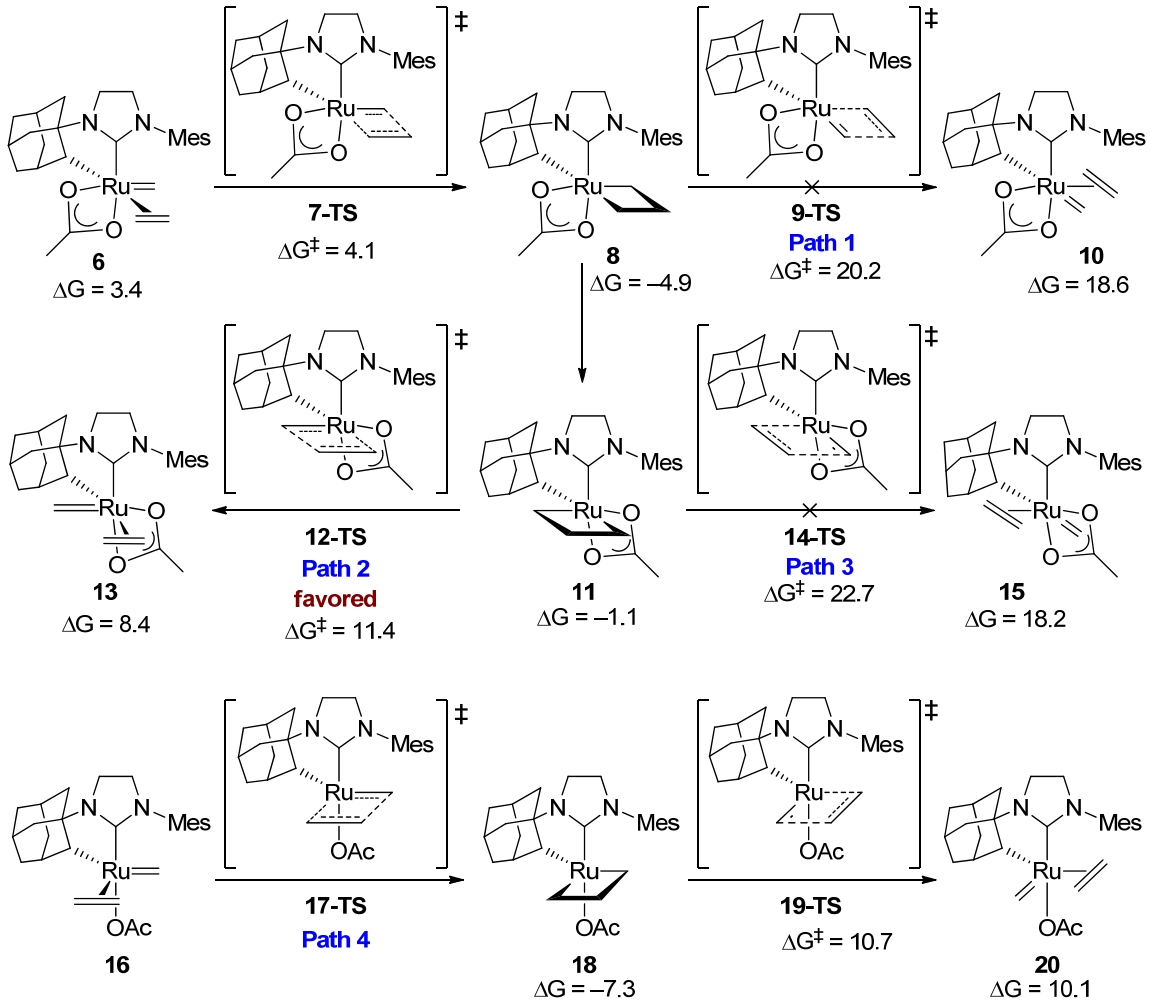


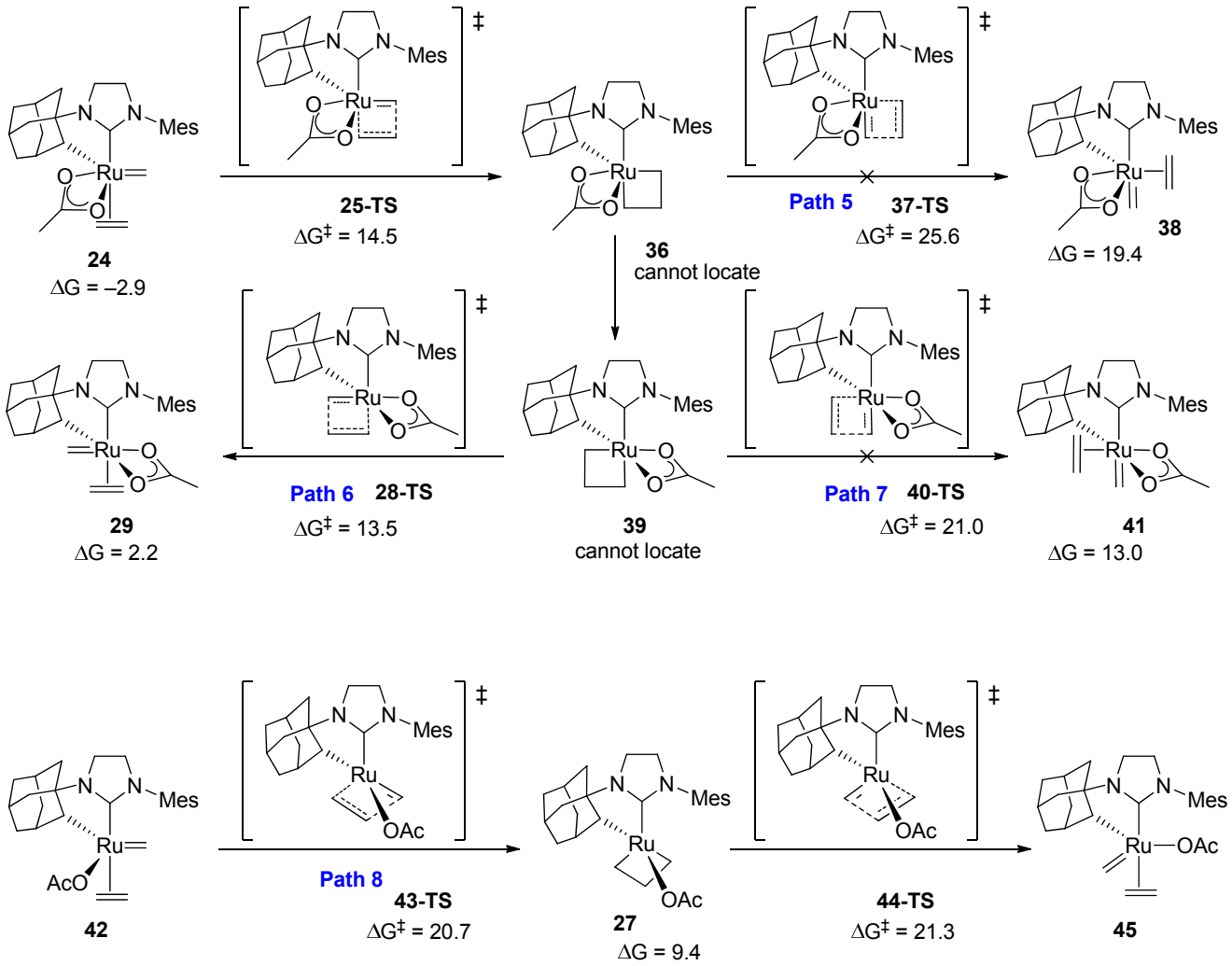
Figure S2. Free energy profiles of the side-(in blue) and bottom-(in green) bound pathways of olefin metathesis with chelated Ru catalyst **1**. Energies were calculated using M06/SDD–6-311+G(d,p) single point calculations in gas phase on geometries optimized by B3LYP/LANL2DZ–6-31G(d).



Scheme S1. Possible side-bound pathways of olefin metathesis of ethylene with chelated Ru catalyst **1**. All energies are free energies in solution calculated by M06 single point energies with B3LYP geometries. All energies are with respect to the active catalyst **21**.

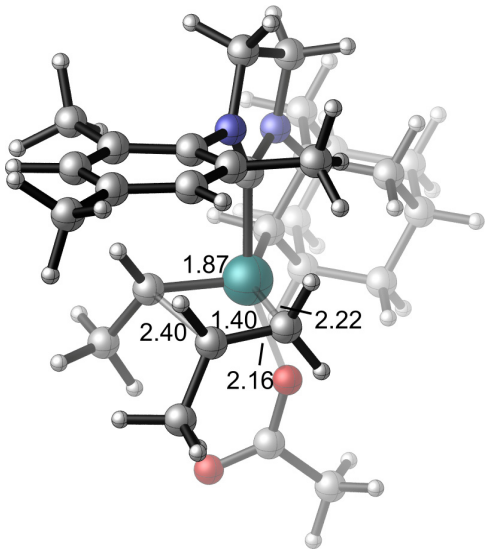
Path 1 and 3 require much higher activation energies than Path 2. In locating the monodentate intermediates and transition states in Path 4, efforts were made to explore rotamers about the Ru–OAc bond. Geometry optimizations of many monodentate conformers lead to bidentate structures as in Path 2. Two rotamers were located for the metallacyclobutane intermediate (**18** and **18'**). Only one rotamer was located for **19-TS**, and no monodentate structure was located for **17-TS**. The monodentate transition state **19-TS** ($\Delta G^{\ddagger}_{sol}$ = 10.7 kcal/mol; $\Delta H^{\ddagger}_{sol}$ = 1.4 kcal/mol) has similar energy compared to the bidentate isomer **12-TS** ($\Delta G^{\ddagger}_{sol}$ = 11.4 kcal/mol; $\Delta H^{\ddagger}_{sol}$ = 0.0 kcal/mol) in solution. In gas phase, the bidentate **12-TS** is 3.5 kcal/mol more stable than **19-TS** in terms of free energies and 5.7 kcal/mol more stable in terms of enthalpies. We also computed the transition states for the metathesis of propene. The bidentate transition state for the metathesis of propene (**46-TS**) is 3.6 kcal/mol less stable than the corresponding

monodentate transition state (**32-TS**, see Figure S3). This suggests that the bidentate transition states are more favorable in metathesis with substituted olefins.

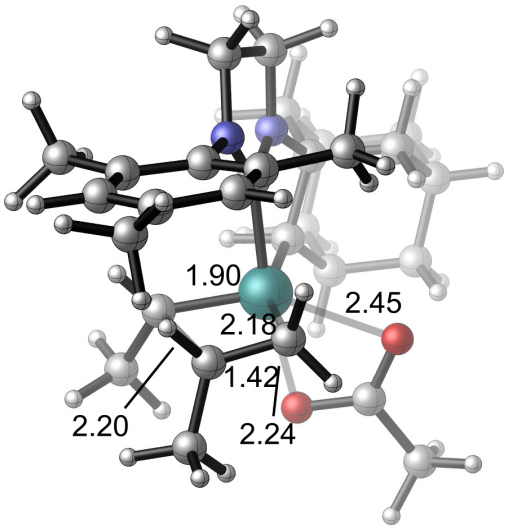


Scheme S2. Possible bottom-bound pathways of olefin metathesis of ethylene with chelated Ru catalyst **1**. All energies are free energies in solution calculated by M06 single point energies with B3LYP geometries. All energies are with respect to the active catalyst **21**.

All transition states in the bottom-bound pathways were located. The most favorable bottom-bound pathway is Path 6 (via **25-TS** and **28-TS**). Both **25-TS** and **28-TS** connect directly to the monodentate intermediates **26** and **27** (see Figure 1 in the manuscript). Bidentate intermediates **36** and **39** could not be located in geometry optimizations.



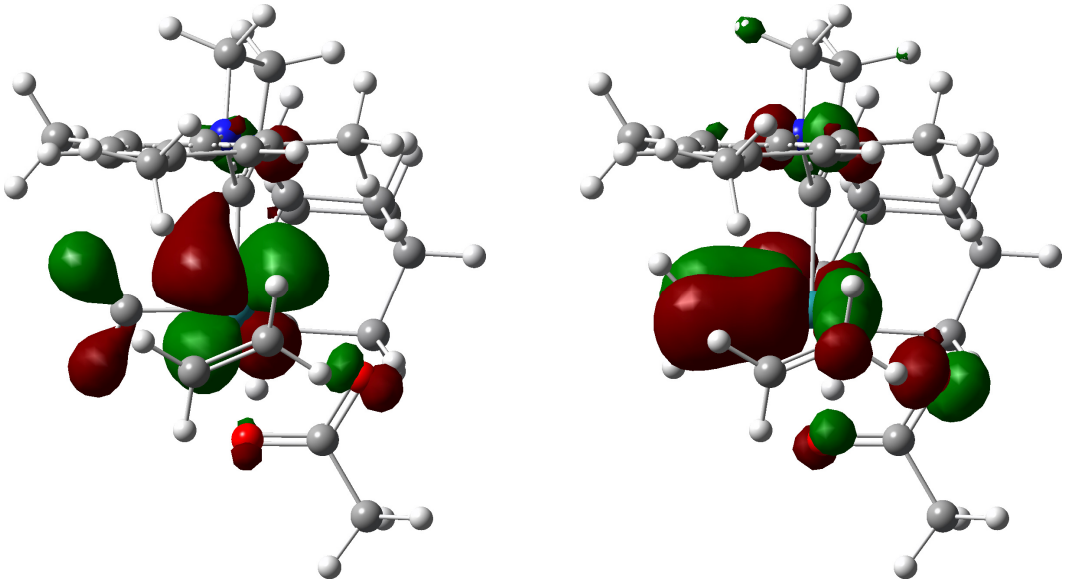
46-TS
$\Delta H^{\ddagger}_{sol}$ = 3.5 kcal/mol
$\Delta G^{\ddagger}_{sol}$ = 18.2 kcal/mol



32-TS
$\Delta H^{\ddagger}_{sol}$ = –1.2 kcal/mol
$\Delta G^{\ddagger}_{sol}$ = 14.6 kcal/mol

Figure S3. Structures of monodentate (**46-TS**) and bidentate (**32-TS**) transition states for the metathesis of propene. Energies were calculated using M06/SDD–6-311+G(d,p) single point calculations with the SMD(THF) solvation model. Geometries were optimized by B3LYP/LANL2DZ–6-31G(d).

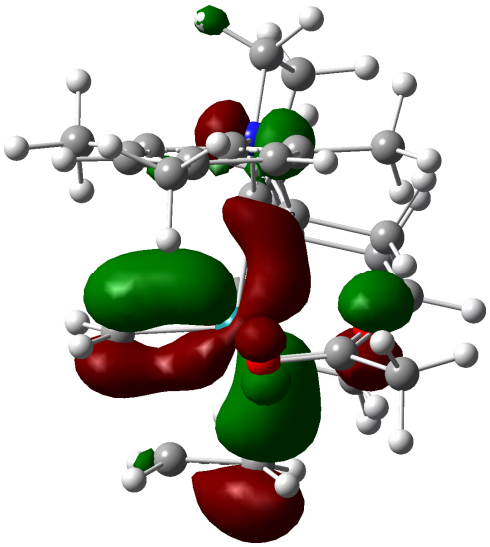
side-bound transition state (**12-TS**)



HOMO
$d \rightarrow \pi^*$(NHC) backdonation

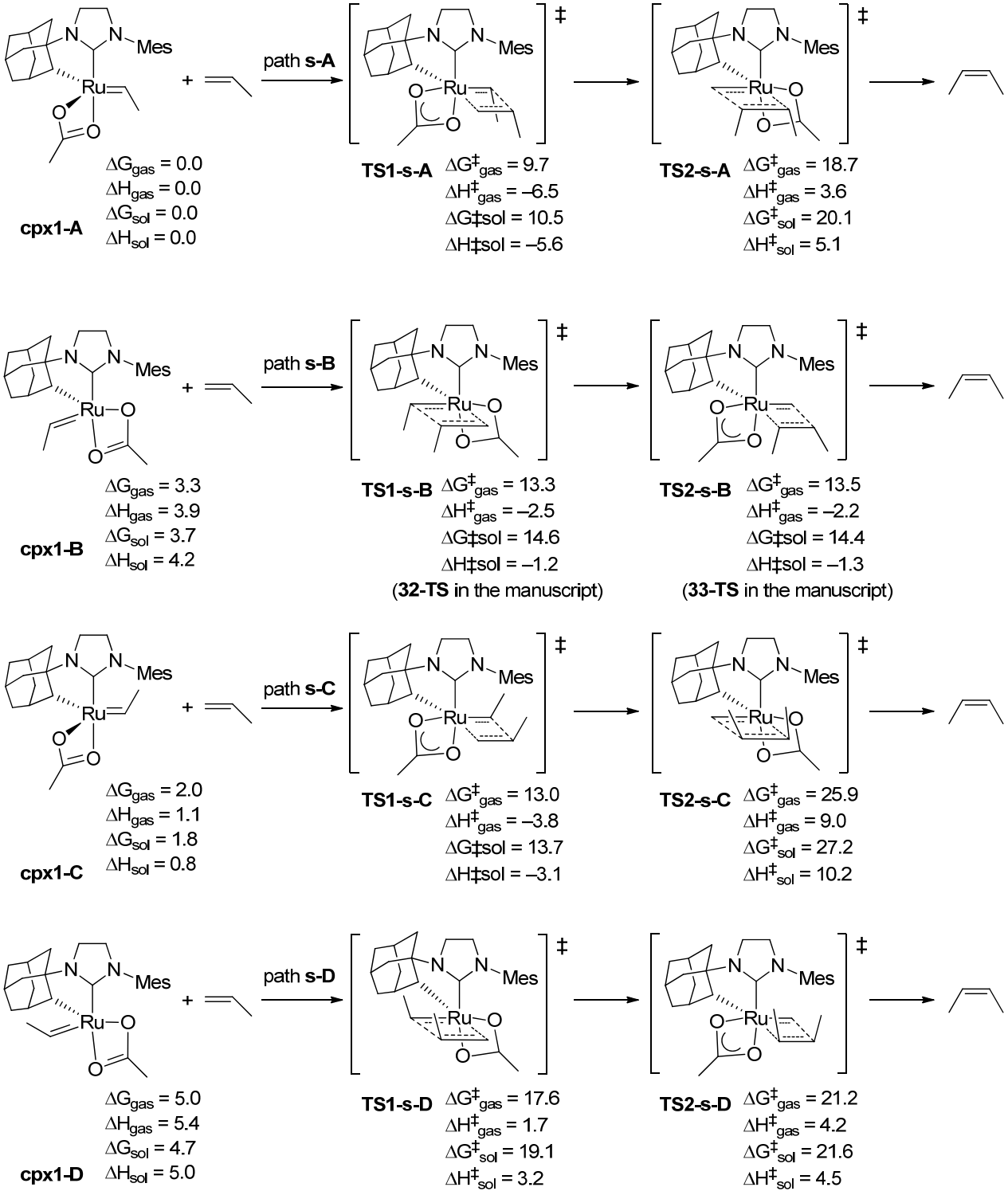
HOMO-4
$d \rightarrow \pi^*$(alkylidene) backdonation

bottom-bound transition state (**28-TS**)

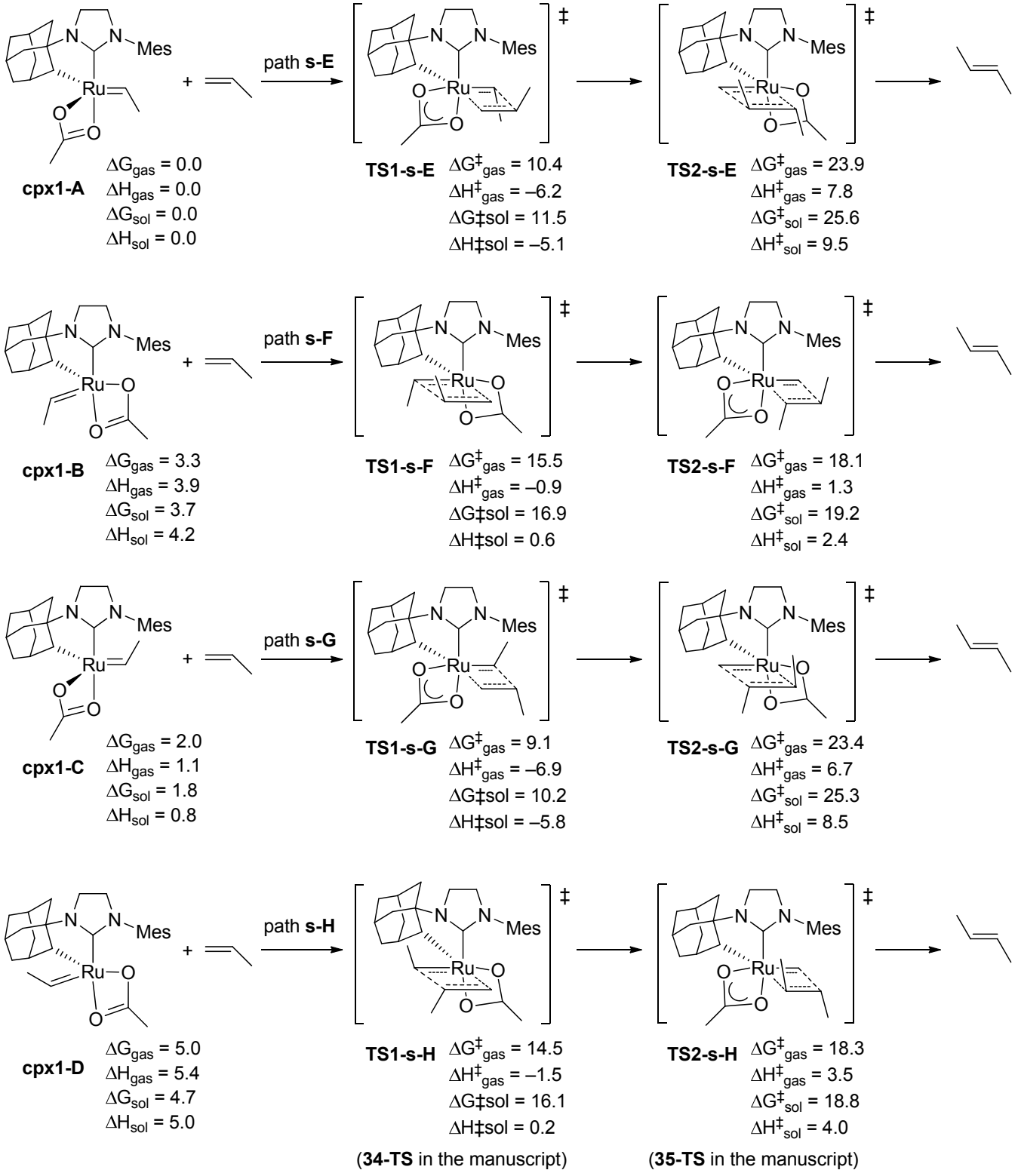


HOMO-6
$d \rightarrow \pi^*$(NHC) and $d \rightarrow \pi^*$(alkylidene) backdonation

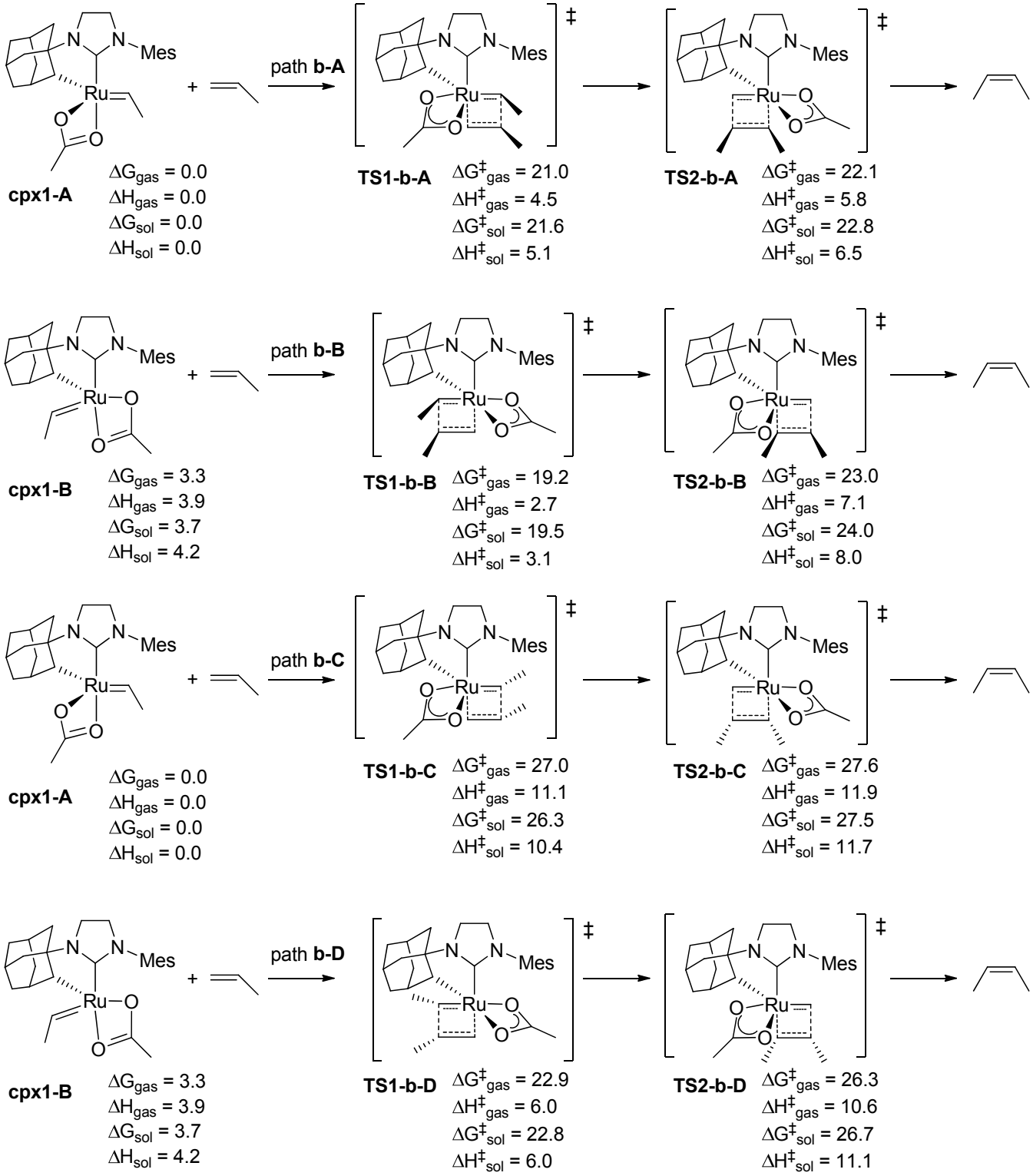
Figure S4. Molecular orbitals related to backdonation in side- and bottom-bound transition states.



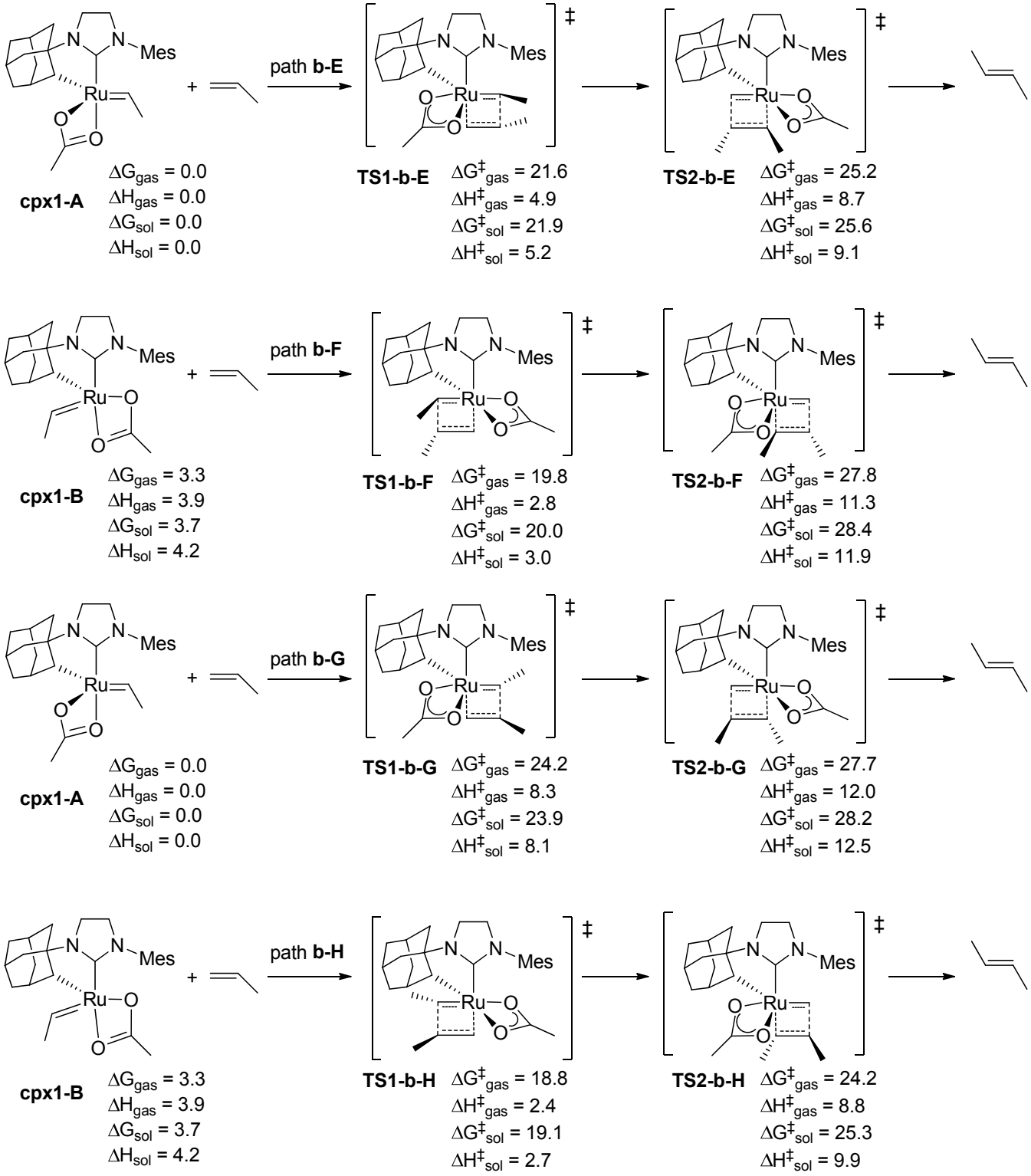
Scheme S3. Computed activation energies for the metathesis of propene via side-bound pathways leading to the *Z*-product. All energies are in kcal/mol with respect to the most stable active catalyst **cpx1-A**. Energies are M06/SDD–6-311+G(d,p) single point energies with geometries optimized at the B3LYP/LANL2DZ–6-31G(d) level.



Scheme S4. Computed activation energies for the metathesis of propene via side-bound pathways leading to the *E*-product. All energies are in kcal/mol with respect to the most stable active catalyst **1a**. Energies are M06/SDD–6-311+G(d,p) single point energies with geometries optimized at the B3LYP/LANL2DZ–6-31G(d) level.



Scheme S5. Computed activation energies for the metathesis of propene via bottom-bound pathways leading to the *Z*-product. All energies are in kcal/mol with respect to the most stable active catalyst **cpx1-A**. Energies are M06/SDD–6-311+G(d,p) single point energies with geometries optimized at the B3LYP/LANL2DZ–6-31G(d) level.

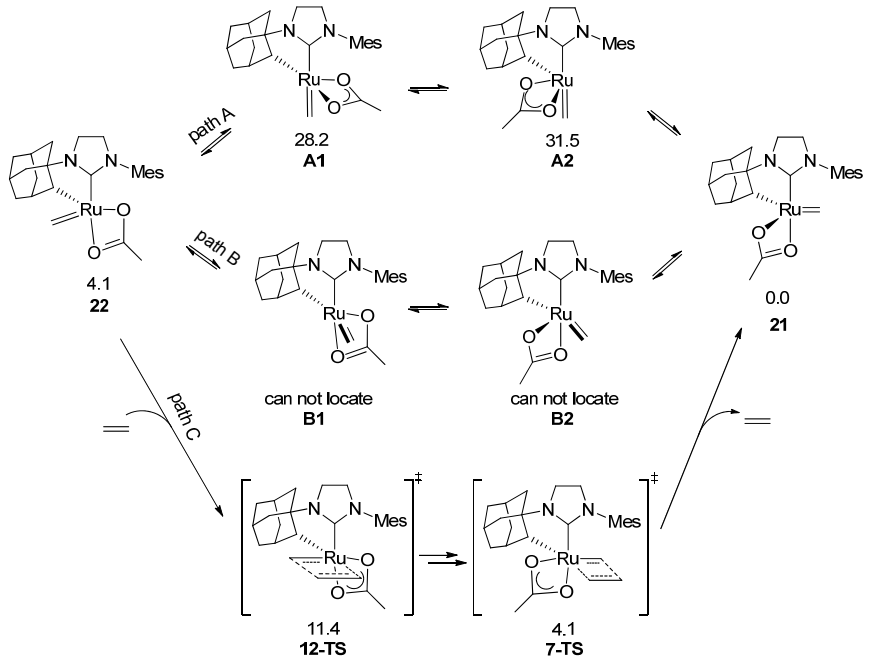


Scheme S6. Computed activation energies for the metathesis of propene via bottom-bound pathways leading to the *E*-product. All energies are in kcal/mol with respect to the most stable active catalyst **1a**. Energies are M06/SDD–6-311+G(d,p) single point energies with geometries optimized at the B3LYP/LANL2DZ–6-31G(d) level.

Transformation of complex 22 to regenerate 21.

The catalytic cycle shown in Figure 1 lead to a Ru alkylidene complex **22**. Since the chelating group is asymmetric, complex 22 and 21 are epimers, and **22** is 4.1 kcal/mol less stable than **21**. We have considered several pathways of the transformation from complex **22** to **21** (Scheme S7). These include direct isomerization via intermediates **A1** and **A2** (path A), or via intermediates **B1** and **B2** (path B), or via an olefin metathesis cycle in which **22** serves as an active catalyst (path C). The calculated free energies in THF solution are shown in Scheme S7.

Direct isomerization of **22** to **21** involves intermediates in which the alkylidene is either *trans* to the NHC (**A1** and **A2**, path A) or *trans* to the chelating adamantyl group (**B1** and **B2**, path B). Due to the *trans* influence of the strong σ-donor NHC and adamantyl, these intermediates are all highly unstable. Intermediates **A1** and **A2** are 31.5 and 28.2 kcal/mol less stable than **21**, respectively. Intermediates **B1** and **B2** cannot be located in the geometry optimizations. In contrast, the barrier of metathesis that transforms **22** to **21** (path C) is much lower than the direct isomerization pathways. Although we cannot rule out other possible pathways of the transformation from **22** to **21**, olefin metathesis via path C is energetically possible and is the most likely pathway based on current mechanistic understandings.



Scheme S7. Possible pathways of the transformation of complex **22** to regenerate complex **21**. All energies are in kcal/mol with respect to complex **21**. Energies are free energies in THF solution calculated using M06/SDD–6-311+G(d,p) single point energies with geometries optimized at the B3LYP/LANL2DZ–6-31G(d) level.

Complete reference of ref. 21:

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**.

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

6
B3LYP SCF energy: -1405.57974860 a.u.
B3LYP enthalpy: -1404.941803 a.u.
B3LYP free energy: -1405.040172 a.u.
M06 SCF energy in solution: -1406.01606477 a.u.
M06 enthalpy in solution: -1405.378119 a.u.
M06 free energy in solution:-1405.476488 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.295975	0.895952	0.509529
O	-0.382231	2.443370	-1.277953
O	-1.163742	2.976383	0.727631
N	-0.698779	-1.781632	-0.503744
N	1.468236	-1.612953	-0.214285
C	0.283730	-0.932602	-0.101432
C	-0.235277	-3.151207	-0.723922
H	-0.666977	-3.585189	-1.630685
H	-0.502526	-3.796852	0.124809
C	1.282724	-2.945761	-0.829232
H	1.858458	-3.707536	-0.295882
H	1.624540	-2.930336	-1.872938
C	-2.095763	-1.376755	-0.322480
C	-2.662953	-1.915314	1.014714
H	-2.003329	-1.621990	1.837921
H	-2.688599	-3.014881	0.991298
C	-4.080525	-1.358259	1.245813
H	-4.468516	-1.738852	2.200522
C	-4.997054	-1.818048	0.093976
H	-5.063085	-2.915592	0.078366
H	-6.016690	-1.438186	0.245434
C	-4.435948	-1.295989	-1.244834
H	-5.082652	-1.625031	-2.069303
C	-3.014480	-1.870339	-1.466073
H	-2.609524	-1.537013	-2.430640
H	-3.064816	-2.969770	-1.491803
C	-4.397944	0.248211	-1.197845
H	-4.044992	0.650338	-2.156907
H	-5.416507	0.633289	-1.043383
C	-3.461161	0.716303	-0.052184
H	-3.429288	1.810360	-0.020862
C	-2.058738	0.164514	-0.362960
H	-1.816714	0.447602	-1.398678
C	-4.009836	0.182451	1.285258
H	-3.368396	0.510231	2.111984
H	-5.010525	0.597858	1.470767
C	2.784370	-1.045214	-0.239090
C	3.666621	-1.336865	0.818163
C	4.976432	-0.850473	0.751052
H	5.660218	-1.069338	1.568755
C	5.429034	-0.097552	-0.336706
C	4.533066	0.160798	-1.379094
H	4.870449	0.735617	-2.239222
C	3.211408	-0.299843	-1.357210
C	3.221757	-2.161616	2.004388
H	3.970244	-2.127924	2.801984
H	3.077393	-3.216621	1.736440
H	2.268657	-1.805300	2.409028
C	6.840678	0.440421	-0.375173
H	6.896421	1.438102	0.080334
H	7.206665	0.532573	-1.403317
H	7.531939	-0.206848	0.175085
C	2.279399	0.025746	-2.502717
H	1.722131	-0.852822	-2.845729
H	2.844052	0.416715	-3.354761
H	1.535576	0.779632	-2.217038
C	-0.473340	0.322971	2.263223
C	-0.976474	3.254656	-0.500321
C	-1.501943	4.567151	-1.051914
H	-0.082086	-0.576705	2.763162
H	-0.980461	1.000868	2.969254
H	-2.484725	4.396595	-1.508688
H	-1.618706	5.304417	-0.253849
H	-0.835746	4.948801	-1.830550
C	1.817178	1.698276	1.920277
H	1.372621	2.227597	2.757616
H	2.350208	0.781367	2.143820
C	1.845432	2.251852	0.682442
H	2.420158	1.806492	-0.119766
H	1.427250	3.235479	0.510219

7-TS
B3LYP SCF energy: -1405.57878818 a.u.
B3LYP enthalpy: -1404.941202 a.u.
B3LYP free energy: -1405.036723 a.u.
M06 SCF energy in solution: -1406.01745065 a.u.
M06 enthalpy in solution: -1405.379864 a.u.
M06 free energy in solution:-1405.475385 a.u.
Imaginary frequency: -152.1336 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	6.539520	5.168699	7.489392
O	5.519291	6.763114	8.688790
O	4.168858	5.487753	7.480245
N	7.206518	2.361841	7.251385
N	7.701785	3.208258	5.291480
C	7.186753	3.510592	6.526184
C	7.930653	1.270167	6.599845
H	7.407817	0.315326	6.706847
H	8.937330	1.159383	7.027442
C	7.979286	1.761843	5.147292
H	8.947644	1.593947	4.667425
H	7.205760	1.289804	4.526614
C	6.900397	2.432248	8.683618
C	8.191975	2.620954	9.517091
H	8.744158	3.486439	9.135173
H	8.840639	1.739161	9.408382
C	7.830643	2.830760	10.999728
H	8.751891	2.972972	11.581035
C	7.079367	1.586800	11.516447
H	7.724477	0.698989	11.446351
H	6.822436	1.712691	12.577109
C	5.795260	1.382771	10.685939
H	5.259695	0.494637	11.047412
C	6.172911	1.167303	9.199604
H	5.273811	0.990624	8.594799
H	6.810864	0.274446	9.110489
C	4.898773	2.630984	10.840366
H	3.957186	2.493863	10.292021
H	4.636763	2.764034	11.900297
C	5.643772	3.882167	10.303942
H	5.005599	4.764517	10.416227
C	5.943573	3.634923	8.815160
H	5.001193	3.347457	8.328450
C	6.934627	4.080641	11.123305

H	7.470647	4.967758	10.764928
H	6.685065	4.257271	12.179120
C	7.572869	3.981724	4.091698
C	8.726834	4.547484	3.519949
C	8.602886	5.245701	2.312695
H	9.491888	5.691640	1.871407
C	7.374675	5.381716	1.661271
C	6.248844	4.788106	2.244274
H	5.284990	4.873507	1.746357
C	6.319980	4.083869	3.449972
C	10.081471	4.401262	4.174436
H	10.801190	5.101046	3.738611
H	10.488950	3.390292	4.039434
H	10.031850	4.580696	5.252852
C	7.256050	6.160109	0.371468
H	6.821489	7.153077	0.546334
H	6.607173	5.647326	-0.347659
H	8.233310	6.307757	-0.099269
C	5.071186	3.477879	4.049215
H	4.763461	4.007901	4.958576
H	5.215513	2.428163	4.328686
H	4.242947	3.522728	3.335633
C	8.295941	5.698344	7.887911
H	9.252402	5.358002	7.467999
C	4.347179	6.419897	8.320030
H	8.427622	6.484895	8.644866
C	3.148605	7.123083	8.930609
H	3.415707	8.131158	9.257816
H	2.321422	7.159806	8.216724
H	2.809867	6.558547	9.808226
C	6.260902	6.669571	5.794864
H	6.061893	6.104488	4.893662
H	5.459876	7.300372	6.160909
C	7.575545	6.964065	6.155178
H	8.396590	6.611666	5.540374
H	7.773553	7.830598	6.778697

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B3LYP SCF energy: -1405.59712547 a.u.
B3LYP enthalpy: -1404.957002 a.u.
B3LYP free energy: -1405.051924 a.u.
M06 SCF energy in solution: -1406.03495012 a.u.
M06 enthalpy in solution: -1405.394827 a.u.
M06 free energy in solution: -1405.489749 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.239694	1.023327	0.185719
O	1.238854	2.266376	-0.946254
O	-0.400485	3.298919	0.114475
N	-0.944846	-1.697189	-0.536914
N	1.225597	-1.697268	-0.215894
C	0.107151	-0.912939	-0.161873
C	-0.596782	-3.110359	-0.687138
H	-1.045082	-3.547777	-1.584811
H	-0.934495	-3.692087	0.181718
C	0.934521	-3.038776	-0.763398
H	1.429441	-3.818354	-0.177757
H	1.299264	-3.106411	-1.797264
C	-2.298944	-1.183880	-0.378343
C	-3.006896	-1.829519	0.841834
H	-2.392072	-1.686692	1.737548
H	-3.100834	-2.912282	0.678688
C	-4.403452	-1.209451	1.039457
H	-4.889614	-1.685643	1.901133
C	-5.254453	-1.433277	-0.226113
H	-5.391461	-2.508450	-0.409585
H	-6.255053	-1.002310	-0.086955
C	-4.556501	-0.772456	-1.432153
H	-5.159760	-0.922201	-2.337152
C	-3.173223	-1.431745	-1.637167
H	-2.666966	-1.014729	-2.517253
H	-3.299406	-2.510365	-1.813732
C	-4.396546	0.740575	-1.161855
H	-3.940527	1.237771	-2.028371
H	-5.385141	1.197522	-1.015362
C	-3.520736	0.960979	0.105392
H	-3.398617	2.035897	0.282400
C	-2.151690	0.333707	-0.196367
H	-1.815394	0.768824	-1.185940
C	-4.243461	0.299519	1.299987
H	-3.693055	0.462065	2.230518
H	-5.231192	0.764315	1.426935
C	2.598484	-1.276018	-0.177877
C	3.386677	-1.649316	0.929713
C	4.735231	-1.285853	0.942828
H	5.344089	-1.561258	1.801761
C	5.320871	-0.582921	-0.115623
C	4.522890	-0.267401	-1.217006
H	4.966198	0.254778	-2.062576
C	3.165555	-0.606175	-1.277941
C	2.813423	-2.448606	2.077574
H	3.473021	-2.400439	2.949420
H	2.702243	-3.509941	1.814881
H	1.824988	-2.086773	2.375699
C	6.773017	-0.168270	-0.061100
H	6.892208	0.783762	0.473180
H	7.188994	-0.032072	-1.064963
H	7.384712	-0.911492	0.462388
C	2.366953	-0.248001	-2.508976
H	1.581003	-0.979318	-2.722707
H	3.023063	-0.192178	-3.384233
H	1.888786	0.728228	-2.378059
C	-1.072948	1.021929	2.176072
C	0.618192	3.343715	-0.634709
C	1.134825	4.665550	-1.158671
H	1.346604	4.588136	-2.229686
H	0.413265	5.463533	-0.972153
H	2.078140	4.909218	-0.656057
C	1.157403	1.063133	1.770373
C	0.185621	1.623484	2.788780
H	1.518703	0.069388	2.030739
H	1.983536	1.698821	1.437198
H	0.373258	1.334005	3.836634
H	0.151059	2.715898	2.737790
H	-1.306286	0.030026	2.568684
H	-1.954359	1.665271	2.195340

9-TS

B3LYP SCF energy: -1405.54593513 a.u.
B3LYP enthalpy: -1404.908586 a.u.
B3LYP free energy: -1405.003816 a.u.
M06 SCF energy in solution: -1405.99184552 a.u.
M06 enthalpy in solution: -1405.354496 a.u.
M06 free energy in solution: -1405.449726 a.u.
Imaginary frequency: -132.8924 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	6.215621	5.134261	7.533976
O	5.522419	6.486817	9.096932
O	3.784355	5.518730	8.119217
N	7.390526	2.438456	7.306753
N	7.729180	3.366175	5.352030
C	7.148897	3.549516	6.581255
C	8.307772	1.495970	6.662045
H	7.943887	0.467514	6.737585
H	9.298933	1.541810	7.132866
C	8.328020	2.017968	5.220219
H	9.335294	2.080734	4.798465
H	7.718891	1.401051	4.547428
C	6.996165	2.384460	8.717999
C	8.186206	2.764276	9.636356
H	8.591504	3.731652	9.324278

H	8.991262	2.020698	9.536185
C	7.711936	2.830136	11.100949
H	8.558327	3.108987	11.743403
C	7.178057	1.444482	11.518455
H	7.980414	0.694784	11.457730
H	6.842006	1.467765	12.564125
C	6.004123	1.048324	10.598993
H	5.624367	0.060152	10.891744
C	6.497825	0.978781	9.132942
H	5.681643	0.667299	8.467551
H	7.296741	0.225044	9.052803
C	4.884099	2.101791	10.737169
H	4.019777	1.822957	10.119698
H	4.536872	2.130348	11.780880
C	5.414151	3.493805	10.302198
H	4.607127	4.224559	10.407890
C	5.849873	3.397256	8.829025
H	5.000023	2.980966	8.263758
C	6.591570	3.884535	11.217761
H	6.965007	4.876736	10.937843
H	6.253168	3.949388	12.261940
C	7.447957	4.062967	4.128537
C	8.435040	4.897372	3.574318
C	8.165238	5.530729	2.355333
H	8.919875	6.188275	1.929122
C	6.961927	5.337894	1.671248
C	6.013051	4.478408	2.235768
H	5.071657	4.310929	1.716379
C	6.232579	3.826328	3.452436
C	9.763227	5.117662	4.261266
H	10.384811	5.809035	3.684358
H	10.325775	4.182123	4.370182
H	9.640713	5.532307	5.266595
C	6.703425	6.010126	0.342755
H	7.335145	6.894545	0.211756
H	5.657762	6.323026	0.249117
H	6.913678	5.329898	-0.493428
C	5.166874	2.919964	4.025025
H	4.725898	3.344974	4.933580
H	5.562693	1.934424	4.295384
H	4.362647	2.767232	3.299179
C	8.198180	5.880153	7.826369
H	9.006452	5.264794	7.437968
C	4.255049	6.302779	8.977770
H	8.258699	6.085758	8.894609
C	3.347791	7.072905	9.919698
H	3.538405	8.147366	9.822830
H	2.298574	6.863293	9.701932
H	3.570762	6.797155	10.956409
C	5.594035	5.858305	5.910139
H	6.078095	6.054075	4.954004
H	4.502073	5.967258	5.895932
C	7.573365	6.846057	6.992704
H	7.867693	6.933133	5.952486
H	7.144525	7.739456	7.433788

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B3LYP SCF energy: -1405.55002110 a.u.
B3LYP enthalpy: -1404.911342 a.u.
B3LYP free energy: -1405.007023 a.u.
M06 SCF energy in solution: -1405.99533827 a.u.
M06 enthalpy in solution: -1405.356659 a.u.
M06 free energy in solution: -1405.452340 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.122961	1.044200	0.463370
O	-0.547500	2.469111	-1.287033
O	-1.210422	2.924667	0.767650
N	-0.636759	-1.731627	-0.459881
N	1.536113	-1.530407	-0.260257
C	0.346399	-0.869189	-0.127883
C	-0.158438	-3.097667	-0.695820
H	-0.597456	-3.522520	-1.602680
H	-0.422927	-3.748106	0.148487
C	1.358312	-2.889935	-0.810369
H	1.936796	-3.620566	-0.237545
H	1.703867	-2.924907	-1.851410
C	-2.052335	-1.361619	-0.315937
C	-2.661284	-1.985594	0.965729
H	-2.054694	-1.726725	1.835557
H	-2.662980	-3.083016	0.883730
C	-4.103166	-1.476847	1.155462
H	-4.521106	-1.909692	2.074700
C	-4.954615	-1.910421	-0.054608
H	-4.987259	-3.007716	-0.120030
H	-5.990691	-1.566246	0.067741
C	-4.350379	-1.313854	-1.342421
H	-4.948843	-1.625477	-2.209177
C	-2.904234	-1.843555	-1.519484
H	-2.465913	-1.464047	-2.451716
H	-2.929248	-2.942720	-1.589124
C	-4.363352	0.227338	-1.225987
H	-3.985099	0.682696	-2.150796
H	-5.401136	0.571447	-1.099095
C	-3.483445	0.667836	-0.024461
H	-3.493947	1.761016	0.056242
C	-2.049865	0.171442	-0.298105
H	-1.823492	0.470547	-1.332076
C	-4.082041	0.061835	1.261290
H	-3.501122	0.373566	2.137115
H	-5.105109	0.436028	1.410748
C	2.852210	-0.966155	-0.251583
C	3.668069	-1.161619	0.879020
C	4.968175	-0.647886	0.859129
H	5.600589	-0.787106	1.733509
C	5.477101	0.033631	-0.251775
C	4.652671	0.180668	-1.371315
H	5.036733	0.694049	-2.250322
C	3.343377	-0.311548	-1.399910
C	3.168956	-1.921111	2.086352
H	3.876612	-1.836659	2.916572
H	3.046931	-2.990380	1.868214
H	2.196356	-1.553856	2.427347
C	6.872967	0.611968	-0.233867
H	6.868679	1.640864	0.149887
H	7.307681	0.642308	-1.238574
H	7.541082	0.028793	0.408791
C	2.496205	-0.141874	-2.640913
H	2.250448	-1.107769	-3.100259
H	3.030761	0.448214	-3.391165
H	1.550270	0.364802	-2.424441
C	1.662465	1.701814	0.207798
C	-1.146292	3.234159	-0.470015
C	-1.815238	4.498461	-0.959231
H	-2.816353	4.253533	-1.334242
H	-1.918779	5.218786	-0.144311
H	-1.245068	4.933905	-1.784119
H	1.869913	2.170541	-0.763869
H	2.576272	1.623595	0.807391
C	-0.476288	0.185154	2.440380
H	-1.457137	0.512292	2.771013
H	-0.307086	-0.885787	2.499802
C	0.619522	1.066663	2.506462
H	1.629653	0.681815	2.607446
H	0.478230	2.081141	2.870774

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B3LYP SCF energy: -1405.59354469 a.u.
B3LYP enthalpy: -1404.952642 a.u.
B3LYP free energy: -1405.047378 a.u.
M06 SCF energy in solution: -1406.02978133 a.u.
M06 enthalpy in solution: -1405.388879 a.u.
M06 free energy in solution: -1405.483615 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.402048	0.876844	0.414421
O	-0.424653	2.205864	-1.202321
O	1.034041	3.062024	0.219924
N	0.772691	-1.920881	-0.206862
N	-1.393189	-1.602156	-0.315312
C	-0.212787	-0.995076	0.002555
C	0.310032	-3.086863	-0.958339
H	0.760677	-4.013028	-0.590526
H	0.546598	-2.989409	-2.028736
C	-1.200806	-3.017216	-0.700663
H	-1.803836	-3.259475	-1.580141
H	-1.503275	-3.681409	0.119296
C	2.134472	-1.387193	-0.224539
C	2.479026	-0.747945	-1.598016
H	1.704673	-0.014835	-1.869250
H	2.476191	-1.517849	-2.383310
C	3.857468	-0.063094	-1.528819
H	4.091625	0.380986	-2.505384
C	4.925736	-1.115946	-1.167482
H	4.972156	-1.891366	-1.945404
H	5.917657	-0.646106	-1.124273
C	4.584293	-1.749427	0.197221
H	5.345349	-2.496731	0.457805
C	3.205732	-2.446351	0.110095
H	2.956412	-2.931784	1.062609
H	3.236336	-3.230378	-0.661722
C	4.555263	-0.641346	1.272837
H	4.351169	-1.074521	2.261126
H	5.541434	-0.158524	1.331122
C	3.469466	0.410836	0.919105
H	3.457663	1.192989	1.686405
C	2.114174	-0.321873	0.892441
H	1.988963	-0.860270	1.835568
C	3.816068	1.036904	-0.449021
H	3.080802	1.808421	-0.708286
H	4.791748	1.538967	-0.388998
C	-2.729659	-1.082150	-0.266445
C	-3.224981	-0.353889	-1.364735
C	-4.552870	0.085630	-1.322104
H	-4.941447	0.650501	-2.167080
C	-5.392095	-0.184550	-0.237675
C	-4.876861	-0.935115	0.823351
H	-5.516364	-1.165744	1.673193
C	-3.557883	-1.398395	0.828279
C	-2.367385	-0.043717	-2.567970
H	-2.994581	0.234750	-3.421143
H	-1.755320	-0.903345	-2.863730
H	-1.686593	0.788292	-2.358634
C	-6.810692	0.335333	-0.204910
H	-6.855241	1.334529	0.248589
H	-7.464689	-0.317565	0.383104
H	-7.230762	0.418243	-1.213120
C	-3.057136	-2.221560	1.993781
H	-3.130549	-3.298407	1.789003
H	-3.653244	-2.024925	2.890346
H	-2.010172	-2.004792	2.226890
C	-1.346628	1.253225	1.535215
C	0.289843	3.189300	-0.798167
C	0.214137	4.508145	-1.534536
H	-0.708530	5.026429	-1.246786
H	0.172017	4.336907	-2.614081
H	1.066590	5.141485	-1.280166
C	0.620428	0.979114	2.554155
C	-0.610261	1.856770	2.713011
H	-1.940461	1.905333	0.886305
H	-1.900680	0.355856	1.798557
H	-0.368325	2.908892	2.536894
H	-1.124624	1.775407	3.685511
H	1.584812	1.430514	2.804350
H	0.507534	0.007662	3.042195

12-TS

B3LYP SCF energy: -1405.56973188 a.u.
B3LYP enthalpy: -1404.932383 a.u.
B3LYP free energy: -1405.029492 a.u.
M06 SCF energy in solution: -1406.00401594 a.u.
M06 enthalpy in solution: -1405.366667 a.u.
M06 free energy in solution:-1405.463776 a.u.
Imaginary frequency: -115.1011 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	6.441019	5.093929	7.654712
O	8.247196	6.082784	8.919651
O	6.153767	6.789974	9.091050
N	6.991099	2.266731	7.302551
N	7.074127	3.083772	5.275037
C	6.877095	3.419757	6.590158
C	7.492672	1.137243	6.517339
H	6.949294	0.215706	6.743865
H	8.559404	0.962747	6.718140
C	7.250644	1.629133	5.085754
H	8.085744	1.422077	4.410087
H	6.342913	1.192862	4.646343
C	7.049640	2.339759	8.765941
C	8.512974	2.502476	9.250952
H	8.949069	3.393132	8.784067
H	9.110059	1.631668	8.941416
C	8.545734	2.643750	10.786545
H	9.588920	2.742020	11.115901
C	7.909479	1.402652	11.441174
H	8.476338	0.496447	11.181694
H	7.941494	1.496967	12.535343
C	6.448972	1.270365	10.963848
H	5.984371	0.391968	11.432179
C	6.442638	1.081071	9.429229
H	5.419029	0.932245	9.059750
H	7.018078	0.178267	9.172648
C	5.663642	2.543564	11.355406
H	4.611070	2.445066	11.056261
H	5.676189	2.659041	12.448997
C	6.299712	3.787642	10.675146
H	5.735311	4.685414	10.953258
C	6.191979	3.562147	9.149877
H	5.154358	3.267296	8.965025
C	7.755059	3.906373	11.179134
H	8.243512	4.783346	10.751541
H	7.755777	4.019210	12.273395
C	7.094251	3.922219	4.114596
C	8.340753	4.424338	3.674981
C	8.382502	5.189865	2.509281
H	9.339485	5.585116	2.174475
C	7.229175	5.460455	1.759582
C	6.021405	4.917430	2.195838
H	5.118523	5.092462	1.613408
C	5.930179	4.135576	3.357488
C	9.609343	4.138968	4.446103
H	10.459548	4.661898	3.998049
H	9.846753	3.067511	4.451539
H	9.528795	4.450580	5.492926
C	7.299015	6.321110	0.519576
H	8.174037	6.073086	-0.091990
H	7.379162	7.384742	0.779844
H	6.405989	6.201346	-0.102053
C	4.598113	3.517752	3.717580
H	4.637731	2.975563	4.663688
H	4.276049	2.816549	2.937139
H	3.816397	4.281960	3.800503
C	7.503631	6.769570	6.101919
H	7.946494	6.240105	5.269536
C	7.378341	6.855224	9.432144
H	8.173346	7.126286	6.875047
C	7.795809	7.850254	10.498032

H	8.818576	8.194238	10.322567
H	7.107080	8.698222	10.530647
H	7.772507	7.353310	11.475947
C	4.702672	5.100127	7.035521
H	4.221540	4.527553	6.233065
H	4.019202	5.817983	7.517203
C	6.197493	7.144316	6.058605
H	5.578294	6.901334	5.199929
H	5.769569	7.794308	6.813863

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B3LYP SCF energy: -1405.57289320 a.u.
B3LYP enthalpy: -1404.934204 a.u.
B3LYP free energy: -1405.033769 a.u.
M06 SCF energy in solution: -1406.00762998 a.u.
M06 enthalpy in solution: -1405.368941 a.u.
M06 free energy in solution: -1405.468506 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.279475	0.960694	-0.588450
O	-1.086585	2.033715	1.407127
O	-1.424650	2.857452	-0.613242
N	-0.601128	-1.851908	0.153011
N	1.557089	-1.523514	0.264767
C	0.365459	-0.926787	-0.022699
C	-0.116333	-3.098447	0.753895
H	-0.529282	-3.973963	0.246010
H	-0.399579	-3.150976	1.813853
C	1.400478	-2.963272	0.565875
H	1.972843	-3.240287	1.455458
H	1.769458	-3.564567	-0.275550
C	-2.009737	-1.443864	0.109689
C	-2.520479	-1.089637	1.528772
H	-1.887911	-0.304991	1.956995
H	-2.456800	-1.973510	2.181323
C	-3.980717	-0.599480	1.448503
H	-4.336196	-0.362754	2.460395
C	-4.870836	-1.693313	0.828260
H	-4.862723	-2.596765	1.455493
H	-5.912707	-1.347667	0.779925
C	-4.356983	-2.022673	-0.587810
H	-4.989253	-2.798637	-1.040250
C	-2.909647	-2.557353	-0.478130
H	-2.528400	-2.853236	-1.464579
H	-2.903649	-3.454877	0.159571
C	-4.402095	-0.743298	-1.454920
H	-4.084194	-0.969838	-2.481641
H	-5.438669	-0.380362	-1.513995
C	-3.482030	0.346585	-0.839181
H	-3.514531	1.249400	-1.459260
C	-2.044994	-0.227363	-0.839096
H	-1.905544	-0.649414	-1.843685
C	-4.019297	0.667193	0.572747
H	-3.426575	1.446224	1.053429
H	-5.051986	1.037749	0.496609
C	2.883120	-0.983050	0.203773
C	3.488959	-0.557002	1.402935
C	4.810816	-0.104982	1.358454
H	5.280901	0.232317	2.280000
C	5.539995	-0.068330	0.164317
C	4.915085	-0.514114	-1.003280
H	5.470105	-0.507173	-1.939081
C	3.595806	-0.983247	-1.008100
C	2.725092	-0.557081	2.706603
H	2.454762	-1.571893	3.025161
H	1.791550	0.010053	2.623262
H	3.325046	-0.111666	3.505693
C	6.957183	0.455397	0.138897
H	6.973261	1.553189	0.122954
H	7.496928	0.107348	-0.747708
H	7.518468	0.137602	1.024677
C	2.972764	-1.477766	-2.291210
H	3.703495	-1.467422	-3.105529
H	2.123546	-0.851668	-2.585487
H	2.594887	-2.502698	-2.195454
C	0.117869	0.610197	-2.356439
C	-1.536443	2.946716	0.655397
C	-2.241013	4.154371	1.240732
H	-1.995016	4.267448	2.298974
H	-1.972573	5.059294	0.688002
H	-3.325094	4.018502	1.146088
H	0.646600	1.333706	-2.996303
H	-0.203821	-0.277607	-2.924533
C	1.519499	2.835602	-0.881093
H	2.116750	2.560960	-1.746570
H	0.764978	3.599267	-1.029960
C	1.788936	2.308470	0.333178
H	1.260805	2.627134	1.225534
H	2.612444	1.619020	0.466052

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B3LYP SCF energy: -1405.54260639 a.u.
B3LYP enthalpy: -1404.905537 a.u.
B3LYP free energy: -1405.000894 a.u.
M06 SCF energy in solution: -1405.98754382 a.u.
M06 enthalpy in solution: -1405.350474 a.u.
M06 free energy in solution: -1405.445831 a.u.
Imaginary frequency: -116.4065 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.274768	1.106202	-0.260610
O	-1.637746	2.449174	1.430780
O	-1.453968	2.882986	-0.734285
N	-0.475300	-1.840003	-0.372190
N	1.671864	-1.427167	-0.272948
C	0.431717	-0.845296	-0.266570
C	0.102729	-3.183431	-0.271876
H	-0.288751	-3.841619	-1.052198
H	-0.131519	-3.633336	0.702240
C	1.600043	-2.896393	-0.436503
H	2.220736	-3.395523	0.313472
H	1.973720	-3.184550	-1.427360
C	-1.896146	-1.551332	-0.131383
C	-2.210837	-1.691043	1.381207
H	-1.536487	-1.034679	1.945082
H	-2.028297	-2.723951	1.713237
C	-3.676525	-1.301775	1.650067
H	-3.890260	-1.414637	2.721634
C	-4.606948	-2.223225	0.835596
H	-4.476860	-3.270198	1.147091
H	-5.656644	-1.961329	1.026005
C	-4.291340	-2.072804	-0.667309
H	-4.957319	-2.722625	-1.251095
C	-2.826321	-2.500810	-0.921444
H	-2.586342	-2.441819	-1.991666
H	-2.695470	-3.549340	-0.610903
C	-4.500669	-0.599986	-1.084250
H	-4.315620	-0.481526	-2.160692
H	-5.548414	-0.315468	-0.905923
C	-3.544456	0.317841	-0.274170
H	-3.700406	1.356369	-0.587266
C	-2.098516	-0.108225	-0.596823
H	-2.009924	-0.115377	-1.697628
C	-3.879188	0.165336	1.224908
H	-3.239997	0.828130	1.814855
H	-4.923054	0.461893	1.405466
C	2.958816	-0.857270	0.007627
C	3.364995	-0.750563	1.358745
C	4.636503	-0.250382	1.638107
H	4.945490	-0.155602	2.677093
C	5.525725	0.125027	0.621307
C	5.115862	-0.040991	-0.700456

H	5.801539	0.214356	-1.506110
C	3.846928	-0.539828	-1.033368
C	2.451015	-1.168872	2.487306
H	2.944079	-1.028379	3.453728
H	2.167649	-2.226169	2.410661
H	1.521721	-0.589153	2.493104
C	6.886893	0.687752	0.957288
H	7.534004	0.725943	0.075382
H	7.391559	0.086168	1.722278
H	6.806239	1.708581	1.352705
C	3.503332	-0.725271	-2.494235
H	4.328841	-1.216775	-3.021518
H	3.333810	0.239205	-2.987407
H	2.603030	-1.326070	-2.636080
C	1.055186	1.625168	0.963070
C	-1.933194	3.144039	0.428047
C	-2.900873	4.306644	0.549494
H	-2.845015	4.746224	1.548595
H	-2.696951	5.063900	-0.212000
H	-3.923177	3.938719	0.397748
H	2.127251	1.430108	0.997828
H	0.639433	2.083585	1.868378
C	0.508635	1.207601	-2.242119
H	0.934584	0.290454	-2.635334
H	-0.329649	1.602129	-2.816399
C	1.303633	2.118430	-1.499740
H	1.058119	3.174934	-1.507032
H	2.333929	1.875386	-1.264251

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B3LYP SCF energy: -1405.55066092 a.u.
B3LYP enthalpy: -1404.912863 a.u.
B3LYP free energy: -1405.009155 a.u.
M06 SCF energy in solution: -1405.99439429 a.u.
M06 enthalpy in solution: -1405.356596 a.u.
M06 free energy in solution:-1405.452888 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.136861	0.955413	0.731671
O	0.497876	1.950854	-1.178758
O	1.228783	2.875952	0.671602
N	0.662382	-1.772825	-0.277818
N	-1.512676	-1.478984	-0.354827
C	-0.330362	-0.908523	0.004638
C	0.197638	-2.952544	-1.019614
H	0.603187	-3.873479	-0.591870
H	0.515755	-2.894262	-2.068310
C	-1.329851	-2.851633	-0.870124
H	-1.865240	-2.979961	-1.815731
H	-1.725110	-3.581937	-0.153198
C	2.066808	-1.312879	-0.256081
C	2.466875	-0.782209	-1.657148
H	1.768420	0.006330	-1.955089
H	2.409012	-1.589646	-2.403026
C	3.903810	-0.226283	-1.607826
H	4.182304	0.143379	-2.604413
C	4.875127	-1.344511	-1.180934
H	4.858539	-2.163753	-1.914635
H	5.904462	-0.961128	-1.153178
C	4.469602	-1.867229	0.212581
H	5.160557	-2.662454	0.524054
C	3.036876	-2.450706	0.135743
H	2.738927	-2.867784	1.107168
H	3.020883	-3.274630	-0.595858
C	4.527482	-0.699394	1.224057
H	4.281815	-1.060507	2.232112
H	5.555163	-0.306877	1.266372
C	3.527452	0.411169	0.802350
H	3.577874	1.237622	1.523578
C	2.104467	-0.192532	0.795772
H	2.005272	-0.707865	1.767414
C	3.953182	0.927513	-0.587332
H	3.296721	1.738681	-0.915155
H	4.972343	1.338652	-0.539375
C	-2.821423	-0.898231	-0.341295
C	-3.207405	-0.068070	-1.416753
C	-4.509479	0.438382	-1.427872
H	-4.813214	1.080470	-2.252114
C	-5.431363	0.140110	-0.417790
C	-5.027185	-0.709733	0.614268
H	-5.735236	-0.968053	1.399273
C	-3.736323	-1.248991	0.668594
C	-2.251672	0.261353	-2.539526
H	-2.773984	0.792917	-3.341007
H	-1.810930	-0.644955	-2.972880
H	-1.420904	0.889182	-2.199483
C	-6.820909	0.733322	-0.440109
H	-6.819782	1.757664	-0.044569
H	-7.517183	0.148118	0.169391
H	-7.219589	0.782004	-1.459562
C	-3.378412	-2.213796	1.775846
H	-3.628647	-3.246612	1.496453
H	-3.939734	-1.985897	2.687812
H	-2.313125	-2.187625	2.015317
C	-1.637244	1.702853	0.695043
C	1.079083	2.923244	-0.589344
C	1.546524	4.124096	-1.373409
H	1.707464	3.858424	-2.420882
H	0.780070	4.907366	-1.327247
H	2.464704	4.525682	-0.936854
H	-2.051767	2.249952	-0.167188
H	-2.417034	1.610631	1.470704
C	0.294923	1.037586	2.928693
H	1.354187	0.972975	3.158214
H	-0.193688	1.961911	3.223161
C	-0.448635	-0.100295	2.645913
H	-1.529801	-0.085975	2.734766
H	0.016676	-1.080944	2.678039

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B3LYP SCF energy: -1405.59423883 a.u.
B3LYP enthalpy: -1404.953849 a.u.
B3LYP free energy: -1405.050297 a.u.
M06 SCF energy in solution: -1406.03747070 a.u.
M06 enthalpy in solution: -1405.397081 a.u.
M06 free energy in solution:-1405.493529 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.384885	0.902902	-0.262895
O	1.630031	2.908599	1.561427
O	1.437142	2.742528	-0.669453
N	0.455016	-1.949794	0.199557
N	-1.679059	-1.552001	-0.082513
C	-0.447994	-0.956855	-0.005163
C	-0.103612	-3.294414	0.050838
H	0.265082	-3.975932	0.822647
H	0.152164	-3.717403	-0.931139
C	-1.605891	-3.008992	0.177397
H	-2.213847	-3.565093	-0.541954
H	-1.982845	-3.232671	1.183800
C	1.878545	-1.612464	0.142082
C	2.431206	-1.745813	-1.302838
H	1.811222	-1.146353	-1.982357
H	2.362099	-2.792581	-1.632918
C	3.897016	-1.269160	-1.352943
H	4.274625	-1.374487	-2.378722
C	4.742239	-2.136259	-0.396970
H	4.719714	-3.187768	-0.717721
H	5.792418	-1.816118	-0.427209
C	4.195081	-2.004409	1.039718
H	4.795923	-2.620601	1.721703
C	2.730372	-2.497533	1.080676

H	2.331479	-2.438618	2.102039
H	2.685126	-3.552074	0.769438
C	4.261452	-0.525723	1.473978
H	3.898582	-0.412979	2.504319
H	5.305591	-0.182183	1.463617
C	3.410178	0.350036	0.515677
H	3.454406	1.388238	0.848107
C	1.960544	-0.145051	0.603618
H	1.609981	-0.069426	1.646668
C	3.961681	0.209182	-0.916874
H	3.382577	0.841092	-1.601197
H	5.001448	0.563017	-0.954813
C	-2.958349	-0.918174	0.075439
C	-3.826841	-0.834970	-1.027829
C	-5.096711	-0.274921	-0.838256
H	-5.770706	-0.207951	-1.689805
C	-5.521700	0.193236	0.406979
C	-4.645468	0.069262	1.491155
H	-4.964286	0.410217	2.474005
C	-3.371012	-0.488096	1.355237
C	-3.424432	-1.321839	-2.401417
H	-4.308314	-1.481547	-3.026790
H	-2.861108	-2.258860	-2.362233
H	-2.786724	-0.591717	-2.914075
C	-6.883101	0.825110	0.581509
H	-6.816875	1.920744	0.551372
H	-7.329592	0.555491	1.544945
H	-7.573043	0.517377	-0.210919
C	-2.469562	-0.612089	2.563210
H	-2.193368	-1.654371	2.764008
H	-2.970657	-0.227199	3.456163
H	-1.536654	-0.053474	2.432152
C	-0.377954	1.154723	-2.080507
C	1.818756	3.342427	0.412434
C	2.568345	4.654354	0.188113
H	2.747121	5.162221	1.138380
H	3.530150	4.448584	-0.297079
H	2.003284	5.307996	-0.484982
C	-1.184245	2.024483	0.291244
C	-1.379384	2.083690	-1.261711
H	-0.876580	0.336509	-2.601007
H	0.281361	1.735970	-2.729149
H	-2.394149	1.745158	-1.482593
H	-1.214531	3.111346	-1.589726
H	-2.018715	1.571966	0.819043
H	-0.851337	2.960895	0.737488

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B3LYP SCF energy: -1405.59357602 a.u.
B3LYP enthalpy: -1404.953294 a.u.
B3LYP free energy: -1405.048669 a.u.
M06 SCF energy in solution: -1406.03834672 a.u.
M06 enthalpy in solution: -1405.398065 a.u.
M06 free energy in solution:-1405.493440 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.331468	0.903361	-0.272726
O	-2.198497	2.972468	1.434558
O	-1.295535	2.794865	-0.628614
N	-0.469546	-1.996517	-0.129561
N	1.661763	-1.578036	0.124345
C	0.445435	-0.989597	-0.078546
C	0.075333	-3.301258	0.256449
H	-0.283711	-4.100363	-0.398150
H	-0.205587	-3.551708	1.288932
C	1.583286	-3.053891	0.120400
H	2.166666	-3.476902	0.943388
H	1.981768	-3.452608	-0.822062
C	-1.890477	-1.647316	-0.063281
C	-2.383166	-1.621008	1.408619
H	-1.743346	-0.941226	1.986498
H	-2.289145	-2.622745	1.852187
C	-3.849853	-1.151759	1.468175
H	-4.183784	-1.153181	2.514078
C	-4.726311	-2.114720	0.641578
H	-4.682106	-3.130282	1.061424
H	-5.776639	-1.796988	0.685269
C	-4.240266	-2.124134	-0.822993
H	-4.865899	-2.803944	-1.416548
C	-2.777099	-2.622314	-0.871686
H	-2.417417	-2.670041	-1.908364
H	-2.718587	-3.639458	-0.456433
C	-4.331707	-0.694977	-1.400553
H	-4.016144	-0.690506	-2.453244
H	-5.375796	-0.352482	-1.378632
C	-3.444562	0.270739	-0.568289
H	-3.501359	1.279863	-0.986964
C	-2.000400	-0.240104	-0.669531
H	-1.709392	-0.289532	-1.741779
C	-3.940720	0.273932	0.892480
H	-3.345749	0.980179	1.479806
H	-4.982572	0.622566	0.924866
C	2.951860	-0.954322	0.096611
C	3.575860	-0.618101	1.313733
C	4.841685	-0.022522	1.272150
H	5.320527	0.254200	2.209212
C	5.507437	0.219718	0.067126
C	4.884774	-0.177293	-1.120953
H	5.398031	-0.022239	-2.068040
C	3.620742	-0.775179	-1.131614
C	2.940964	-0.933380	2.649487
H	3.305647	-0.253343	3.425657
H	3.195385	-1.953525	2.969817
H	1.851270	-0.866739	2.616725
C	6.855927	0.900999	0.044735
H	6.751116	1.979069	-0.135383
H	7.494076	0.501078	-0.750832
H	7.382702	0.779185	0.996775
C	3.032230	-1.257166	-2.439674
H	3.300140	-2.306530	-2.624653
H	3.422520	-0.675372	-3.280702
H	1.941648	-1.189284	-2.455338
C	1.084837	1.668000	-1.451299
C	-1.997174	3.390343	0.285655
C	-2.611780	4.715541	-0.172563
H	-3.076335	5.233604	0.669360
H	-1.848938	5.354342	-0.630537
H	-3.371481	4.523537	-0.940090
C	1.551541	2.283591	-0.074344
C	0.748312	1.754979	1.178180
H	1.832690	1.033877	-1.920196
H	0.664267	2.418562	-2.123744
H	1.409763	3.364051	-0.129736
H	2.600709	2.015387	0.066778
H	1.347681	1.137132	1.843792
H	0.178488	2.524879	1.695444

19-TS

B3LYP SCF energy: -1405.56100186 a.u.
B3LYP enthalpy: -1404.924221 a.u.
B3LYP free energy: -1405.024750 a.u.
M06 SCF energy in solution: -1406.00116770 a.u.
M06 enthalpy in solution: -1405.364387 a.u.
M06 free energy in solution:-1405.464916 a.u.
Imaginary frequency: -123.4740 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.350895	0.845068	-0.085477
O	-1.516309	2.609801	0.298146
O	-0.443340	4.242979	-0.844370
N	-0.581614	-2.032397	-0.342493
N	1.577138	-1.692494	-0.215673

C	0.365244	-1.062732	-0.228855
C	-0.047934	-3.386037	-0.169801
H	-0.483134	-4.087454	-0.886916
H	-0.250241	-3.763269	0.843430
C	1.453055	-3.152588	-0.405722
H	2.090454	-3.695511	0.298012
H	1.757483	-3.428718	-1.424617
C	-1.978800	-1.634992	-0.125903
C	-2.309588	-1.606107	1.390224
H	-1.580513	-0.963229	1.906285
H	-2.210360	-2.613430	1.821441
C	-3.736850	-1.068712	1.609880
H	-3.960181	-1.062443	2.685375
C	-4.737496	-1.987719	0.878429
H	-4.692719	-3.005451	1.292723
H	-5.762476	-1.624746	1.033441
C	-4.410376	-2.010243	-0.629407
H	-5.124072	-2.661817	-1.150976
C	-2.981598	-2.570035	-0.833795
H	-2.738403	-2.624747	-1.903331
H	-2.927834	-3.593085	-0.430474
C	-4.510112	-0.572989	-1.187835
H	-4.314575	-0.572330	-2.268923
H	-5.534274	-0.197193	-1.048314
C	-3.493968	0.346104	-0.462632
H	-3.557884	1.364906	-0.857064
C	-2.083148	-0.214072	-0.724711
H	-1.965104	-0.322658	-1.809761
C	-3.826151	0.362314	1.043058
H	-3.135274	1.035847	1.562875
H	-4.838998	0.759870	1.199640
C	2.869071	-1.088423	-0.084056
C	3.434901	-0.984205	1.206230
C	4.695432	-0.400325	1.339760
H	5.128701	-0.307398	2.333656
C	5.418121	0.062827	0.232112
C	4.853375	-0.098063	-1.033428
H	5.409135	0.231053	-1.909488
C	3.590367	-0.678756	-1.218563
C	2.721699	-1.527438	2.424097
H	3.184882	-1.155446	3.343048
H	2.771349	-2.624374	2.457408
H	1.661709	-1.257734	2.438967
C	6.765661	0.722567	0.411072
H	7.324110	0.755173	-0.529767
H	7.376315	0.192202	1.150549
H	6.656010	1.756083	0.764759
C	3.076091	-0.878622	-2.626015
H	2.045351	-1.237129	-2.641813
H	3.696273	-1.608912	-3.161757
H	3.117400	0.055403	-3.197676
C	1.074776	1.787897	1.615150
H	1.522494	0.951793	2.141589
C	-1.361534	3.825963	-0.122017
H	0.274562	2.325902	2.116752
C	-2.463890	4.781508	0.342664
H	-3.410724	4.511175	-0.140132
H	-2.617658	4.693355	1.423650
H	-2.211718	5.812355	0.084276
C	0.357618	1.340781	-1.701899
H	0.804077	0.686085	-2.458581
H	0.282713	2.408669	-1.939640
C	1.676919	2.325795	0.514841
H	2.579704	1.882020	0.106360
H	1.315995	3.251981	0.075681

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B3LYP SCF energy: -1405.56318251 a.u.
B3LYP enthalpy: -1404.925256 a.u.
B3LYP free energy: -1405.024715 a.u.
M06 SCF energy in solution: -1406.00423231 a.u.
M06 enthalpy in solution: -1405.366306 a.u.
M06 free energy in solution:-1405.465765 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.331161	0.878561	-0.098502
O	-0.883298	4.008095	-1.048723
O	-1.494226	2.493424	0.515430
N	-0.545366	-2.031392	-0.173665
N	1.612901	-1.691271	-0.057274
C	0.402719	-1.076299	-0.121147
C	-0.018156	-3.383588	0.041742
H	-0.440262	-4.096895	-0.670858
H	-0.251958	-3.733587	1.056829
C	1.491594	-3.162120	-0.162365
H	2.105942	-3.659767	0.592934
H	1.826859	-3.499258	-1.151753
C	-1.953820	-1.623249	-0.061154
C	-2.366737	-1.539420	1.431042
H	-1.678059	-0.864014	1.959789
H	-2.277365	-2.527800	1.906610
C	-3.811154	-1.017746	1.548628
H	-4.093738	-0.971411	2.609108
C	-4.758324	-1.978680	0.801160
H	-4.723908	-2.979905	1.255304
H	-5.794694	-1.625241	0.886841
C	-4.347712	-2.051750	-0.684297
H	-5.023060	-2.731904	-1.220377
C	-2.904746	-2.600453	-0.784672
H	-2.601454	-2.696388	-1.835741
H	-2.863813	-3.605345	-0.336369
C	-4.428077	-0.638685	-1.303784
H	-4.174323	-0.679384	-2.371886
H	-5.461443	-0.268438	-1.235237
C	-3.460354	0.318936	-0.561400
H	-3.522265	1.319687	-1.002514
C	-2.025316	-0.227041	-0.730911
H	-1.877272	-0.403264	-1.808408
C	-3.883983	0.388156	0.921010
H	-3.236108	1.089375	1.456103
H	-4.911482	0.772350	0.996968
C	2.902808	-1.066131	-0.021379
C	3.548719	-0.913889	1.220680
C	4.817161	-0.325199	1.245527
H	5.315804	-0.195268	2.203840
C	5.458426	0.098651	0.077516
C	4.804594	-0.100212	-1.142838
H	5.296126	0.203144	-2.064821
C	3.535940	-0.685192	-1.219328
C	2.912854	-1.394604	2.505726
H	2.971970	-2.487665	2.598756
H	1.853864	-1.126006	2.565918
H	3.424550	-0.969467	3.374457
C	6.811286	0.768876	0.134749
H	6.708706	1.851241	0.288641
H	7.370388	0.624041	-0.795528
H	7.417265	0.380219	0.960229
C	2.888153	-0.918219	-2.563785
H	3.495392	-0.487087	-3.365174
H	1.890183	-0.472164	-2.613919
H	2.775300	-1.989080	-2.777033
C	0.117120	1.191143	-1.840808
C	-1.524452	3.668747	-0.052216
C	-2.476518	4.644466	0.640826
H	-2.405538	5.633093	0.182966
H	-3.505983	4.277670	0.557539
H	-2.244553	4.712128	1.709334
H	0.780506	2.014039	-2.125995
H	-0.317916	0.641998	-2.689873
C	1.685287	2.470514	0.348415
H	2.528293	2.032143	-0.178083
H	1.206000	3.334984	-0.100835
C	1.287161	1.976857	1.542677
H	0.500469	2.459409	2.115437
H	1.829297	1.170396	2.026122

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B3LYP SCF energy: -1326.99566518 a.u.
B3LYP enthalpy: -1326.415616 a.u.
B3LYP free energy: -1326.506007 a.u.
M06 SCF energy in solution: -1327.46521485 a.u.
M06 enthalpy in solution: -1326.885166 a.u.
M06 free energy in solution: -1326.975557 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.230223	1.034533	0.272430
O	1.295253	2.346294	-0.578107
O	-0.331759	3.328720	0.553895
N	-0.964365	-1.582751	-0.696610
N	1.205317	-1.634246	-0.328537
C	0.100766	-0.846973	-0.270122
C	-0.628783	-2.998265	-0.879622
H	-1.075369	-3.407728	-1.790562
H	-0.977699	-3.596868	-0.026570
C	0.908032	-2.944602	-0.944148
H	1.391064	-3.757721	-0.395330
H	1.276796	-2.964336	-1.978614
C	-2.300705	-1.056527	-0.389362
C	-2.791857	-1.586214	0.980946
H	-2.032304	-1.365297	1.738046
H	-2.916624	-2.677639	0.936744
C	-4.128406	-0.918963	1.358752
H	-4.464315	-1.307509	2.329538
C	-5.179563	-1.242688	0.278161
H	-5.349049	-2.327770	0.226822
H	-6.142492	-0.780791	0.535447
C	-4.692778	-0.712276	-1.086338
H	-5.438791	-0.941171	-1.858867
C	-3.356829	-1.401999	-1.463115
H	-3.007768	-1.058459	-2.446063
H	-3.509608	-2.489601	-1.532229
C	-4.501382	0.817566	-0.986827
H	-4.193364	1.227741	-1.958315
H	-5.459211	1.291871	-0.729680
C	-3.432980	1.145050	0.090841
H	-3.287037	2.230295	0.149188
C	-2.121878	0.475505	-0.343470
H	-1.905932	0.806252	-1.386429
C	-3.914381	0.605588	1.451881
H	-3.174859	0.835372	2.228298
H	-4.852743	1.100630	1.737902
C	2.567250	-1.207586	-0.163634
C	3.251183	-1.582213	1.009460
C	4.592343	-1.216587	1.145356
H	5.124613	-1.501888	2.050549
C	5.264975	-0.495640	0.152640
C	4.561116	-0.151458	-1.003034
H	5.069327	0.401166	-1.790686
C	3.215870	-0.492832	-1.186582
C	2.562824	-2.353714	2.111083
H	3.251548	-2.536565	2.941412
H	2.193116	-3.328180	1.768028
H	1.699540	-1.804666	2.502204
C	6.707173	-0.083534	0.337358
H	6.779229	0.873217	0.871676
H	7.214541	0.042742	-0.624933
H	7.265362	-0.823383	0.921575
C	2.503792	-0.061539	-2.446371
H	1.748821	-0.784477	-2.771133
H	3.218481	0.071908	-3.265251
H	1.998484	0.896001	-2.276679
C	-0.253993	0.635683	2.050744
C	0.725813	3.411652	-0.125402
C	1.365927	4.747779	-0.426741
H	0.064827	-0.293040	2.537855
H	-0.532166	1.448648	2.737401
H	1.536493	4.843663	-1.504103
H	0.736287	5.565928	-0.072213
H	2.344821	4.799801	0.063051

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B3LYP SCF energy: -1326.98939170 a.u.
B3LYP enthalpy: -1326.409194 a.u.
B3LYP free energy: -1326.500412 a.u.
M06 SCF energy in solution: -1327.45804345 a.u.
M06 enthalpy in solution: -1326.877846 a.u.
M06 free energy in solution: -1326.969064 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.298157	0.868944	-0.558367
O	0.375837	2.366038	0.867169
O	-0.848094	3.125602	-0.810979
N	-0.777707	-1.753638	0.448391
N	1.401929	-1.488462	0.540519
C	0.240945	-0.900517	0.151397
C	-0.353440	-2.848385	1.322376
H	-0.815548	-3.798269	1.038993
H	-0.608776	-2.640190	2.372076
C	1.171409	-2.839264	1.094547
H	1.744951	-2.981642	2.014942
H	1.477962	-3.609053	0.374862
C	-2.138489	-1.227188	0.274092
C	-2.595723	-0.418517	1.517334
H	-1.847148	0.351645	1.755693
H	-2.659859	-1.079552	2.394084
C	-3.963177	0.239307	1.242424
H	-4.278918	0.802529	2.130609
C	-4.998532	-0.861329	0.929909
H	-5.113692	-1.530285	1.794756
H	-5.982043	-0.409602	0.742515
C	-4.543074	-1.661655	-0.307771
H	-5.279783	-2.444501	-0.531698
C	-3.178114	-2.329826	-0.011426
H	-2.848805	-2.931106	-0.869117
H	-3.280044	-3.009771	0.848328
C	-4.422396	-0.701133	-1.512818
H	-4.129626	-1.258046	-2.413262
H	-5.402666	-0.248572	-1.720629
C	-3.373917	0.399992	-1.205526
H	-3.288360	1.078080	-2.063098
C	-2.025262	-0.297749	-0.963596
H	-1.809326	-0.940659	-1.821702
C	-3.831998	1.192568	0.036049
H	-3.115451	1.995115	0.251033
H	-4.799016	1.675167	-0.163324
C	2.727792	-0.997389	0.297971
C	3.309591	-0.104314	1.217233
C	4.614995	0.337367	0.974798
H	5.070484	1.028624	1.680955
C	5.347046	-0.081215	-0.139595
C	4.745888	-0.983102	-1.022769
H	5.301603	-1.328863	-1.892360
C	3.445142	-1.455707	-0.824373
C	2.558933	0.390025	2.430577
H	3.255000	0.798889	3.170308
H	1.985588	-0.411230	2.909821
H	1.850503	1.179723	2.155339
C	6.741316	0.442323	-0.396326
H	6.717033	1.333273	-1.037933
H	7.364281	-0.303824	-0.901580
H	7.240730	0.727126	0.535825
C	2.854392	-2.449481	-1.799453
H	2.974672	-3.482521	-1.445065
H	3.357235	-2.384220	-2.769391
H	1.785063	-2.282465	-1.959668
C	0.546675	0.722732	-2.159538
C	-0.191625	3.342282	0.239930

C	-0.033202	4.737597	0.799874
H	1.018275	5.038591	0.729309
H	-0.652124	5.446719	0.247145
H	-0.303156	4.747388	1.860856
H	0.372746	1.535273	-2.880835
H	1.294562	-0.020243	-2.453443

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B3LYP SCF energy: -1326.98664658 a.u.
B3LYP enthalpy: -1326.406542 a.u.
B3LYP free energy: -1326.498690 a.u.
M06 SCF energy in solution: -1327.46171336 a.u.
M06 enthalpy in solution: -1326.881609 a.u.
M06 free energy in solution: -1326.973757 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.289138	0.983700	0.724272
O	0.487816	2.412093	-1.048692
O	1.662206	2.028442	0.781954
N	-1.092405	-1.396308	-0.653092
N	1.077402	-1.535015	-0.292515
C	-0.021741	-0.751751	-0.127549
C	-0.793120	-2.775130	-1.040961
H	-1.199086	-3.012706	-2.029098
H	-1.218613	-3.484534	-0.318265
C	0.749410	-2.784451	-1.013452
H	1.161383	-3.650306	-0.486221
H	1.178999	-2.766972	-2.021793
C	-2.421309	-0.817787	-0.435072
C	-3.113571	-1.468558	0.787359
H	-2.446117	-1.410050	1.652510
H	-3.302948	-2.532876	0.584968
C	-4.439569	-0.744135	1.087437
H	-4.919704	-1.212650	1.957041
C	-5.366370	-0.855194	-0.139816
H	-5.599063	-1.910283	-0.343167
H	-6.321455	-0.350170	0.059253
C	-4.676848	-0.213099	-1.361511
H	-5.332868	-0.290249	-2.238647
C	-3.353441	-0.962561	-1.659520
H	-2.862658	-0.541172	-2.546375
H	-3.570894	-2.020041	-1.874349
C	-4.402911	1.275872	-1.049429
H	-3.949626	1.771706	-1.917824
H	-5.354965	1.787702	-0.848085
C	-3.455861	1.391196	0.176208
H	-3.261084	2.452307	0.382896
C	-2.143537	0.683531	-0.201815
H	-1.817813	1.099822	-1.171704
C	-4.136723	0.737312	1.394344
H	-3.488055	0.810193	2.276227
H	-5.068451	1.269180	1.633121
C	2.452028	-1.129340	-0.172951
C	3.161616	-1.451012	0.995704
C	4.517780	-1.115273	1.064879
H	5.072500	-1.361347	1.967967
C	5.175336	-0.476513	0.010826
C	4.440942	-0.178488	-1.141550
H	4.938095	0.309407	-1.977845
C	3.082454	-0.488953	-1.258014
C	2.487580	-2.124109	2.167064
H	3.227098	-2.442026	2.908387
H	1.911812	-3.005978	1.863530
H	1.789394	-1.437395	2.658904
C	6.634162	-0.097627	0.118959
H	6.748749	0.925775	0.500301
H	7.133238	-0.138241	-0.855491
H	7.171917	-0.761646	0.804065
C	2.330409	-0.116681	-2.516372
H	1.847650	-0.981204	-2.987564
H	3.014235	0.314333	-3.254181
H	1.548882	0.622770	-2.309377
C	-0.589382	0.260284	2.381791
H	-0.459084	-0.761172	2.760423
C	1.510241	2.628144	-0.337282
C	2.594019	3.580287	-0.797950
H	-0.895346	0.968243	3.175171
H	3.503011	3.008784	-1.017960
H	2.839124	4.285393	0.002640
H	2.279119	4.121840	-1.692244

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B3LYP SCF energy: -1405.58816366 a.u.
B3LYP enthalpy: -1404.949189 a.u.
B3LYP free energy: -1405.045690 a.u.
M06 SCF energy in solution: -1406.02906890 a.u.
M06 enthalpy in solution: -1405.390094 a.u.
M06 free energy in solution: -1405.486595 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.331435	1.092369	-0.460909
O	-0.301206	1.995636	1.697157
O	-1.743005	1.727020	0.048062
N	0.947894	-1.639988	0.378709
N	-1.216193	-1.610898	0.046138
C	-0.090819	-0.850625	0.036764
C	0.594784	-3.058186	0.501196
H	0.972715	-3.486178	1.434596
H	1.016012	-3.635913	-0.331757
C	-0.942097	-3.007869	0.451786
H	-1.371601	-3.705010	-0.274627
H	-1.394289	-3.217435	1.427621
C	2.314161	-1.120943	0.294802
C	2.990938	-1.573759	-1.024995
H	2.372926	-1.276938	-1.877481
H	3.069034	-2.670647	-1.042522
C	4.392580	-0.948449	-1.141003
H	4.853956	-1.265989	-2.085722
C	5.257880	-1.422215	0.044025
H	5.373891	-2.515067	0.012689
H	6.266504	-0.992255	-0.025429
C	4.593139	-0.991063	1.367360
H	5.202256	-1.330650	2.215678
C	3.186926	-1.622732	1.473534
H	2.710825	-1.346546	2.423389
H	3.275360	-2.719374	1.456239
C	4.476791	0.545480	1.388204
H	4.040450	0.882197	2.337966
H	5.478197	0.994439	1.317980
C	3.592956	1.025642	0.206109
H	3.542447	2.116608	0.246161
C	2.186656	0.419467	0.384773
H	1.859514	0.654073	1.410706
C	4.249825	0.586775	-1.117393
H	3.639951	0.915293	-1.968994
H	5.237297	1.058084	-1.221698
C	-2.588179	-1.195059	-0.058694
C	-3.218123	-1.198256	-1.313670
C	-4.577381	-0.871574	-1.377369
H	-5.069659	-0.871423	-2.347813
C	-5.315738	-0.549969	-0.236797
C	-4.661155	-0.571187	0.999225
H	-5.220432	-0.331682	1.901777
C	-3.305420	-0.889412	1.114021
C	-2.465841	-1.527231	-2.580459
H	-3.160805	-1.744057	-3.397824
H	-1.805034	-2.392501	-2.456945
H	-1.835195	-0.685252	-2.888288
C	-6.774535	-0.168034	-0.335707
H	-6.893494	0.920771	-0.415571
H	-7.336020	-0.491144	0.547863
H	-7.246479	-0.611770	-1.218825

C	-2.646166	-0.892493	2.474868
H	-2.453670	-1.911555	2.836729
H	-3.292843	-0.410067	3.214056
H	-1.688556	-0.362651	2.467620
C	0.594354	0.568008	-2.211855
H	0.471344	-0.443284	-2.620094
C	-1.466733	2.120309	1.232740
C	-2.564229	2.781713	2.044485
H	0.878440	1.286948	-2.996664
H	-3.530956	2.320044	1.827082
H	-2.629461	3.841147	1.766980
H	-2.340125	2.720859	3.112226
C	0.212034	3.324438	-1.269290
H	-0.080392	3.224457	-2.309880
H	-0.528530	3.769316	-0.616426
C	1.500760	3.136160	-0.861490
H	1.808411	3.430041	0.136975
H	2.292459	2.900204	-1.564476

25-TS
B3LYP SCF energy: -1405.56116117 a.u.
B3LYP enthalpy: -1404.923911 a.u.
B3LYP free energy: -1405.019414 a.u.
M06 SCF energy in solution: -1406.00050331 a.u.
M06 enthalpy in solution: -1405.363253 a.u.
M06 free energy in solution:-1405.458756 a.u.
Imaginary frequency: -141.8986 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	6.828174	5.401115	7.549016
O	4.854615	5.655092	6.329535
O	6.635390	6.836124	5.724358
N	6.856797	2.471608	7.328314
N	7.005589	3.167246	5.259758
C	6.904771	3.562460	6.548925
C	6.969604	1.208795	6.588187
H	6.078974	0.589425	6.739133
H	7.840875	0.634348	6.922947
C	7.110369	1.696055	5.131619
H	8.075766	1.429424	4.685905
H	6.322027	1.307746	4.480190
C	6.834824	2.596090	8.790948
C	8.261583	2.388727	9.359843
H	8.949892	3.089496	8.877002
H	8.613183	1.372895	9.124743
C	8.253934	2.596368	10.886723
H	9.269690	2.452276	11.279183
C	7.297890	1.573817	11.533258
H	7.646255	0.550436	11.332768
H	7.289740	1.700899	12.624457
C	5.876576	1.774175	10.968130
H	5.192115	1.047771	11.426311
C	5.899310	1.545719	9.438651
H	4.889773	1.645217	9.019028
H	6.243517	0.520895	9.230394
C	5.404687	3.208879	11.288366
H	4.377855	3.359566	10.929909
H	5.388775	3.355358	12.378645
C	6.354739	4.234713	10.614730
H	6.005032	5.245367	10.866270
C	6.294564	4.015819	9.084141
H	5.218871	3.974098	8.833801
C	7.769970	4.027594	11.195764
H	8.473663	4.757861	10.779514
H	7.754297	4.187240	12.283678
C	7.061140	3.972686	4.072339
C	8.286354	4.534666	3.673206
C	8.331557	5.243311	2.469494
H	9.275909	5.684402	2.157065
C	7.202606	5.397300	1.659355
C	6.003657	4.814840	2.080530
H	5.114188	4.921818	1.462882
C	5.904896	4.102831	3.281275
C	9.528824	4.386699	4.517010
H	10.398884	4.804363	4.001273
H	9.747162	3.336393	4.747309
H	9.413521	4.908566	5.472574
C	7.271355	6.195185	0.377592
H	7.108516	7.264343	0.568584
H	6.507928	5.872367	-0.338294
H	8.250868	6.098956	-0.103651
C	4.577352	3.526005	3.716262
H	4.591975	2.429288	3.760307
H	3.789105	3.809205	3.011758
H	4.303658	3.898785	4.708950
C	8.613832	5.688861	8.043649
H	9.212731	5.284870	8.874083
C	5.413639	6.531970	5.588416
H	9.202736	6.405696	7.446212
C	4.576272	7.267359	4.555637
H	3.631498	6.749176	4.375589
H	4.355217	8.276385	4.925352
H	5.134802	7.370964	3.621734
C	5.917248	7.125136	8.646065
C	7.239916	7.201013	9.081690
H	5.569429	7.814488	7.884648
H	5.159813	6.669934	9.276604
H	7.523465	6.807017	10.051328
H	7.890669	7.963240	8.662771

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B3LYP SCF energy: -1405.56648408 a.u.
B3LYP enthalpy: -1404.926322 a.u.
B3LYP free energy: -1405.020867 a.u.
M06 SCF energy in solution: -1406.01027922 a.u.
M06 enthalpy in solution: -1405.370117 a.u.
M06 free energy in solution:-1405.464662 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.349148	1.186124	0.113892
O	1.200214	1.184745	-1.768337
O	1.734830	2.108908	0.178430
N	-1.002635	-1.665895	-0.267308
N	1.177179	-1.596570	-0.076925
C	0.047930	-0.851914	-0.108861
C	-0.635216	-3.082664	-0.384042
H	-0.854817	-3.452681	-1.392281
H	-1.192450	-3.694701	0.331977
C	0.874283	-3.047087	-0.085290
H	1.123672	-3.480172	0.891606
H	1.468908	-3.562229	-0.843710
C	-2.369411	-1.148165	-0.159463
C	-2.919045	-1.420631	1.264489
H	-2.248154	-0.961211	1.999809
H	-2.936502	-2.502930	1.461254
C	-4.339058	-0.838734	1.399926
H	-4.721531	-1.046074	2.408458
C	-5.267908	-1.479923	0.350119
H	-5.340070	-2.564562	0.515533
H	-6.283845	-1.073801	0.449476
C	-4.717248	-1.191060	-1.061508
H	-5.378115	-1.640295	-1.814779
C	-3.310714	-1.818318	-1.189302
H	-2.910300	-1.668596	-2.200383
H	-3.380516	-2.904089	-1.020573
C	-4.644804	0.337165	-1.277120
H	-4.293509	0.559679	-2.293389
H	-5.652405	0.768560	-1.183471
C	-3.683097	0.968233	-0.233213
H	-3.661035	2.054882	-0.391821
C	-2.273042	0.363051	-0.458761
H	-2.104581	0.426156	-1.547707

C	-4.267592	0.681540	1.167767
H	-3.663295	1.146478	1.952300
H	-5.274206	1.117996	1.242858
C	2.537707	-1.190411	0.135999
C	2.970922	-0.859611	1.433322
C	4.326210	-0.581914	1.628766
H	4.667283	-0.323702	2.629271
C	5.251233	-0.632013	0.580581
C	4.785949	-0.964953	-0.694438
H	5.488431	-1.003162	-1.524381
C	3.437043	-1.242987	-0.944485
C	2.008040	-0.789754	2.593791
H	2.550091	-0.703055	3.540429
H	1.365211	-1.676029	2.653205
H	1.350411	0.082171	2.501660
C	6.709187	-0.315107	0.822160
H	6.860284	0.760555	0.981152
H	7.330143	-0.613027	-0.028793
H	7.088942	-0.827675	1.713815
C	2.968628	-1.538887	-2.349432
H	2.529449	-2.539762	-2.446384
H	3.805801	-1.482584	-3.052092
H	2.210302	-0.807421	-2.648651
C	-0.976068	2.021214	1.775469
C	1.998169	1.848858	-1.040103
C	3.297576	2.376271	-1.625112
H	4.146151	1.962987	-1.071148
H	3.332201	3.465840	-1.513727
H	3.386367	2.114661	-2.681839
C	-1.078612	3.262720	0.690838
C	-0.984235	2.869384	-0.796734
H	-0.312030	3.994649	0.942769
H	-2.088350	3.637542	0.866622
H	-0.174803	2.240587	2.490383
H	-1.934032	1.879898	2.274011
H	-0.187942	3.361299	-1.353883
H	-1.931767	2.846554	-1.332139

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B3LYP SCF energy: -1405.56984810 a.u.
B3LYP enthalpy: -1404.929739 a.u.
B3LYP free energy: -1405.024106 a.u.
M06 SCF energy in solution: -1406.01266240 a.u.
M06 enthalpy in solution: -1405.372553 a.u.
M06 free energy in solution: -1405.466920 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.303193	1.135056	-0.304072
O	1.680771	2.066366	0.280955
O	0.645988	1.028349	1.949439
N	-0.982870	-1.724403	-0.014565
N	1.204713	-1.622453	-0.020827
C	0.064554	-0.894712	-0.080603
C	-0.592596	-3.103399	0.302019
H	-1.146180	-3.825618	-0.302774
H	-0.778153	-3.322425	1.362147
C	0.907918	-3.073658	-0.027292
H	1.521111	-3.600409	0.707128
H	1.123590	-3.491901	-1.019716
C	-2.336158	-1.162688	0.036693
C	-2.792169	-1.007821	1.508157
H	-2.071595	-0.378096	2.043350
H	-2.803806	-1.991362	2.001112
C	-4.196048	-0.376181	1.554090
H	-4.516681	-0.277510	2.599796
C	-5.198400	-1.256881	0.783657
H	-5.272096	-2.250136	1.249476
H	-6.200828	-0.809109	0.823604
C	-4.735864	-1.388890	-0.681174
H	-5.447858	-2.011031	-1.239916
C	-3.347937	-2.068187	-0.704263
H	-3.009543	-2.226381	-1.736869
H	-3.422815	-3.057585	-0.226850
C	-4.658790	0.015497	-1.320798
H	-4.376117	-0.065704	-2.378800
H	-5.652946	0.485639	-1.288919
C	-3.621166	0.885334	-0.560695
H	-3.595360	1.880898	-1.026593
C	-2.234894	0.201885	-0.694268
H	-2.138055	-0.053043	-1.761490
C	-4.111789	1.015360	0.902009
H	-3.440531	1.639982	1.498915
H	-5.099411	1.498800	0.916859
C	2.559592	-1.177196	-0.181046
C	3.404452	-1.175043	0.944270
C	4.742929	-0.810689	0.764071
H	5.403665	-0.805816	1.628740
C	5.251358	-0.450424	-0.487731
C	4.385793	-0.478919	-1.585021
H	4.765662	-0.215386	-2.569959
C	3.041939	-0.843031	-1.459022
C	2.888492	-1.536146	2.317959
H	3.650382	-1.336089	3.077644
H	2.628449	-2.600345	2.395076
H	1.993191	-0.954875	2.560891
C	6.691186	-0.020791	-0.647490
H	6.792787	1.066470	-0.531713
H	7.079298	-0.278564	-1.638866
H	7.336632	-0.489747	0.102949
C	2.148188	-0.877141	-2.676509
H	1.625895	-1.836413	-2.776289
H	2.733498	-0.720028	-3.587587
H	1.379743	-0.097616	-2.632052
C	-0.472077	2.004020	-2.059678
C	1.605152	1.729376	1.507006
C	2.705474	2.189850	2.448763
H	2.456971	1.955122	3.486154
H	2.859530	3.268397	2.338511
H	3.645866	1.697658	2.177597
C	-1.215556	2.796306	0.394195
C	-0.795705	3.231053	-1.032202
H	0.468631	2.212580	-2.579864
H	-1.300693	1.834043	-2.754013
H	-1.676381	3.693607	-1.482789
H	0.057262	3.907302	-1.003644
H	-0.641764	3.253471	1.200515
H	-2.285110	2.827725	0.561392

28-TS

B3LYP SCF energy: -1405.56472023 a.u.
B3LYP enthalpy: -1404.926898 a.u.
B3LYP free energy: -1405.020897 a.u.
M06 SCF energy in solution: -1406.00427585 a.u.
M06 enthalpy in solution: -1405.366454 a.u.
M06 free energy in solution: -1405.460453 a.u.
Imaginary frequency: -137.0719 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.329449	1.074099	-0.494526
O	0.154565	1.297564	1.775627
O	1.612133	2.096725	0.304284
N	-0.918278	-1.761641	-0.005833
N	1.266525	-1.643735	0.030859
C	0.128775	-0.929678	-0.119100
C	-0.529605	-3.105130	0.442508
H	-1.048251	-3.882811	-0.124135
H	-0.764130	-3.238852	1.507165
C	0.986685	-3.089487	0.181474
H	1.570055	-3.516579	1.001137
H	1.252996	-3.620003	-0.741967
C	-2.268719	-1.185392	0.079702
C	-2.612125	-0.875615	1.559578

H	-1.844255	-0.215239	1.976616
H	-2.605985	-1.807261	2.145033
C	-3.998760	-0.211431	1.646462
H	-4.235641	-0.000478	2.697851
C	-5.065646	-1.150403	1.051055
H	-5.113564	-2.085620	1.627228
H	-6.058618	-0.684241	1.114699
C	-4.717902	-1.447964	-0.421802
H	-5.476012	-2.115113	-0.853705
C	-3.338759	-2.145297	-0.486949
H	-3.087183	-2.408051	-1.523258
H	-3.379150	-3.082949	0.089068
C	-4.684810	-0.119663	-1.208935
H	-4.482672	-0.313188	-2.270995
H	-5.671860	0.362943	-1.152393
C	-3.589920	0.812420	-0.624409
H	-3.596078	1.752410	-1.194154
C	-2.219109	0.104901	-0.782678
H	-2.187266	-0.246484	-1.829059
C	-3.951013	1.105602	0.849880
H	-3.215608	1.772348	1.313109
H	-4.925697	1.612366	0.900082
C	2.617922	-1.173826	-0.078931
C	3.342830	-0.925340	1.100351
C	4.671755	-0.506526	0.984454
H	5.238584	-0.305497	1.891421
C	5.287279	-0.333248	-0.258960
C	4.545035	-0.617110	-1.408984
H	5.012659	-0.506880	-2.385322
C	3.215230	-1.044743	-1.344611
C	2.712774	-1.109242	2.461895
H	3.369080	-0.718640	3.245516
H	2.536202	-2.169893	2.687460
H	1.749058	-0.595558	2.529790
C	6.709546	0.167560	-0.357320
H	7.199523	-0.190219	-1.269249
H	7.309889	-0.155184	0.500286
H	6.739336	1.265068	-0.380533
C	2.461552	-1.379287	-2.610573
H	2.186262	-2.441348	-2.650747
H	3.073359	-1.165622	-3.492276
H	1.533958	-0.803976	-2.690447
C	-1.160408	3.118662	-0.240799
H	-2.157489	3.020516	0.167463
C	1.237618	1.915537	1.498730
H	-0.434538	3.656975	0.359288
C	2.081564	2.474375	2.632419
H	1.729232	2.113096	3.601112
H	3.131025	2.201266	2.485461
H	2.025407	3.569368	2.619662
C	-0.128448	1.168835	-2.359326
C	-0.974438	3.057528	-1.631067
H	0.788396	1.591019	-2.797229
H	-0.832832	0.824261	-3.136664
H	-1.832541	2.918043	-2.282417
H	-0.124583	3.576725	-2.064607

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B3LYP SCF energy: -1405.58150201 a.u.
B3LYP enthalpy: -1404.942492 a.u.
B3LYP free energy: -1405.038380 a.u.
M06 SCF energy in solution: -1406.02158335 a.u.
M06 enthalpy in solution: -1405.382573 a.u.
M06 free energy in solution: -1405.478461 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.309693	1.023578	-0.713324
O	1.435645	1.718003	0.508404
O	-0.501718	1.810738	1.560023
N	-0.872958	-1.785975	-0.094218
N	1.310871	-1.594936	-0.048324
C	0.151098	-0.916229	-0.237075
C	-0.444275	-3.088983	0.428220
H	-0.932176	-3.913357	-0.098769
H	-0.681252	-3.175810	1.497411
C	1.070240	-3.037882	0.175507
H	1.661826	-3.405611	1.018005
H	1.360851	-3.607046	-0.717540
C	-2.218007	-1.219898	0.079428
C	-2.450170	-0.833409	1.563558
H	-1.660251	-0.150590	1.889189
H	-2.404760	-1.735376	2.192338
C	-3.825840	-0.158444	1.719443
H	-3.976334	0.115449	2.772085
C	-4.929699	-1.137812	1.273483
H	-4.922919	-2.033082	1.911912
H	-5.919426	-0.673636	1.385014
C	-4.699770	-1.530442	-0.200547
H	-5.482050	-2.230169	-0.524254
C	-3.321524	-2.216268	-0.344784
H	-3.154986	-2.533648	-1.383092
H	-3.295580	-3.120338	0.282538
C	-4.747443	-0.256030	-1.067190
H	-4.630158	-0.512519	-2.129048
H	-5.730373	0.225711	-0.960765
C	-3.624220	0.723620	-0.632577
H	-3.690898	1.615920	-1.263001
C	-2.270006	0.015045	-0.853681
H	-2.290745	-0.382670	-1.872338
C	-3.849045	1.110904	0.844172
H	-3.069072	1.800269	1.185406
H	-4.816002	1.623354	0.951629
C	2.660759	-1.102831	-0.041874
C	3.248163	-0.792254	1.202480
C	4.577597	-0.371607	1.227382
H	5.031469	-0.123851	2.185037
C	5.340687	-0.260024	0.058732
C	4.740252	-0.605065	-1.151498
H	5.321858	-0.547883	-2.069717
C	3.407552	-1.032654	-1.228045
C	2.475902	-0.928198	2.493398
H	2.344892	-1.981076	2.779588
H	1.478223	-0.487136	2.420297
H	3.007836	-0.437032	3.313747
C	6.768750	0.230707	0.111972
H	6.807274	1.324969	0.194546
H	7.323048	-0.049022	-0.789924
H	7.302307	-0.176847	0.978279
C	2.834804	-1.396408	-2.577202
H	3.600049	-1.862469	-3.207403
H	2.474998	-0.503486	-3.102030
H	1.989158	-2.084734	-2.499686
C	0.023526	0.640949	-2.485736
C	0.743859	2.017112	1.538424
C	1.436689	2.668532	2.720220
H	1.286731	3.754081	2.670409
H	2.510184	2.467316	2.700267
H	0.998198	2.317448	3.658511
H	0.074485	1.430811	-3.252012
H	0.141837	-0.358130	-2.923319
C	-1.505735	2.976186	-1.342800
H	-1.987700	2.748144	-2.287766
H	-2.160685	3.152420	-0.496556
C	-0.179711	3.304527	-1.277098
H	0.246349	3.751217	-0.386953
H	0.446890	3.338535	-2.163278

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B3LYP SCF energy: -1326.97937731 a.u.
B3LYP enthalpy: -1326.399082 a.u.
B3LYP free energy: -1326.490417 a.u.
M06 SCF energy in solution: -1327.45066746 a.u.
M06 enthalpy in solution: -1326.870372 a.u.

M06 free energy in solution:-1326.961707 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.263176	0.752371	-0.946314
O	0.987703	2.513436	-0.376975
O	-1.056886	2.566413	0.453708
N	-0.850995	-1.379521	0.852218
N	1.333131	-1.089429	0.908176
C	0.175377	-0.659588	0.329669
C	-0.449810	-2.154152	2.025885
H	-0.904797	-3.148806	2.027752
H	-0.740768	-1.640476	2.953144
C	1.079428	-2.199332	1.852058
H	1.623556	-2.038979	2.787292
H	1.411831	-3.151740	1.420501
C	-2.217314	-0.988867	0.478593
C	-2.792696	0.058206	1.465144
H	-2.102509	0.899736	1.564346
H	-2.913831	-0.400983	2.458072
C	-4.157282	0.558305	0.950009
H	-4.552491	1.306828	1.649274
C	-5.131576	-0.632457	0.856037
H	-5.285411	-1.076213	1.850341
H	-6.114998	-0.294623	0.501040
C	-4.557108	-1.684772	-0.114872
H	-5.244205	-2.538729	-0.184788
C	-3.190970	-2.187068	0.418121
H	-2.782325	-2.964015	-0.241901
H	-3.330673	-2.638416	1.412402
C	-4.395062	-1.036671	-1.509144
H	-4.031489	-1.777466	-2.234397
H	-5.376328	-0.692722	-1.866957
C	-3.402397	0.154428	-1.424642
H	-3.291272	0.603235	-2.421482
C	-2.052804	-0.419601	-0.953452
H	-1.828148	-1.280325	-1.591028
C	-3.963305	1.202109	-0.440104
H	-3.280688	2.053976	-0.357733
H	-4.926210	1.581470	-0.811573
C	2.677003	-0.822463	0.474827
C	3.395724	0.231017	1.070488
C	4.720280	0.439556	0.675378
H	5.278079	1.255516	1.130281
C	5.344651	-0.363595	-0.283372
C	4.612527	-1.416707	-0.837093
H	5.084007	-2.063571	-1.574601
C	3.286949	-1.671549	-0.469420
C	2.763428	1.140567	2.093660
H	3.530471	1.660639	2.676375
H	2.114163	0.594980	2.786138
H	2.149276	1.889472	1.583845
C	6.764455	-0.087471	-0.720764
H	6.791409	0.661493	-1.523368
H	7.251059	-0.991566	-1.101845
H	7.369700	0.302184	0.105099
C	2.574607	-2.865317	-1.067370
H	2.748178	-3.771804	-0.470932
H	2.949355	-3.073126	-2.074962
H	1.493598	-2.717896	-1.133215
C	0.581502	-0.013700	-2.371983
C	0.068177	3.110754	0.282938
C	0.369447	4.466771	0.887773
H	-0.547445	5.053391	0.982958
H	1.107512	5.002636	0.285835
H	0.788272	4.326473	1.892175
H	0.422914	0.511433	-3.334049
H	1.279066	-0.852870	-2.453038

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B3LYP SCF energy: -1484.20505563 a.u.

B3LYP enthalpy: -1483.507505 a.u.

B3LYP free energy: -1483.608001 a.u.

M06 SCF energy in solution: -1484.60295414 a.u.

M06 enthalpy in solution: -1483.905404 a.u.

M06 free energy in solution:-1484.005900 a.u.

Imaginary frequency: -221.1622 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.299628	0.901423	0.225208
O	1.459526	1.779851	-1.750810
O	1.285701	2.915830	0.143133
N	0.671284	-1.982652	0.186183
N	-1.493909	-1.729530	0.022068
C	-0.308564	-1.042966	0.116478
C	0.202729	-3.349302	-0.054535
H	0.636360	-4.053773	0.660606
H	0.471057	-3.682388	-1.066783
C	-1.312363	-3.192096	0.116488
H	-1.889985	-3.705530	-0.658035
H	-1.657537	-3.555346	1.094087
C	2.078005	-1.579573	0.099250
C	2.586108	-1.669269	-1.363321
H	1.947975	-1.048123	-2.002350
H	2.517416	-2.706985	-1.722174
C	4.048255	-1.183717	-1.443815
H	4.397700	-1.269793	-2.481566
C	4.936724	-2.044072	-0.524337
H	4.920473	-3.095752	-0.846128
H	5.980351	-1.706678	-0.588182
C	4.430453	-1.925839	0.927613
H	5.064238	-2.529800	1.591202
C	2.981758	-2.461528	0.994808
H	2.605318	-2.436892	2.026534
H	2.968400	-3.512067	0.665874
C	4.479093	-0.444912	1.368365
H	4.157486	-0.351441	2.415039
H	5.516349	-0.082412	1.319294
C	3.565520	0.410462	0.447262
H	3.601215	1.457290	0.770820
C	2.129081	-0.129361	0.608343
H	1.944928	-0.177737	1.694652
C	4.102077	0.288788	-0.995628
H	3.506884	0.900248	-1.675798
H	5.140524	0.650018	-1.033280
C	-2.825174	-1.225860	-0.133429
C	-3.317860	-1.014262	-1.440604
C	-4.631248	-0.567863	-1.596958
H	-5.009163	-0.391327	-2.601951
C	-5.475484	-0.350505	-0.500190
C	-4.978674	-0.622995	0.774910
H	-5.628044	-0.490603	1.638379
C	-3.667572	-1.074958	0.982712
C	-2.461777	-1.300273	-2.654176
H	-2.967094	-0.974823	-3.568371
H	-2.262325	-2.375472	-2.753535
H	-1.489084	-0.801184	-2.605087
C	-6.881112	0.167394	-0.698146
H	-7.362111	-0.300169	-1.564705
H	-6.882397	1.251089	-0.874670
H	-7.506018	-0.022586	0.180437
C	-3.229446	-1.437780	2.384182
H	-2.143513	-1.504291	2.474334
H	-3.649210	-2.408703	2.680174
H	-3.587721	-0.701877	3.112492
C	-1.321722	1.793757	-0.927330
H	-1.841579	1.028106	-1.487217
C	1.703564	2.807927	-1.059449
C	2.539880	3.932491	-1.643371
H	2.369941	4.017145	-2.720107
H	2.319440	4.881143	-1.147186
H	3.602004	3.704799	-1.488870
C	-0.576164	1.164176	1.885944
H	-1.369015	0.522727	2.283677
C	-1.809722	2.149947	0.360497

H	-2.642793	1.556171	0.729061
C	-1.790524	3.601917	0.790435
H	-2.568186	4.145093	0.235644
H	-2.000892	3.732162	1.855685
H	-0.823407	4.056873	0.562865
H	-0.869900	2.573906	-1.533537
C	-0.058206	2.144156	2.903630
H	-0.859125	2.655802	3.456349
H	0.511738	1.563919	3.647777
H	0.616436	2.883162	2.465312

33-TS

B3LYP SCF energy: -1484.20270299 a.u.
B3LYP enthalpy: -1483.505090 a.u.
B3LYP free energy: -1483.605740 a.u.
M06 SCF energy in solution: -1484.60315057 a.u.
M06 enthalpy in solution: -1483.905538 a.u.
M06 free energy in solution:-1484.006188 a.u.
Imaginary frequency: -227.8930 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.373454	0.817943	0.290245
O	-1.319630	2.845252	0.380717
O	-0.753826	2.177099	-1.654794
N	-0.768332	-2.002096	-0.241750
N	1.399391	-1.815448	0.007748
C	0.224934	-1.101566	-0.025941
C	-0.332316	-3.396162	-0.161920
H	-0.775351	-4.005854	-0.954715
H	-0.611932	-3.837911	0.805086
C	1.186241	-3.246950	-0.305530
H	1.750107	-3.885442	0.380433
H	1.527044	-3.461444	-1.327598
C	-2.160482	-1.554414	-0.153402
C	-2.726003	-1.768150	1.273150
H	-2.059013	-1.294200	2.000985
H	-2.760457	-2.843172	1.504420
C	-4.140489	-1.165094	1.369663
H	-4.527210	-1.310440	2.387628
C	-5.061663	-1.878105	0.359170
H	-5.131664	-2.948722	0.600449
H	-6.079767	-1.469730	0.419878
C	-4.503172	-1.685761	-1.066150
H	-5.152538	-2.197819	-1.789040
C	-3.083294	-2.296195	-1.150898
H	-2.680424	-2.194223	-2.167228
H	-3.133980	-3.371930	-0.922636
C	-4.455749	-0.175649	-1.384287
H	-4.098273	-0.013375	-2.410044
H	-5.471059	0.243800	-1.328378
C	-3.516607	0.543493	-0.379939
H	-3.493635	1.612603	-0.611230
C	-2.111827	-0.062574	-0.541549
H	-1.846055	-0.017125	-1.606248
C	-4.066822	0.342201	1.046280
H	-3.422480	0.854943	1.770403
H	-5.067620	0.789488	1.128983
C	2.727313	-1.310372	-0.182607
C	3.655080	-1.418042	0.868966
C	4.968617	-0.984445	0.650116
H	5.685532	-1.052841	1.465832
C	5.381998	-0.471820	-0.581415
C	4.439578	-0.394043	-1.613923
H	4.742354	0.001719	-2.581408
C	3.115824	-0.808750	-1.444296
C	3.266794	-2.001165	2.208347
H	3.983440	-1.708852	2.982245
H	3.252773	-3.099408	2.179849
H	2.268245	-1.679121	2.518364
C	6.811107	-0.034672	-0.806284
H	7.364623	-0.775899	-1.397887
H	7.344199	0.094224	0.141048
H	6.858867	0.913731	-1.353317
C	2.129940	-0.678836	-2.582847
H	1.399278	0.116876	-2.392451
H	1.557074	-1.599536	-2.740308
H	2.650654	-0.444022	-3.516094
C	-0.278161	0.571394	2.153858
H	0.164858	-0.245251	2.739544
C	-1.284477	3.027707	-0.881923
C	-1.857226	4.311928	-1.453818
H	-1.056221	5.056842	-1.541753
H	-2.261039	4.136483	-2.454501
H	-2.630641	4.718428	-0.797276
C	1.654675	1.878665	0.251143
H	2.264077	1.155065	-0.275767
C	1.521369	1.657461	1.648256
H	2.078789	0.806605	2.031675
C	1.357917	2.821213	2.608522
H	1.215713	2.478579	3.637605
H	2.259805	3.449399	2.585059
H	0.504901	3.446192	2.331471
C	1.720731	3.269220	-0.337023
H	2.733632	3.676091	-0.190572
H	1.519811	3.244302	-1.409924
H	1.014097	3.957935	0.129093
H	-0.781294	1.314418	2.785860

34-TS

B3LYP SCF energy: -1484.20049010 a.u.
B3LYP enthalpy: -1483.502807 a.u.
B3LYP free energy: -1483.603034 a.u.
M06 SCF energy in solution: -1484.60084258 a.u.
M06 enthalpy in solution: -1483.903159 a.u.
M06 free energy in solution:-1484.003386 a.u.
Imaginary frequency: -208.5019 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.323017	0.974200	0.415549
O	1.144017	1.807684	-1.701609
O	1.261608	2.989279	0.170295
N	0.699799	-1.905215	0.443111
N	-1.482151	-1.652265	0.357262
C	-0.282318	-0.969921	0.385659
C	0.231692	-3.290913	0.385450
H	0.568250	-3.853844	1.262885
H	0.615825	-3.801560	-0.506062
C	-1.296728	-3.122325	0.350618
H	-1.750120	-3.555659	-0.548016
H	-1.787519	-3.574955	1.219830
C	2.084086	-1.512361	0.148409
C	2.366780	-1.688892	-1.366860
H	1.635512	-1.102955	-1.935028
H	2.249006	-2.744533	-1.653304
C	3.794021	-1.212102	-1.698833
H	3.983483	-1.362203	-2.770387
C	4.816906	-2.017022	-0.873432
H	4.759259	-3.085828	-1.126991
H	5.836719	-1.686148	-1.113090
C	4.534861	-1.811297	0.629161
H	5.266768	-2.375166	1.223299
C	3.116061	-2.341179	0.948668
H	2.901925	-2.253007	2.022327
H	3.059601	-3.409970	0.689767
C	4.642041	-0.305992	0.963768
H	4.486124	-0.145099	2.039389
H	5.657402	0.047505	0.731276
C	3.590906	0.493000	0.144795
H	3.665748	1.557175	0.397126
C	2.202257	-0.036971	0.559472
H	2.198425	-0.030277	1.659582
C	3.896833	0.285364	-1.354827

H	3.193078	0.854159	-1.966594
H	4.910889	0.649023	-1.577652
C	-2.739950	-1.175097	-0.147586
C	-2.876275	-0.949834	-1.538943
C	-4.121297	-0.560381	-2.035933
H	-4.223583	-0.378463	-3.103882
C	-5.239140	-0.407911	-1.205495
C	-5.085877	-0.683396	0.152463
H	-5.947971	-0.602289	0.812001
C	-3.856143	-1.075876	0.701289
C	-1.708751	-1.113652	-2.485148
H	-2.042873	-1.023924	-3.523110
H	-1.225699	-2.091796	-2.374554
H	-0.935916	-0.355553	-2.312654
C	-6.566364	0.041264	-1.770562
H	-6.780447	-0.446757	-2.728257
H	-6.572672	1.124003	-1.952578
H	-7.390306	-0.181210	-1.084910
C	-3.792875	-1.388225	2.179822
H	-2.904486	-1.964815	2.443562
H	-4.676035	-1.958439	2.488953
H	-3.776686	-0.471304	2.781892
C	-1.468310	1.965662	-0.402140
H	-2.053833	1.239107	-0.948420
C	1.490919	2.853236	-1.078263
C	2.227038	3.959103	-1.811758
H	1.884738	4.025786	-2.848040
H	2.094283	4.917880	-1.304140
H	3.298972	3.725856	-1.827821
C	-0.184559	1.280413	2.210291
C	-1.744865	2.175066	0.972947
H	-2.480932	1.509345	1.418660
C	-1.681595	3.579171	1.546129
H	-2.550297	4.151007	1.191749
H	-1.704607	3.589868	2.640731
H	-0.774148	4.085805	1.205928
H	-1.116084	2.812793	-0.983951
H	0.248307	2.222787	2.577999
C	-0.831350	0.489338	3.306910
H	-1.318341	-0.417632	2.947511
H	-0.038276	0.192091	4.011197
H	-1.552816	1.081426	3.891072

35-TS

B3LYP SCF energy: -1484.19445826 a.u.
B3LYP enthalpy: -1483.496603 a.u.
B3LYP free energy: -1483.598728 a.u.
M06 SCF energy in solution: -1484.59481589 a.u.
M06 enthalpy in solution: -1483.896961 a.u.
M06 free energy in solution: -1483.999086 a.u.
Imaginary frequency: -237.4141 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.452918	0.894661	0.235086
O	-1.646494	2.785017	0.305453
O	-0.989301	2.226067	-1.736799
N	-0.636414	-1.976531	-0.117980
N	1.513308	-1.670114	0.143836
C	0.311907	-1.012030	0.017589
C	-0.146340	-3.337046	0.105869
H	-0.531964	-4.033655	-0.644207
H	-0.451242	-3.700800	1.096688
C	1.367893	-3.138434	0.010383
H	1.922100	-3.655219	0.799526
H	1.768774	-3.470896	-0.955535
C	-2.055868	-1.613996	-0.082476
C	-2.633846	-1.766510	1.347123
H	-2.018721	-1.191185	2.047028
H	-2.594138	-2.821060	1.657197
C	-4.090425	-1.265298	1.378327
H	-4.486290	-1.367532	2.397970
C	-4.936637	-2.113042	0.406805
H	-4.934208	-3.166548	0.722365
H	-5.982626	-1.777544	0.422911
C	-4.364836	-1.980865	-1.019837
H	-4.961086	-2.587970	-1.714362
C	-2.904075	-2.490391	-1.038032
H	-2.487624	-2.432120	-2.052332
H	-2.882158	-3.547740	-0.732919
C	-4.415375	-0.498015	-1.444444
H	-4.047385	-0.383055	-2.472906
H	-5.458417	-0.149040	-1.435911
C	-3.553109	0.355314	-0.477803
H	-3.605815	1.402822	-0.785115
C	-2.103690	-0.154504	-0.571289
H	-1.814497	-0.158874	-1.632193
C	-4.118190	0.216419	0.949324
H	-3.527973	0.826498	1.643013
H	-5.150208	0.593772	0.982516
C	2.838060	-1.166964	-0.080504
C	3.722397	-1.050655	1.007205
C	5.044283	-0.663698	0.755975
H	5.728810	-0.562904	1.595799
C	5.510948	-0.421159	-0.538860
C	4.614957	-0.575868	-1.602141
H	4.959764	-0.396524	-2.618432
C	3.281448	-0.944412	-1.400758
C	3.284273	-1.366283	2.418731
H	4.043324	-1.048602	3.140199
H	3.129674	-2.444150	2.560376
H	2.340089	-0.876407	2.673354
C	6.936211	0.017506	-0.783147
H	7.311115	-0.354129	-1.742925
H	7.607042	-0.339931	0.005206
H	7.015138	1.112612	-0.806644
C	2.341084	-1.061777	-2.577826
H	1.493235	-0.375568	-2.478317
H	1.924683	-2.071480	-2.677289
H	2.861659	-0.826863	-3.510911
C	-0.280008	0.707506	2.094603
H	0.294787	-0.029899	2.670668
C	-1.623802	2.990778	-0.956376
C	-2.404564	4.167532	-1.515273
H	-1.925029	4.548473	-2.420842
H	-3.415363	3.835929	-1.783906
H	-2.496506	4.961369	-0.769367
C	1.201024	2.444109	0.146552
C	1.354941	2.055038	1.498591
H	2.161855	1.356293	1.711764
C	1.053933	3.068591	2.593217
H	0.986379	2.616054	3.587205
H	1.866160	3.808941	2.620353
H	0.120954	3.599487	2.381655
H	-0.858019	1.383735	2.736224
H	0.621778	3.354695	0.014096
C	2.238046	2.234456	-0.924600
H	2.879979	1.379757	-0.722925
H	1.765830	2.115510	-1.904327
H	2.878777	3.128716	-0.980320

37-TS

B3LYP SCF energy: -1405.54006680 a.u.
B3LYP enthalpy: -1404.902912 a.u.
B3LYP free energy: -1405.000640 a.u.
M06 SCF energy in solution: -1405.98061917 a.u.
M06 enthalpy in solution: -1405.343464 a.u.
M06 free energy in solution: -1405.441192 a.u.
Imaginary frequency: -301.8455 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	6.845592	5.704505	7.555179
O	4.998194	5.932442	6.303495

O	6.759440	7.144419	5.726517
N	6.844601	2.687327	7.273774
N	7.202372	3.328162	5.221875
C	7.011113	3.761813	6.490230
C	6.950822	1.402505	6.563432
H	6.019719	0.832666	6.651531
H	7.760126	0.791385	6.978162
C	7.234100	1.850706	5.117724
H	8.213227	1.519309	4.752792
H	6.476952	1.497500	4.410691
C	6.776871	2.814738	8.735084
C	8.170813	2.522338	9.347569
H	8.917538	3.174632	8.887989
H	8.465531	1.487359	9.118344
C	8.131427	2.721209	10.873875
H	9.128992	2.530810	11.292507
C	7.116681	1.731969	11.482052
H	7.430926	0.697847	11.280260
H	7.080373	1.848173	12.573887
C	5.721835	1.995927	10.878566
H	4.996374	1.288783	11.302697
C	5.777333	1.796902	9.345708
H	4.784445	1.945647	8.901968
H	6.084111	0.762927	9.126409
C	5.300680	3.441340	11.212462
H	4.288989	3.640833	10.835408
H	5.268326	3.572496	12.304270
C	6.305690	4.436779	10.575447
H	5.990055	5.453345	10.837660
C	6.267397	4.245800	9.041102
H	5.200453	4.231388	8.766257
C	7.700606	4.169828	11.179670
H	8.437789	4.875858	10.778668
H	7.671590	4.326814	12.267578
C	7.358562	4.110603	4.029274
C	8.640750	4.543367	3.646969
C	8.776605	5.244600	2.444969
H	9.764896	5.590669	2.149171
C	7.683728	5.504935	1.613515
C	6.427409	5.034737	2.008615
H	5.566487	5.212961	1.367032
C	6.238021	4.340419	3.208806
C	9.857378	4.238273	4.488461
H	10.731112	4.782028	4.116874
H	10.103920	3.167948	4.468323
H	9.703750	4.510991	5.535542
C	7.851555	6.291724	0.334277
H	7.113812	5.995751	-0.419392
H	8.849892	6.153149	-0.094604
H	7.721424	7.367513	0.512597
C	4.858510	3.866814	3.605823
H	4.803515	2.773262	3.681713
H	4.118246	4.177569	2.862038
H	4.567602	4.280446	4.576984
C	8.927235	5.825651	8.102207
H	9.312351	5.081896	8.790192
C	5.551618	6.816261	5.557083
H	9.462329	5.907213	7.156753
C	4.733942	7.476531	4.464927
H	3.687647	7.167229	4.515962
H	4.803187	8.564837	4.565387
H	5.148652	7.209984	3.487317
C	6.055548	7.061192	8.619073
C	8.348370	7.017003	8.612350
H	5.467399	7.860056	8.139022
H	5.998129	7.119857	9.711253
H	8.251312	7.133296	9.688226
H	8.441960	7.942483	8.050661

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B3LYP SCF energy: -1405.55228349 a.u.
B3LYP enthalpy: -1404.913507 a.u.
B3LYP free energy: -1405.009908 a.u.
M06 SCF energy in solution: -1405.99347225 a.u.
M06 enthalpy in solution: -1405.354696 a.u.
M06 free energy in solution: -1405.451097 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.445258	1.320085	0.462925
O	0.438883	1.983628	-1.456959
O	1.736433	2.007011	0.332314
N	-0.898850	-1.606849	-0.303987
N	1.263536	-1.597261	-0.027824
C	0.151559	-0.819756	-0.021206
C	-0.561384	-3.037142	-0.405187
H	-0.969669	-3.482423	-1.316455
H	-0.965750	-3.589737	0.452664
C	0.974021	-3.002330	-0.402270
H	1.418547	-3.693963	0.320063
H	1.399445	-3.227199	-1.387561
C	-2.273458	-1.088029	-0.301144
C	-3.009552	-1.462631	1.009211
H	-2.448102	-1.078237	1.866529
H	-3.054434	-2.556375	1.114579
C	-4.441259	-0.884543	0.995999
H	-4.947981	-1.155329	1.932011
C	-5.218489	-1.466823	-0.201762
H	-5.294434	-2.560063	-0.112891
H	-6.244678	-1.074917	-0.210207
C	-4.496806	-1.088168	-1.511057
H	-5.044715	-1.501792	-2.368311
C	-3.073088	-1.682923	-1.491589
H	-2.545993	-1.459406	-2.428284
H	-3.140878	-2.777567	-1.406253
C	-4.416240	0.447073	-1.631252
H	-3.931061	0.728514	-2.575392
H	-5.429335	0.874112	-1.651247
C	-3.617488	1.019997	-0.431288
H	-3.567076	2.111721	-0.527613
C	-2.183513	0.442345	-0.478348
H	-1.812357	0.618295	-1.499675
C	-4.374230	0.650279	0.859243
H	-3.889639	1.096217	1.732473
H	-5.393351	1.060845	0.821582
C	2.637269	-1.174667	-0.013976
C	3.387635	-1.299878	1.167973
C	4.743453	-0.956329	1.136809
H	5.327495	-1.049337	2.050234
C	5.365955	-0.504513	-0.029068
C	4.598418	-0.420640	-1.195153
H	5.070509	-0.095170	-2.120187
C	3.240192	-0.753331	-1.215291
C	2.772351	-1.792105	2.457227
H	3.551864	-2.065227	3.175287
H	2.133878	-2.669095	2.305366
H	2.149077	-1.021444	2.922144
C	6.824142	-0.108043	-0.027207
H	6.944126	0.956561	0.214214
H	7.287086	-0.273290	-1.006111
H	7.393191	-0.674872	0.717624
C	2.458788	-0.666242	-2.507330
H	2.067231	-1.644285	-2.815094
H	3.100329	-0.305185	-3.317075
H	1.604749	0.012684	-2.421768
C	1.547285	2.279641	-0.891113
C	2.625433	2.990609	-1.678360
H	3.598234	2.535571	-1.472275
H	2.409828	2.961374	-2.748725
H	2.672707	4.037294	-1.354763
C	-1.316930	2.993587	0.468051
H	-1.864847	3.527568	1.254031
H	-1.412992	3.500597	-0.504362
C	-1.205422	1.352385	2.582149
H	-1.065163	2.368643	2.935325
H	-2.209219	0.959768	2.686651

C	-0.119548	0.492802	2.493848
H	-0.257364	-0.582808	2.536462
H	0.882201	0.844144	2.730697

40-TS
B3LYP SCF energy: -1405.54917788 a.u.
B3LYP enthalpy: -1404.911874 a.u.
B3LYP free energy: -1405.007727 a.u.
M06 SCF energy in solution: -1405.98995731 a.u.
M06 enthalpy in solution: -1405.352653 a.u.
M06 free energy in solution:-1405.448506 a.u.
Imaginary frequency: -309.6596 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.408474	-1.131174	0.596606
O	1.465503	-2.347571	-0.202468
O	-0.121694	-1.567699	-1.533590
N	-0.852640	1.720177	-0.211029
N	1.326621	1.625131	-0.227044
C	0.199673	0.917006	0.015280
C	-0.477498	3.010112	-0.813409
H	-0.992082	3.843627	-0.328138
H	-0.731706	3.025898	-1.881617
C	1.042660	3.034722	-0.577772
H	1.611719	3.339881	-1.460675
H	1.322122	3.694907	0.253740
C	-2.212810	1.151634	-0.228122
C	-2.563025	0.634103	-1.647506
H	-1.805486	-0.085218	-1.969352
H	-2.554481	1.472919	-2.360144
C	-3.958944	-0.019431	-1.633610
H	-4.194204	-0.390416	-2.640131
C	-5.008397	1.026681	-1.207270
H	-5.030451	1.856680	-1.928220
H	-6.012642	0.580585	-1.203306
C	-4.663449	1.553065	0.200975
H	-5.405126	2.302892	0.507996
C	-3.264813	2.210147	0.178898
H	-3.016841	2.617551	1.168595
H	-3.270074	3.051625	-0.530343
C	-4.670950	0.373859	1.193734
H	-4.463677	0.733048	2.211285
H	-5.669725	-0.086612	1.214083
C	-3.604678	-0.670059	0.773858
H	-3.638685	-1.499776	1.492578
C	-2.210383	-0.003367	0.808020
H	-2.124444	0.482242	1.795382
C	-3.950592	-1.194195	-0.634374
H	-3.213871	-1.942797	-0.950386
H	-4.934623	-1.684960	-0.623658
C	2.677007	1.162273	-0.091614
C	3.325370	0.636276	-1.225844
C	4.644712	0.197462	-1.093988
H	5.148532	-0.217958	-1.964493
C	5.331592	0.273633	0.122689
C	4.672348	0.835838	1.218059
H	5.197005	0.922817	2.167673
C	3.352680	1.295888	1.133496
C	2.629853	0.576751	-2.566130
H	3.223383	0.002230	-3.283840
H	2.493639	1.581756	-2.989020
H	1.638108	0.121747	-2.494272
C	6.740619	-0.257204	0.249796
H	6.737507	-1.336018	0.454723
H	7.281362	0.228901	1.068709
H	7.312100	-0.104845	-0.672515
C	2.713297	1.961709	2.330588
H	2.884096	3.047228	2.314488
H	3.143698	1.584239	3.263777
H	1.633602	1.801163	2.362780
C	-1.263552	-2.829231	0.805900
C	0.961442	-2.238417	-1.348774
C	1.597831	-2.923438	-2.542445
H	1.374533	-3.996224	-2.500702
H	2.685094	-2.811602	-2.502831
H	1.208052	-2.522940	-3.481075
H	-2.227715	-3.054865	1.275572
H	-0.802390	-3.743651	0.395287
C	-0.545408	-1.829044	2.765074
H	-1.565249	-1.833584	3.138691
H	0.025642	-2.736971	2.940703
C	0.133725	-0.599929	2.620567
H	1.220758	-0.604373	2.660859
H	-0.352798	0.316479	2.945670

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B3LYP SCF energy: -1405.56387411 a.u.
B3LYP enthalpy: -1404.925307 a.u.
B3LYP free energy: -1405.021945 a.u.
M06 SCF energy in solution: -1406.00320264 a.u.
M06 enthalpy in solution: -1405.364636 a.u.
M06 free energy in solution:-1405.461274 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.406109	1.112139	0.798665
O	-1.237047	2.189491	-0.324493
O	0.792370	2.083668	-1.171168
N	0.781492	-1.670246	-0.450163
N	-1.387314	-1.491062	-0.553672
C	-0.254963	-0.869832	-0.146203
C	0.402189	-2.833669	-1.271355
H	0.856283	-3.755129	-0.896929
H	0.724689	-2.692942	-2.311402
C	-1.129298	-2.829339	-1.134842
H	-1.648476	-2.945169	-2.090943
H	-1.486785	-3.614212	-0.456488
C	2.157557	-1.156576	-0.335811
C	2.590677	-0.473517	-1.657807
H	1.877747	0.313967	-1.911695
H	2.584348	-1.214514	-2.471372
C	4.006026	0.116106	-1.504298
H	4.294161	0.609752	-2.441937
C	5.000679	-1.017734	-1.186590
H	5.023028	-1.744020	-2.011881
H	6.018329	-0.615737	-1.086237
C	4.580559	-1.712285	0.124817
H	5.279256	-2.528411	0.353207
C	3.159454	-2.300611	-0.035164
H	2.856020	-2.829412	0.878451
H	3.161328	-3.035727	-0.853730
C	4.596447	-0.674162	1.265321
H	4.347056	-1.153801	2.221760
H	5.608144	-0.256159	1.370694
C	3.579693	0.454397	0.957230
H	3.596076	1.181033	1.779841
C	2.173519	-0.179064	0.869506
H	2.051315	-0.802617	1.759187
C	3.990382	1.148398	-0.357764
H	3.291011	1.955357	-0.599456
H	4.987591	1.597334	-0.243744
C	-2.735796	-1.058039	-0.320597
C	-3.397311	-0.318126	-1.317580
C	-4.720346	0.071331	-1.091436
H	-5.233037	0.651806	-1.855743
C	-5.398969	-0.259770	0.085481
C	-4.724176	-1.021722	1.043029
H	-5.239956	-1.305204	1.958267
C	-3.400504	-1.437706	0.860550
C	-2.713069	0.026973	-2.618014
H	-3.312967	0.738096	-3.193972
H	-2.568647	-0.863334	-3.245189
H	-1.728219	0.466502	-2.446470

C	-6.815254	0.210598	0.322948
H	-6.829099	1.226669	0.739229
H	-7.340598	-0.439069	1.030976
H	-7.391947	0.234929	-0.608256
C	-2.732868	-2.299883	1.907776
H	-2.633629	-3.339849	1.569136
H	-3.322364	-2.314250	2.829392
H	-1.728880	-1.944560	2.155011
C	1.315786	2.547085	1.577049
C	-0.404441	2.516222	-1.226148
C	-0.814808	3.449166	-2.343255
H	-0.478095	4.464750	-2.102595
H	-1.901283	3.461224	-2.454155
H	-0.337257	3.154624	-3.281980
H	1.943437	3.234071	0.990298
H	1.373523	2.769533	2.655694
C	-0.956463	0.998435	2.506346
H	-1.079431	2.006157	2.893646
H	-1.866574	0.536045	2.137259
C	0.163876	0.238504	2.833434
H	0.140768	-0.844008	2.759939
H	0.931040	0.634936	3.493335

43-TS

B3LYP SCF energy: -1405.54473980 a.u.
B3LYP enthalpy: -1404.908353 a.u.
B3LYP free energy: -1405.006264 a.u.
M06 SCF energy in solution: -1405.98746079 a.u.
M06 enthalpy in solution: -1405.351074 a.u.
M06 free energy in solution:-1405.448985 a.u.
Imaginary frequency: -195.4985 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.380495	1.084751	-0.174167
O	1.743562	1.697110	-0.448868
O	2.051775	3.241935	1.178420
N	-1.174988	-1.740259	-0.363193
N	1.008700	-1.796716	-0.173740
C	-0.067077	-0.987490	-0.231588
C	-0.897805	-3.181236	-0.262386
H	-1.394283	-3.739404	-1.060568
H	-1.250692	-3.572657	0.700476
C	0.636444	-3.216226	-0.375963
H	1.112275	-3.853599	0.373846
H	0.974948	-3.545911	-1.366539
C	-2.499511	-1.125878	-0.168150
C	-2.921674	-1.246358	1.319176
H	-2.143376	-0.798206	1.946935
H	-3.009254	-2.304486	1.606110
C	-4.271621	-0.536740	1.539543
H	-4.560986	-0.630086	2.594972
C	-5.343368	-1.196281	0.647904
H	-5.467871	-2.253283	0.923570
H	-6.315754	-0.709774	0.803972
C	-4.924307	-1.075579	-0.831991
H	-5.686198	-1.542252	-1.470291
C	-3.577325	-1.806268	-1.042831
H	-3.275964	-1.760934	-2.097954
H	-3.694506	-2.869047	-0.780670
C	-4.783061	0.418410	-1.194810
H	-4.520059	0.527561	-2.255818
H	-5.749392	0.924408	-1.052029
C	-3.689208	1.070800	-0.309785
H	-3.608994	2.133369	-0.576978
C	-2.341473	0.359208	-0.567750
H	-2.222702	0.342858	-1.677240
C	-4.125864	0.951699	1.165268
H	-3.395466	1.435888	1.824279
H	-5.084177	1.468574	1.317444
C	2.401294	-1.454329	-0.070430
C	3.023374	-1.574468	1.185073
C	4.402284	-1.363337	1.265421
H	4.890691	-1.450426	2.233628
C	5.165931	-1.042949	0.138384
C	4.510947	-0.920156	-1.090283
H	5.086155	-0.659017	-1.976347
C	3.130667	-1.107110	-1.218434
C	2.228300	-1.901781	2.427539
H	2.867348	-1.862939	3.314570
H	1.783327	-2.904794	2.387671
H	1.407699	-1.189934	2.569359
C	6.652252	-0.795780	0.253012
H	7.092121	-1.365878	1.078278
H	6.860335	0.265633	0.442410
H	7.177128	-1.070263	-0.668414
C	2.456605	-0.865383	-2.545303
H	1.636076	-1.564151	-2.740032
H	3.172383	-0.941965	-3.369898
H	2.042335	0.150278	-2.543955
C	-0.442413	1.538062	1.616570
H	-1.293986	1.363966	2.289867
C	2.422744	2.594689	0.181530
H	0.437257	2.029035	2.048870
C	3.812499	2.861253	-0.409599
H	4.364153	1.920991	-0.510989
H	3.712249	3.287072	-1.415840
H	4.370894	3.557836	0.220207
C	-0.850635	3.081379	-1.047997
C	-0.950808	3.378112	0.310519
H	0.064032	3.332797	-1.577586
H	-1.752783	2.957618	-1.642161
H	-1.928213	3.452690	0.778539
H	-0.096802	3.818241	0.817905

44-TS

B3LYP SCF energy: -1405.54678644 a.u.
B3LYP enthalpy: -1404.909801 a.u.
B3LYP free energy: -1405.006136 a.u.
M06 SCF energy in solution: -1405.98870532 a.u.
M06 enthalpy in solution: -1405.351720 a.u.
M06 free energy in solution:-1405.448055 a.u.
Imaginary frequency: -143.3282 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	6.790372	5.341486	7.553796
O	6.138351	8.098517	5.521488
O	7.744868	6.572732	5.974812
N	6.960776	2.423339	7.385916
N	7.006880	3.105796	5.304120
C	6.940562	3.503546	6.591831
C	7.216202	1.176512	6.652626
H	6.511633	0.393147	6.944184
H	8.233003	0.812545	6.850819
C	7.033015	1.629011	5.189540
H	7.851535	1.313743	4.536020
H	6.093245	1.266064	4.757254
C	6.952585	2.596639	8.846464
C	8.407841	2.609673	9.378218
H	8.970189	3.406999	8.871884
H	8.906568	1.658929	9.138338
C	8.411701	2.845288	10.899570
H	9.447061	2.845319	11.265836
C	7.612798	1.728600	11.599640
H	8.083066	0.751741	11.417020
H	7.618766	1.887617	12.686479
C	6.163836	1.732853	11.072198
H	5.587382	0.942106	11.570396
C	6.182779	1.455918	9.550635
H	5.160031	1.406292	9.154143
H	6.653934	0.477517	9.367844
C	5.522884	3.107789	11.365108
H	4.475087	3.113972	11.036485

H	5.519526	3.283877	12.451038
C	6.312067	4.224097	10.630550
H	5.846314	5.193493	10.859278
C	6.235419	3.954191	9.105262
H	5.168330	3.755458	8.899140
C	7.758923	4.212033	11.176245
H	8.365943	4.995887	10.709332
H	7.752732	4.413541	12.256933
C	6.875257	3.906913	4.117692
C	8.030386	4.419885	3.504818
C	7.886914	5.102649	2.292540
H	8.777465	5.496308	1.806746
C	6.638167	5.302939	1.697173
C	5.508764	4.791035	2.343041
H	4.526686	4.943688	1.900297
C	5.601425	4.088996	3.548090
C	9.385085	4.302129	4.156647
H	10.184319	4.513537	3.439322
H	9.562068	3.308074	4.582037
H	9.446251	5.034547	4.970682
C	6.506962	6.082745	0.409698
H	5.680179	5.709286	-0.204443
H	7.424226	6.030455	-0.186376
H	6.308126	7.143378	0.612252
C	4.351289	3.550316	4.205325
H	4.265497	2.460157	4.099991
H	3.459322	3.989104	3.748484
H	4.328454	3.776775	5.276193
C	7.365944	7.000428	8.951851
H	7.519815	6.624951	9.955505
C	7.280252	7.624864	5.386045
H	8.232626	7.393841	8.425393
C	8.267956	8.306081	4.432425
H	7.907750	9.299546	4.154522
H	9.260122	8.381002	4.890288
H	8.371332	7.699830	3.524809
C	5.028327	5.830356	7.323397
C	6.095709	7.423540	8.561592
H	4.805451	6.540859	6.518238
H	4.179635	5.458544	7.920357
H	5.270619	7.333871	9.264939
H	5.972542	8.091720	7.714199

46-TS

B3LYP SCF energy: -1484.19406043 a.u.
B3LYP enthalpy: -1483.497142 a.u.
B3LYP free energy: -1483.599484 a.u.
M06 SCF energy in solution: -1484.59469012 a.u.
M06 enthalpy in solution: -1483.897772 a.u.
M06 free energy in solution: -1484.000114 a.u.
Imaginary frequency: -121.8449 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.365391	0.723010	0.027968
O	1.654641	2.368940	-0.514050
O	1.501290	4.279066	0.683806
N	0.552758	-2.163263	0.160356
N	-1.593052	-1.810624	-0.082577
C	-0.381698	-1.180646	0.049294
C	0.030954	-3.503290	-0.117189
H	0.420772	-4.242245	0.588088
H	0.299558	-3.825699	-1.133377
C	-1.478942	-3.279392	0.031008
H	-2.068545	-3.775329	-0.745745
H	-1.849749	-3.615396	1.008608
C	1.971720	-1.796833	0.090817
C	2.461041	-1.793799	-1.382038
H	1.811773	-1.135070	-1.976330
H	2.380696	-2.803727	-1.810690
C	3.920568	-1.304708	-1.451764
H	4.255342	-1.315390	-2.497879
C	4.810178	-2.245343	-0.613179
H	4.778039	-3.266097	-1.021450
H	5.856502	-1.914979	-0.662354
C	4.325248	-2.241462	0.851707
H	4.958946	-2.908360	1.451537
C	2.866993	-2.756477	0.906000
H	2.509803	-2.796011	1.943892
H	2.825922	-3.780631	0.504277
C	4.406729	-0.802621	1.408428
H	4.096337	-0.786601	2.462398
H	5.450166	-0.456587	1.377864
C	3.501267	0.138525	0.571974
H	3.557654	1.157317	0.967868
C	2.054610	-0.376742	0.686494
H	1.816291	-0.467684	1.758049
C	3.993659	0.128444	-0.889659
H	3.379704	0.812679	-1.484017
H	5.030098	0.492316	-0.938469
C	-2.899564	-1.222799	-0.082149
C	-3.547083	-0.977715	-1.308940
C	-4.825800	-0.407326	-1.289199
H	-5.319687	-0.199606	-2.236455
C	-5.483805	-0.103335	-0.095551
C	-4.841658	-0.417753	1.107580
H	-5.350568	-0.220034	2.049143
C	-3.566608	-0.989496	1.140605
C	-2.931269	-1.356582	-2.637496
H	-3.121024	-0.587537	-3.393897
H	-3.372843	-2.289513	-3.013794
H	-1.852766	-1.509398	-2.564119
C	-6.845104	0.552122	-0.098372
H	-7.483984	0.153549	0.697465
H	-7.359515	0.404120	-1.053341
H	-6.762500	1.634698	0.065092
C	-2.972186	-1.397182	2.471719
H	-1.879970	-1.384935	2.465502
H	-3.289341	-2.414332	2.740038
H	-3.315622	-0.734625	3.272702
C	-0.898093	1.532923	-1.607306
H	-1.283111	0.678050	-2.151518
C	1.994607	3.578946	-0.212160
H	-0.212774	2.182089	-2.148590
C	3.125633	4.140173	-1.080281
H	4.047329	3.575404	-0.896658
H	2.884591	4.024776	-2.143036
H	3.297305	5.194326	-0.851613
C	-0.698914	1.259125	1.469473
H	-1.607696	0.718281	1.748621
C	-1.662194	2.081948	-0.566950
H	-2.549981	1.527369	-0.274968
C	-0.319756	2.357079	2.412657
H	-1.207996	2.905510	2.761385
H	0.128043	1.890178	3.306056
H	0.401633	3.059402	1.978856
C	-1.661443	3.554775	-0.233720
H	-2.211727	4.093177	-1.019082
H	-2.171935	3.754747	0.713111
H	-0.652327	3.969179	-0.167085

cpx1-A

B3LYP SCF energy: -1366.31596711 a.u.
B3LYP enthalpy: -1365.705984 a.u.
B3LYP free energy: -1365.801653 a.u.
M06 SCF energy in solution: -1366.76425247 a.u.
M06 enthalpy in solution: -1366.154269 a.u.
M06 free energy in solution: -1366.249938 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.218828	0.992595	0.112004
O	1.374365	2.231673	-0.773349
O	-0.345002	3.315862	0.098882

N	-0.940440	-1.717404	-0.571767
N	1.229516	-1.718241	-0.208497
C	0.119787	-0.932980	-0.231025
C	-0.599039	-3.142044	-0.606933
H	-1.046762	-3.647989	-1.467540
H	-0.941849	-3.648940	0.306065
C	0.936609	-3.087057	-0.683852
H	1.426510	-3.836676	-0.056611
H	1.300922	-3.211880	-1.712703
C	-2.283720	-1.162812	-0.371811
C	-2.840495	-1.543713	1.024284
H	-2.116709	-1.247277	1.790840
H	-2.968430	-2.633885	1.090498
C	-4.190216	-0.839575	1.263525
H	-4.572308	-1.120544	2.254206
C	-5.192998	-1.279441	0.177967
H	-5.364017	-2.363960	0.237270
H	-6.164702	-0.793619	0.341119
C	-4.641221	-0.899759	-1.211860
H	-5.351608	-1.211583	-1.988996
C	-3.293307	-1.625692	-1.446866
H	-2.898861	-1.392945	-2.444866
H	-3.448211	-2.714405	-1.401943
C	-4.447137	0.632212	-1.270806
H	-4.091162	0.932462	-2.265794
H	-5.413654	1.131939	-1.113489
C	-3.427939	1.075622	-0.186793
H	-3.281176	2.161157	-0.239326
C	-2.100388	0.365233	-0.481284
H	-1.844502	0.579976	-1.546541
C	-3.976630	0.686687	1.199701
H	-3.274981	1.002766	1.979822
H	-4.927125	1.206164	1.385805
C	2.590955	-1.267980	-0.121054
C	3.311038	-1.527641	1.061582
C	4.652160	-1.142263	1.124658
H	5.211872	-1.338124	2.037110
C	5.290981	-0.513142	0.050424
C	4.552445	-0.283397	-1.111819
H	5.033510	0.196347	-1.961841
C	3.205709	-0.648482	-1.224053
C	2.661213	-2.200158	2.248066
H	3.361362	-2.261997	3.086696
H	2.332821	-3.221913	2.018279
H	1.776687	-1.648608	2.584082
C	6.733578	-0.075293	0.155029
H	6.811594	0.922201	0.607733
H	7.209095	-0.023096	-0.830122
H	7.318184	-0.760568	0.778758
C	2.456526	-0.341193	-2.498655
H	1.696531	-1.093639	-2.731597
H	3.147606	-0.283632	-3.346187
H	1.951825	0.627214	-2.405597
C	-0.238410	0.741095	1.928110
C	0.768146	3.331498	-0.494125
C	1.426846	4.635844	-0.886048
H	0.063011	-0.205200	2.400689
H	1.683572	4.617802	-1.950369
H	0.768259	5.480288	-0.674047
H	2.362972	4.752342	-0.328367
C	-0.555786	1.832734	2.915026
H	-1.360841	1.511753	3.595459
H	0.321583	2.040313	3.547776
H	-0.853275	2.762976	2.424788

cpx1-B

B3LYP SCF energy: -1366.31090746 a.u.
B3LYP enthalpy: -1365.700779 a.u.
B3LYP free energy: -1365.797327 a.u.
M06 SCF energy in solution: -1366.75764722 a.u.
M06 enthalpy in solution: -1366.147519 a.u.
M06 free energy in solution: -1366.244067 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.315524	0.855044	0.397565
O	-0.438009	2.231941	-1.144308
O	0.924182	3.125166	0.351441
N	0.789546	-1.854930	-0.342847
N	-1.390894	-1.605308	-0.448501
C	-0.229124	-0.976522	-0.127297
C	0.363768	-3.029320	-1.104962
H	0.832753	-3.946259	-0.737003
H	0.608976	-2.921276	-2.172171
C	-1.158452	-3.004254	-0.864952
H	-1.739716	-3.241976	-1.760508
H	-1.454101	-3.698135	-0.067391
C	2.148675	-1.307000	-0.236208
C	2.578589	-0.606530	-1.553338
H	1.819896	0.136412	-1.842867
H	2.629841	-1.339793	-2.371760
C	3.946552	0.078848	-1.362860
H	4.242804	0.563584	-2.302635
C	4.993145	-0.987210	-0.976690
H	5.096450	-1.728459	-1.782159
H	5.977480	-0.517136	-0.847213
C	4.565290	-1.679289	0.334333
H	5.311154	-2.436000	0.611689
C	3.199371	-2.376134	0.124559
H	2.889402	-2.899908	1.038512
H	3.288942	-3.130022	-0.672793
C	4.460197	-0.618884	1.453486
H	4.186573	-1.097362	2.403759
H	5.441177	-0.145347	1.603542
C	3.399631	0.447587	1.071128
H	3.326580	1.197097	1.868741
C	2.046969	-0.268810	0.912710
H	1.847799	-0.833085	1.829691
C	3.834369	1.132340	-0.241299
H	3.113072	1.912968	-0.511770
H	4.804447	1.629613	-0.100965
C	-2.719062	-1.087642	-0.290580
C	-3.271599	-0.290732	-1.312826
C	-4.580141	0.175006	-1.154383
H	-5.012356	0.791269	-1.940295
C	-5.346328	-0.128356	-0.024290
C	-4.775351	-0.937276	0.961187
H	-5.357826	-1.193059	1.844247
C	-3.470945	-1.431200	0.848729
C	-2.483968	0.072762	-2.548236
H	-3.155224	0.414157	-3.343032
H	-1.910341	-0.779008	-2.930498
H	-1.773589	0.878036	-2.330392
C	-6.746427	0.419316	0.130038
H	-6.728499	1.457321	0.487812
H	-7.329398	-0.164877	0.849648
H	-7.284829	0.417013	-0.824417
C	-2.918259	-2.328723	1.933119
H	-3.078406	-3.390035	1.697642
H	-3.418177	-2.134983	2.887515
H	-1.843412	-2.185824	2.077564
C	-0.502391	0.813034	2.029974
C	0.198601	3.246588	-0.671390
C	0.046234	4.578468	-1.372917
H	-0.994273	4.913533	-1.295196
H	0.704867	5.327098	-0.928693
H	0.271075	4.465449	-2.438657
H	-1.194497	0.013803	2.325572
C	-0.359521	1.906219	3.052485
H	-1.342955	2.332710	3.305074
H	0.048527	1.486571	3.986634
H	0.293837	2.715046	2.715145

cpx1-C

B3LYP SCF energy: -1366.31253175 a.u.
B3LYP enthalpy: -1365.702707 a.u.
B3LYP free energy: -1365.796893 a.u.
M06 SCF energy in solution: -1366.76275841 a.u.
M06 enthalpy in solution: -1366.152934 a.u.
M06 free energy in solution: -1366.247120 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.246989	1.034454	0.268500
O	1.415008	2.329492	-0.410308
O	-0.379103	3.325616	0.416814
N	-0.948492	-1.642891	-0.561061
N	1.225353	-1.667018	-0.224039
C	0.108964	-0.880717	-0.168918
C	-0.609752	-3.058822	-0.708862
H	-1.071629	-3.498822	-1.597705
H	-0.938334	-3.633985	0.168896
C	0.923358	-2.992937	-0.806339
H	1.423401	-3.792210	-0.252888
H	1.269513	-3.029409	-1.848592
C	-2.295239	-1.083722	-0.415986
C	-2.938765	-1.510733	0.928148
H	-2.259089	-1.260609	1.747815
H	-3.086371	-2.600705	0.938687
C	-4.289776	-0.793483	1.116289
H	-4.733286	-1.104673	2.071713
C	-5.232676	-1.177065	-0.041924
H	-5.421771	-2.260153	-0.033098
H	-6.205621	-0.682196	0.081665
C	-4.595275	-0.756084	-1.382536
H	-5.262607	-1.029883	-2.210493
C	-3.245200	-1.493873	-1.565528
H	-2.790180	-1.231287	-2.529926
H	-3.417727	-2.580719	-1.569499
C	-4.380932	0.774146	-1.372654
H	-3.963652	1.106339	-2.333139
H	-5.349462	1.280422	-1.253395
C	-3.421091	1.162696	-0.216292
H	-3.257563	2.246994	-0.218983
C	-2.088889	0.443812	-0.464466
H	-1.774289	0.688430	-1.506899
C	-4.050526	0.730675	1.122599
H	-3.387560	1.005835	1.951675
H	-5.001689	1.259014	1.277010
C	2.585855	-1.203495	-0.218736
C	3.435813	-1.604284	0.831844
C	4.768820	-1.185996	0.811734
H	5.424280	-1.486410	1.626840
C	5.280998	-0.397470	-0.223377
C	4.423681	-0.049300	-1.268445
H	4.807067	0.545552	-2.095167
C	3.080170	-0.440049	-1.294107
C	2.950907	-2.493946	1.952541
H	3.645568	-2.464038	2.797676
H	2.876869	-3.543205	1.633826
H	1.963073	-2.195313	2.310904
C	6.715487	0.077037	-0.202632
H	6.805424	1.038397	0.320602
H	7.104703	0.222214	-1.216155
H	7.368105	-0.635643	0.313400
C	2.219240	-0.022813	-2.463191
H	1.405946	-0.727583	-2.659732
H	2.824409	0.058341	-3.372644
H	1.774365	0.958664	-2.265034
C	-0.441753	0.821700	2.073385
C	0.773854	3.397829	-0.092534
C	1.437685	4.736123	-0.330952
H	-0.789303	1.758586	2.543120
H	1.804847	4.792526	-1.360789
H	0.740924	5.553313	-0.134631
H	2.306873	4.832002	0.329767
C	-0.125876	-0.261857	3.060130
H	0.739281	0.025686	3.677697
H	-0.965950	-0.407779	3.757424
H	0.099190	-1.219426	2.584548

cpx1-D
B3LYP SCF energy: -1366.30606165 a.u.
B3LYP enthalpy: -1365.695948 a.u.
B3LYP free energy: -1365.792236 a.u.
M06 SCF energy in solution: -1366.75635013 a.u.
M06 enthalpy in solution: -1366.146236 a.u.
M06 free energy in solution: -1366.242524 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.355153	0.895874	0.501605
O	-0.604333	2.420624	-0.803433
O	0.908392	3.121605	0.649861
N	0.821751	-1.774932	-0.434275
N	-1.358203	-1.520186	-0.528424
C	-0.199295	-0.918470	-0.136048
C	0.405083	-2.874118	-1.306574
H	0.857046	-3.824206	-1.006806
H	0.684581	-2.677353	-2.352221
C	-1.122423	-2.857507	-1.111405
H	-1.676588	-2.969887	-2.048151
H	-1.454532	-3.644155	-0.422206
C	2.181578	-1.229363	-0.327615
C	2.583923	-0.460449	-1.614992
H	1.818772	0.294971	-1.850314
H	2.621955	-1.148388	-2.472291
C	3.953743	0.218736	-1.415335
H	4.229626	0.754688	-2.333325
C	5.011260	-0.861931	-1.107203
H	5.100239	-1.558029	-1.953586
H	5.996404	-0.395091	-0.972664
C	4.611589	-1.624621	0.172769
H	5.364428	-2.392991	0.393606
C	3.242746	-2.313193	-0.047270
H	2.952366	-2.887612	0.842324
H	3.317571	-3.022137	-0.886244
C	4.526822	-0.625387	1.349102
H	4.274709	-1.155235	2.277839
H	5.509506	-0.156894	1.503893
C	3.455096	0.453679	1.045705
H	3.394096	1.159566	1.883036
C	2.102569	-0.259259	0.874989
H	1.928416	-0.879540	1.761824
C	3.858542	1.210091	-0.236739
H	3.125556	1.998094	-0.450588
H	4.827434	1.707932	-0.090409
C	-2.692824	-1.013553	-0.386308
C	-3.186164	-0.094735	-1.335642
C	-4.493377	0.377620	-1.184499
H	-4.875249	1.091747	-1.911402
C	-5.322599	-0.044597	-0.140737
C	-4.823397	-0.998197	0.749007
H	-5.462321	-1.367616	1.549185
C	-3.523402	-1.504511	0.639764
C	-2.352870	0.371323	-2.505059
H	-2.999877	0.738189	-3.308873
H	-1.734739	-0.437361	-2.910236
H	-1.684426	1.185379	-2.207039
C	-6.715700	0.518182	0.020317
H	-6.699114	1.459125	0.586426
H	-7.369579	-0.175227	0.559889
H	-7.176005	0.734009	-0.950175
C	-3.082459	-2.598731	1.586034
H	-3.425284	-3.581614	1.233917
H	-3.509793	-2.450377	2.583207
H	-1.996865	-2.646166	1.688221
C	-0.225059	0.822962	2.226294
C	0.082878	3.368581	-0.274139
C	-0.133375	4.782983	-0.764892

H	-1.101911	5.145593	-0.400689
H	0.655134	5.443042	-0.397872
H	-0.167762	4.801764	-1.858423
H	-0.045254	1.786882	2.734840
C	-0.878152	-0.212825	3.083287
H	-0.451956	-0.191418	4.097903
H	-1.954216	-0.005935	3.189207
H	-0.764841	-1.220475	2.678184

TS1-s-A

B3LYP SCF energy: -1484.20985367 a.u.
B3LYP enthalpy: -1483.511681 a.u.
B3LYP free energy: -1483.611607 a.u.
M06 SCF energy in solution: -1484.61053393 a.u.
M06 enthalpy in solution: -1483.912361 a.u.
M06 free energy in solution: -1484.012287 a.u.
Imaginary frequency: -225.4738 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.341587	0.865722	0.114428
O	-1.332672	2.870546	0.052122
O	-0.866293	2.091790	-1.970418
N	-0.607969	-2.010773	-0.167279
N	1.546128	-1.708097	0.083599
C	0.343902	-1.052942	-0.027695
C	-0.115111	-3.371487	0.048113
H	-0.519507	-4.070548	-0.689532
H	-0.392181	-3.732265	1.048715
C	1.398086	-3.171557	-0.088452
H	1.974954	-3.713962	0.665978
H	1.766076	-3.472231	-1.078383
C	-2.019361	-1.620010	-0.121085
C	-2.578583	-1.726509	1.319744
H	-1.936671	-1.152352	1.996548
H	-2.559900	-2.774042	1.655219
C	-4.022242	-1.188812	1.360386
H	-4.407698	-1.261565	2.386588
C	-4.901855	-2.033226	0.415986
H	-4.920125	-3.080579	0.750760
H	-5.938989	-1.671933	0.440761
C	-4.347249	-1.940969	-1.020693
H	-4.969230	-2.544491	-1.695362
C	-2.900738	-2.490524	-1.048756
H	-2.497042	-2.460677	-2.069407
H	-2.902758	-3.542808	-0.725246
C	-4.367198	-0.464389	-1.472877
H	-4.011010	-0.377371	-2.507957
H	-5.401527	-0.090325	-1.456529
C	-3.470565	0.385070	-0.533861
H	-3.493319	1.428848	-0.860907
C	-2.037332	-0.166801	-0.632432
H	-1.761181	-0.194996	-1.695581
C	-4.023816	0.284757	0.901933
H	-3.417520	0.896144	1.580133
H	-5.047849	0.683187	0.938185
C	2.858746	-1.168434	-0.126650
C	3.758677	-1.116337	0.953291
C	5.060734	-0.658147	0.717725
H	5.756967	-0.608120	1.552530
C	5.489896	-0.271307	-0.553977
C	4.579637	-0.362485	-1.613217
H	4.898743	-0.079065	-2.614113
C	3.268025	-0.809774	-1.429112
C	3.359915	-1.568427	2.339330
H	4.057490	-1.183016	3.089410
H	3.368268	-2.663892	2.422459
H	2.351006	-1.237667	2.601457
C	6.891013	0.247553	-0.779977
H	6.914941	1.345195	-0.759448
H	7.282031	-0.065393	-1.754363
H	7.580277	-0.108402	-0.007208
C	2.319993	-0.880702	-2.604870
H	1.495451	-0.165591	-2.502471
H	1.867230	-1.873618	-2.709469
H	2.847952	-0.656628	-3.536485
C	-0.060689	0.844353	1.999923
H	0.550167	0.093667	2.518803
C	-1.355654	2.980353	-1.223560
C	-2.018606	4.208886	-1.824024
H	-1.759386	5.102667	-1.248298
H	-1.725596	4.333926	-2.868923
H	-3.108439	4.093498	-1.777319
C	1.500393	1.914298	-0.248442
H	2.223997	1.278443	-0.741087
H	1.249592	2.821917	-0.791777
C	1.523787	1.992878	1.183901
H	2.240524	1.328836	1.663368
C	-0.882484	1.667444	2.960939
H	-1.630984	0.999419	3.412787
H	-0.288008	2.069807	3.793210
H	-1.411123	2.483138	2.462308
C	1.366004	3.357976	1.827059
H	1.256284	3.307734	2.913552
H	2.265457	3.952050	1.616715
H	0.503134	3.880329	1.405806

TS1-s-C

B3LYP SCF energy: -1484.20403744 a.u.
B3LYP enthalpy: -1483.505694 a.u.
B3LYP free energy: -1483.604657 a.u.
M06 SCF energy in solution: -1484.60671016 a.u.
M06 enthalpy in solution: -1483.908367 a.u.
M06 free energy in solution: -1484.007330 a.u.
Imaginary frequency: -242.7746 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.398394	0.912573	0.326998
O	-1.383977	2.887253	0.452477
O	-0.855663	2.427378	-1.655577
N	-0.657034	-1.913734	-0.267003
N	1.509310	-1.644854	-0.076634
C	0.299899	-0.982517	-0.025599
C	-0.163513	-3.288928	-0.282915
H	-0.610607	-3.872614	-1.092409
H	-0.387168	-3.795441	0.667277
C	1.339864	-3.063413	-0.473128
H	1.955491	-3.720528	0.147180
H	1.646485	-3.195597	-1.519773
C	-2.066781	-1.516560	-0.248508
C	-2.703420	-1.757770	1.141825
H	-2.100952	-1.254425	1.902982
H	-2.702100	-2.833527	1.372766
C	-4.143955	-1.211125	1.160972
H	-4.583804	-1.382759	2.152908
C	-4.977566	-1.944007	0.090671
H	-5.022049	-3.019433	0.315838
H	-6.011625	-1.573244	0.096531
C	-4.345604	-1.714159	-1.297727
H	-4.934434	-2.238109	-2.062568
C	-2.904295	-2.278316	-1.304647
H	-2.446371	-2.153294	-2.294931
H	-2.934364	-3.357246	-1.088577
C	-4.329875	-0.199561	-1.597002
H	-3.917852	-0.012238	-2.597562
H	-5.360323	0.185006	-1.597477
C	-3.478119	0.539148	-0.530623
H	-3.475452	1.610082	-0.751994
C	-2.047138	-0.019597	-0.614301
H	-1.714740	0.057108	-1.659098
C	-4.107241	0.301504	0.857217
H	-3.530962	0.830300	1.626249
H	-5.127515	0.709948	0.880180

C	2.793244	-1.067909	-0.356846
C	3.849608	-1.275991	0.550061
C	5.113772	-0.757676	0.241406
H	5.926634	-0.905793	0.949685
C	5.359140	-0.064732	-0.945082
C	4.300842	0.085388	-1.848768
H	4.476639	0.599419	-2.791703
C	3.020286	-0.410113	-1.587272
C	3.667884	-2.071769	1.822355
H	4.356090	-1.727411	2.601110
H	3.879843	-3.137351	1.656912
H	2.647558	-1.999952	2.205641
C	6.721384	0.515980	-1.245712
H	6.747362	1.593770	-1.037325
H	6.988682	0.386156	-2.300493
H	7.501278	0.045898	-0.637856
C	1.924831	-0.218421	-2.610708
H	1.236349	0.584355	-2.321716
H	1.319354	-1.121755	-2.740976
H	2.354660	0.041672	-3.582992
C	-0.300735	0.817543	2.223607
C	-1.374075	3.184916	-0.794123
C	-2.040238	4.485554	-1.213740
H	-1.783148	5.288753	-0.516247
H	-1.747381	4.759287	-2.229846
H	-3.129782	4.362377	-1.182347
C	1.433425	2.042169	0.214806
H	2.297440	1.494561	-0.146874
H	1.153726	2.902279	-0.384357
C	1.247947	2.114520	1.639175
H	0.709261	2.998243	1.974107
C	2.394978	1.687054	2.537569
H	2.114397	1.638386	3.592950
H	2.810509	0.722513	2.235544
H	3.197199	2.431320	2.447810
H	-0.925748	1.590739	2.694061
C	0.159957	-0.225616	3.204291
H	0.609886	0.201755	4.110541
H	-0.725613	-0.784029	3.540692
H	0.856648	-0.942915	2.764946

TS1-s-D
B3LYP SCF energy: -1484.19483469 a.u.
B3LYP enthalpy: -1483.497078 a.u.
B3LYP free energy: -1483.597419 a.u.
M06 SCF energy in solution: -1484.59604337 a.u.
M06 enthalpy in solution: -1483.898287 a.u.
M06 free energy in solution:-1483.998628 a.u.
Imaginary frequency: -243.7541 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.381506	1.006023	0.467373
O	1.284832	1.998955	-1.618073
O	1.396264	2.973986	0.371847
N	0.669209	-1.891949	0.397664
N	-1.503392	-1.585191	0.273399
C	-0.291430	-0.927065	0.351689
C	0.163697	-3.254003	0.210316
H	0.574035	-3.935681	0.961170
H	0.434461	-3.639643	-0.781456
C	-1.348635	-3.056033	0.361274
H	-1.925962	-3.547751	-0.427220
H	-1.714315	-3.421041	1.328693
C	2.060943	-1.527164	0.097824
C	2.330073	-1.671611	-1.424101
H	1.610554	-1.051829	-1.971729
H	2.185728	-2.715064	-1.739171
C	3.767146	-1.224467	-1.754311
H	3.944919	-1.354731	-2.830421
C	4.773057	-2.076968	-0.955712
H	4.684324	-3.137268	-1.234751
H	5.799898	-1.768519	-1.194899
C	4.506537	-1.901276	0.553581
H	5.227444	-2.498322	1.128389
C	3.076847	-2.401143	0.870279
H	2.870679	-2.333351	1.946969
H	2.990322	-3.461260	0.586109
C	4.654100	-0.408205	0.924379
H	4.506801	-0.269608	2.004370
H	5.676777	-0.074133	0.695604
C	3.620763	0.437537	0.129776
H	3.723834	1.491988	0.410119
C	2.221454	-0.067052	0.537084
H	2.215599	-0.076397	1.638871
C	3.912698	0.260533	-1.375920
H	3.221602	0.866608	-1.966321
H	4.934999	0.602252	-1.595645
C	-2.745428	-1.090841	-0.243425
C	-2.823123	-0.688099	-1.597606
C	-4.057467	-0.267289	-2.099602
H	-4.114374	0.053117	-3.137961
C	-5.219140	-0.262499	-1.318574
C	-5.123584	-0.723901	-0.005580
H	-6.018049	-0.757700	0.613422
C	-3.909105	-1.152342	0.547187
C	-1.619290	-0.721567	-2.510039
H	-1.924579	-0.565371	-3.549151
H	-1.099964	-1.685519	-2.454266
H	-0.885347	0.050494	-2.253321
C	-6.531040	0.229193	-1.884111
H	-6.674889	-0.109864	-2.916301
H	-6.570786	1.326430	-1.897321
H	-7.380942	-0.122516	-1.290288
C	-3.903479	-1.707661	1.953119
H	-2.943984	-1.557799	2.451910
H	-4.105347	-2.787608	1.951182
H	-4.683023	-1.238012	2.561696
C	-1.354082	2.093328	-0.288027
H	-2.137980	1.477373	-0.713671
C	1.655559	2.954603	-0.880055
C	2.461213	4.098394	-1.469733
H	2.161989	4.283394	-2.504907
H	2.346379	5.006045	-0.871759
H	3.523229	3.822798	-1.472452
C	-0.122862	1.286574	2.270253
C	-1.477810	2.460804	1.088766
H	-0.904820	2.804353	-0.972117
H	-0.969006	3.383674	1.358162
C	-2.782125	2.208786	1.820140
H	-2.697906	2.352062	2.900977
H	-3.527499	2.927500	1.453367
H	-3.171292	1.207338	1.623226
H	0.394323	2.158720	2.697893
C	-0.772701	0.432123	3.316297
H	-1.399350	-0.353582	2.892360
H	0.042220	-0.058157	3.872717
H	-1.353154	1.001878	4.054863

TS1-s-E
B3LYP SCF energy: -1484.20837319 a.u.
B3LYP enthalpy: -1483.510118 a.u.
B3LYP free energy: -1483.609317 a.u.
M06 SCF energy in solution: -1484.60981630 a.u.
M06 enthalpy in solution: -1483.911561 a.u.
M06 free energy in solution:-1484.010760 a.u.
Imaginary frequency: -242.8084 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.384629	0.898910	0.185475
O	-1.407041	2.882626	0.150744
O	-0.840681	2.193425	-1.879295
N	-0.607481	-1.967274	-0.196806

N	1.547856	-1.656154	0.017784
C	0.336306	-1.006605	-0.025698
C	-0.098613	-3.331776	-0.068206
H	-0.524381	-3.997113	-0.824438
H	-0.334959	-3.744203	0.923272
C	1.404165	-3.106427	-0.252320
H	2.017107	-3.696346	0.434134
H	1.731161	-3.326304	-1.277869
C	-2.022592	-1.593793	-0.161311
C	-2.605376	-1.741780	1.265895
H	-1.981470	-1.176908	1.966785
H	-2.579388	-2.797366	1.574878
C	-4.055277	-1.219448	1.293192
H	-4.458801	-1.321300	2.309908
C	-4.909399	-2.047555	0.311818
H	-4.923107	-3.103436	0.618795
H	-5.950447	-1.697116	0.327119
C	-4.330121	-1.912594	-1.111630
H	-4.934033	-2.503871	-1.813022
C	-2.878805	-2.449048	-1.126474
H	-2.456702	-2.390825	-2.138531
H	-2.878151	-3.508875	-0.828907
C	-4.354740	-0.425258	-1.526867
H	-3.980346	-0.309683	-2.552741
H	-5.392428	-0.060401	-1.520713
C	-3.483600	0.408430	-0.550386
H	-3.511320	1.460251	-0.850195
C	-2.043723	-0.128861	-0.637283
H	-1.746250	-0.127015	-1.695351
C	-4.063536	0.265236	0.871496
H	-3.479091	0.865630	1.577766
H	-5.092683	0.651184	0.896208
C	2.847789	-1.101632	-0.222291
C	3.827156	-1.210629	0.782083
C	5.117182	-0.735109	0.515418
H	5.873059	-0.806450	1.294946
C	5.458475	-0.177810	-0.718637
C	4.471118	-0.115663	-1.709156
H	4.722222	0.297026	-2.684310
C	3.168447	-0.573866	-1.492236
C	3.522388	-1.844355	2.120565
H	4.227562	-1.500551	2.883868
H	3.607690	-2.938887	2.074565
H	2.507031	-1.614390	2.455897
C	6.848318	0.354957	-0.979280
H	6.872671	1.450484	-0.909935
H	7.197457	0.088913	-1.983481
H	7.570209	-0.035824	-0.254907
C	2.143113	-0.481121	-2.598669
H	1.406641	0.307235	-2.402349
H	1.580970	-1.414207	-2.717432
H	2.630193	-0.258981	-3.553063
C	-0.185101	0.846245	2.075091
H	0.457561	0.120392	2.591003
C	-1.382957	3.040484	-1.119473
C	-2.055863	4.272867	-1.700154
H	-1.853498	5.149111	-1.076867
H	-1.718769	4.450267	-2.723967
H	-3.142290	4.121501	-1.711043
C	1.470532	2.036233	-0.011994
H	2.334389	1.463653	-0.330867
H	1.171411	2.833246	-0.683791
C	1.261234	2.208126	1.391230
C	-1.029004	1.650630	3.034675
H	-1.718608	0.967305	3.551373
H	-0.420169	2.128835	3.817625
H	-1.617144	2.414485	2.520106
H	0.680243	3.087822	1.659984
C	2.363455	1.846546	2.372010
H	2.003567	1.770537	3.403329
H	2.854095	0.910274	2.096348
H	3.125839	2.636910	2.348098

TS1-s-F
B3LYP SCF energy: -1484.20205843 a.u.
B3LYP enthalpy: -1483.504127 a.u.
B3LYP free energy: -1483.603798 a.u.
M06 SCF energy in solution: -1484.60042382 a.u.
M06 enthalpy in solution: -1483.902492 a.u.
M06 free energy in solution:-1484.002163 a.u.
Imaginary frequency: -243.2735 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	0.360990	0.944357	0.229533
O	1.565526	1.855755	-1.753724
O	1.429393	2.908386	0.192118
N	0.655132	-1.953383	0.168061
N	-1.503120	-1.659987	0.018854
C	-0.306754	-0.992748	0.109562
C	0.163093	-3.310311	-0.076667
H	0.587904	-4.024811	0.633726
H	0.422490	-3.643029	-1.091388
C	-1.346285	-3.127198	0.101515
H	-1.936753	-3.621768	-0.675530
H	-1.693779	-3.492531	1.076950
C	2.070233	-1.586230	0.090405
C	2.584595	-1.679739	-1.370128
H	1.964236	-1.041466	-2.010000
H	2.493937	-2.713806	-1.734298
C	4.057717	-1.226823	-1.439844
H	4.410894	-1.314886	-2.476129
C	4.921522	-2.111892	-0.520337
H	4.884095	-3.161037	-0.848519
H	5.972680	-1.797289	-0.576213
C	4.409566	-1.991136	0.929469
H	5.025817	-2.613096	1.592907
C	2.948926	-2.494951	0.984973
H	2.566900	-2.469295	2.014594
H	2.914137	-3.542345	0.648066
C	4.488136	-0.514526	1.379640
H	4.161635	-0.420144	2.424700
H	5.533310	-0.174518	1.339365
C	3.600062	0.366616	0.457916
H	3.656793	1.410174	0.787929
C	2.151939	-0.143898	0.608591
H	1.956743	-0.192141	1.692917
C	4.140937	0.241426	-0.982965
H	3.562552	0.869922	-1.662255
H	5.186941	0.580855	-1.013785
C	-2.830645	-1.157047	-0.157880
C	-3.283413	-0.885418	-1.467706
C	-4.607231	-0.478134	-1.645907
H	-4.956281	-0.255764	-2.652261
C	-5.498999	-0.364822	-0.571164
C	-5.034654	-0.686782	0.705056
H	-5.716264	-0.622546	1.551125
C	-3.712048	-1.091353	0.935622
C	-2.371883	-1.068085	-2.659870
H	-2.868230	-0.743182	-3.579237
H	-2.095070	-2.122741	-2.788469
H	-1.438944	-0.505461	-2.555874
C	-6.919044	0.102296	-0.791786
H	-7.356085	-0.352504	-1.688016
H	-6.961367	1.190730	-0.929812
H	-7.559512	-0.145496	0.060770
C	-3.285498	-1.474420	2.334490
H	-2.209364	-1.355416	2.480855
H	-3.534351	-2.522716	2.549445
H	-3.803408	-0.864265	3.081920
C	-1.260003	1.935694	-0.902613
H	-2.027164	1.284419	-1.306438
C	1.845741	2.839199	-1.014184
C	2.727191	3.957635	-1.541425
H	2.562596	4.101829	-2.612621
H	2.544702	4.888838	-0.999049

H	3.778847	3.679029	-1.398947
C	-0.532799	1.287631	1.858872
H	-1.407993	0.725760	2.204476
C	-1.501954	2.528927	0.365358
H	-0.667296	2.468020	-1.637430
C	-0.004676	2.248669	2.891807
H	-0.795820	2.894195	3.303745
H	0.389918	1.660572	3.735228
H	0.801574	2.872992	2.499538
H	-0.916657	3.418149	0.587096
C	-2.881209	2.501807	0.994314
H	-2.857877	2.714019	2.068603
H	-3.489731	3.286230	0.522723
H	-3.389117	1.548953	0.833894

TS1-s-G

B3LYP SCF energy: -1484.20957809 a.u.
B3LYP enthalpy: -1483.511349 a.u.
B3LYP free energy: -1483.611536 a.u.
M06 SCF energy in solution: -1484.61089199 a.u.
M06 enthalpy in solution: -1483.912663 a.u.
M06 free energy in solution:-1484.012850 a.u.
Imaginary frequency: -236.6451 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.353306	0.890516	0.272916
O	-1.278303	2.923250	0.215298
O	-0.624905	2.206082	-1.779735
N	-0.660273	-1.945225	-0.219706
N	1.505175	-1.695169	0.035048
C	0.302679	-1.018545	0.014488
C	-0.184453	-3.325417	-0.152919
H	-0.614201	-3.942887	-0.946753
H	-0.444150	-3.781594	0.813398
C	1.327687	-3.127338	-0.306146
H	1.915357	-3.765155	0.359745
H	1.662611	-3.309173	-1.336322
C	-2.065208	-1.527889	-0.217930
C	-2.701508	-1.720141	1.179775
H	-2.088437	-1.206423	1.925197
H	-2.717122	-2.789052	1.440399
C	-4.133267	-1.151882	1.186541
H	-4.573015	-1.286787	2.184272
C	-4.980427	-1.904679	0.141092
H	-5.038862	-2.972134	0.398792
H	-6.009321	-1.519745	0.138294
C	-4.349128	-1.725127	-1.254952
H	-4.947304	-2.263472	-2.002354
C	-2.915085	-2.309259	-1.249075
H	-2.458508	-2.219084	-2.243670
H	-2.959313	-3.381045	-1.001757
C	-4.316288	-0.219641	-1.598810
H	-3.907803	-0.067286	-2.606746
H	-5.342321	0.176834	-1.605369
C	-3.448647	0.538499	-0.559093
H	-3.431015	1.604159	-0.807961
C	-2.026014	-0.042962	-0.634597
H	-1.704638	-0.010965	-1.684445
C	-4.074632	0.350466	0.837725
H	-3.486010	0.891350	1.588864
H	-5.088034	0.776001	0.853637
C	2.799344	-1.138938	-0.249140
C	3.821124	-1.253941	0.712268
C	5.096880	-0.771691	0.397361
H	5.884779	-0.851423	1.143550
C	5.386987	-0.200626	-0.843868
C	4.360294	-0.132086	-1.791458
H	4.568872	0.292077	-2.771643
C	3.067773	-0.595447	-1.525350
C	3.582795	-1.907525	2.053916
H	4.404503	-1.687926	2.742601
H	3.518098	-3.000593	1.965556
H	2.650501	-1.569634	2.512692
C	6.764186	0.338967	-1.152730
H	6.802796	1.427973	-1.017423
H	7.052119	0.133048	-2.189704
H	7.523197	-0.099267	-0.496425
C	1.999883	-0.476449	-2.588833
H	1.313335	0.352864	-2.379086
H	1.387366	-1.381040	-2.665627
H	2.456218	-0.295519	-3.566995
C	-0.327413	0.828476	2.172647
C	-1.169054	3.080585	-1.049457
C	-1.744584	4.341141	-1.671676
H	-1.622115	5.193571	-0.997419
H	-1.270195	4.546434	-2.634405
H	-2.819739	4.202615	-1.840269
C	1.532048	1.968876	0.203732
H	2.288328	1.366122	-0.281394
H	1.337461	2.930680	-0.263091
C	1.397641	1.883284	1.624740
H	2.038411	1.143783	2.101782
C	1.167848	3.160937	2.416822
H	0.904414	2.965690	3.461641
H	2.089204	3.758791	2.413506
H	0.371348	3.751392	1.955456
H	-0.902205	1.665232	2.595588
C	0.092155	-0.154902	3.232775
H	0.658592	-0.997103	2.827619
H	0.681540	0.319802	4.032004
H	-0.809640	-0.556223	3.716955

TS2-s-A

B3LYP SCF energy: -1484.19451211 a.u.
B3LYP enthalpy: -1483.497032 a.u.
B3LYP free energy: -1483.598688 a.u.
M06 SCF energy in solution: -1484.59283054 a.u.
M06 enthalpy in solution: -1483.895350 a.u.
M06 free energy in solution:-1483.997006 a.u.
Imaginary frequency: -196.9448 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.325751	0.846471	-0.481633
O	-1.376004	1.961545	1.349441
O	-1.274292	2.865768	-0.668669
N	-0.757512	-2.011182	-0.164161
N	1.415128	-1.788365	-0.052947
C	0.240006	-1.086407	-0.179725
C	-0.309631	-3.361971	0.180730
H	-0.771266	-4.114693	-0.464210
H	-0.561243	-3.605189	1.222862
C	1.203715	-3.250144	-0.032975
H	1.788686	-3.714952	0.766400
H	1.519750	-3.693030	-0.987177
C	-2.148695	-1.566121	-0.043154
C	-2.567549	-1.502604	1.448581
H	-1.881578	-0.835764	1.983782
H	-2.492054	-2.500917	1.904685
C	-4.012467	-0.980383	1.569883
H	-4.299629	-0.959004	2.629997
C	-4.969587	-1.904491	0.792368
H	-4.949509	-2.921193	1.211933
H	-6.001931	-1.540601	0.887066
C	-4.552412	-1.934476	-0.692145
H	-5.236659	-2.583069	-1.256000
C	-3.120430	-2.507622	-0.794217
H	-2.808037	-2.589724	-1.844041
H	-3.105785	-3.522171	-0.366984
C	-4.603539	-0.500405	-1.267268
H	-4.349692	-0.512653	-2.336167
H	-5.629064	-0.110890	-1.186982
C	-3.617054	0.416526	-0.491719

H	-3.657072	1.427414	-0.913731
C	-2.203158	-0.173405	-0.697639
H	-2.110034	-0.344584	-1.777803
C	-4.066841	0.443699	0.986481
H	-3.422051	1.102758	1.570238
H	-5.094959	0.830372	1.049191
C	2.748548	-1.302297	0.130050
C	3.173393	-0.972946	1.436980
C	4.492856	-0.558900	1.627769
H	4.819651	-0.294337	2.631386
C	5.405647	-0.481689	0.567607
C	4.969575	-0.856958	-0.703643
H	5.669559	-0.826792	-1.536613
C	3.655010	-1.281332	-0.944834
C	2.229836	-1.085868	2.613180
H	2.717073	-0.748428	3.532842
H	1.909294	-2.123916	2.769600
H	1.320144	-0.492858	2.470446
C	6.818343	0.002266	0.798728
H	7.234137	-0.403081	1.728154
H	6.853843	1.096628	0.880409
H	7.480874	-0.286800	-0.023431
C	3.268974	-1.743439	-2.331605
H	2.187257	-1.733431	-2.479521
H	3.619810	-2.768481	-2.512634
H	3.726748	-1.110631	-3.099782
C	1.550904	1.940856	0.442265
H	1.965887	1.116060	1.006968
C	-1.665569	2.896443	0.543501
C	-2.517501	4.059040	1.016037
H	-2.297462	4.295933	2.060633
H	-2.362001	4.937705	0.384972
H	-3.575345	3.774937	0.954266
C	0.400257	0.846992	-2.205436
H	1.095956	0.153581	-2.692601
H	0.084906	1.664413	-2.868636
C	1.900918	1.987457	-0.915380
H	2.577998	1.212066	-1.260247
C	1.299720	3.186805	1.258339
H	2.268339	3.611736	1.564766
H	0.764960	3.956374	0.698287
H	0.728459	2.959377	2.159777
C	1.905922	3.283009	-1.698862
H	2.688352	3.949577	-1.307822
H	2.114000	3.111610	-2.758919
H	0.946661	3.800458	-1.613315

TS2-s-C
B3LYP SCF energy: -1484.18604170 a.u.
B3LYP enthalpy: -1483.488025 a.u.
B3LYP free energy: -1483.586691 a.u.
M06 SCF energy in solution: -1484.58516532 a.u.
M06 enthalpy in solution: -1483.887149 a.u.
M06 free energy in solution:-1483.985815 a.u.
Imaginary frequency: -196.3713 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.426593	0.975836	-0.284839
O	-2.108957	2.122882	1.237610
O	-1.573608	2.792229	-0.808681
N	-0.615834	-1.812746	0.500385
N	1.536194	-1.447346	0.655825
C	0.330576	-0.859533	0.308496
C	-0.134302	-3.002378	1.202477
H	-0.547543	-3.920515	0.777994
H	-0.411525	-2.960594	2.265168
C	1.373962	-2.879380	0.997773
H	1.952795	-3.136786	1.889003
H	1.728031	-3.504996	0.167034
C	-2.024386	-1.565318	0.182835
C	-2.856764	-1.294018	1.459205
H	-2.435311	-0.433245	1.990129
H	-2.805703	-2.165320	2.129472
C	-4.324251	-1.007068	1.075703
H	-4.906162	-0.834617	1.990981
C	-4.916010	-2.200263	0.300840
H	-4.911701	-3.107305	0.923107
H	-5.963847	-1.995371	0.041857
C	-4.088324	-2.432371	-0.979173
H	-4.507210	-3.276614	-1.543694
C	-2.640202	-2.776585	-0.566732
H	-2.026519	-3.005937	-1.448410
H	-2.654406	-3.675866	0.067415
C	-4.115094	-1.158483	-1.853974
H	-3.561568	-1.330269	-2.787482
H	-5.153416	-0.930134	-2.135431
C	-3.496058	0.032504	-1.070956
H	-3.516808	0.931601	-1.697735
C	-2.028951	-0.351717	-0.765130
H	-1.605457	-0.706030	-1.716263
C	-4.360088	0.253339	0.192026
H	-3.997760	1.103909	0.768543
H	-5.396557	0.464435	-0.110184
C	2.848673	-1.075182	0.212688
C	3.840666	-0.790330	1.173049
C	5.129473	-0.463358	0.732965
H	5.888649	-0.222945	1.474846
C	5.469051	-0.448998	-0.621550
C	4.488225	-0.825296	-1.545698
H	4.746363	-0.878217	-2.601665
C	3.189694	-1.168609	-1.156023
C	3.577487	-0.903391	2.658566
H	4.136830	-0.146522	3.218326
H	3.906669	-1.883681	3.030598
H	2.518076	-0.795784	2.896969
C	6.852668	-0.047153	-1.076435
H	7.598707	-0.222697	-0.294270
H	6.891512	1.020448	-1.330746
H	7.158653	-0.603248	-1.969273
C	2.238601	-1.736490	-2.188655
H	1.201524	-1.439172	-2.025562
H	2.274521	-2.834783	-2.172539
H	2.528832	-1.423040	-3.196482
C	0.807428	2.424954	1.021414
C	-2.258157	2.912501	0.263278
C	-3.294949	4.019773	0.333685
H	-3.423981	4.359685	1.364622
H	-3.017592	4.856572	-0.312635
H	-4.258545	3.626705	-0.013996
C	0.667429	1.231725	-1.770013
H	1.639967	0.793202	-2.003744
H	0.304617	1.941773	-2.526941
C	1.367114	2.759648	-0.224780
H	0.822217	3.512473	-0.787076
C	2.845147	2.655065	-0.530666
H	3.278215	1.704766	-0.212990
H	3.045830	2.783126	-1.598331
H	3.376179	3.457108	0.003202
H	-0.066028	2.991425	1.319725
C	1.601845	1.888150	2.182265
H	1.999411	2.726084	2.776376
H	0.969075	1.293929	2.849002
H	2.446022	1.278990	1.864253

TS2-s-D
B3LYP SCF energy: -1484.19177596 a.u.
B3LYP enthalpy: -1483.493410 a.u.
B3LYP free energy: -1483.591911 a.u.
M06 SCF energy in solution: -1484.59462215 a.u.
M06 enthalpy in solution: -1483.896256 a.u.
M06 free energy in solution:-1483.994757 a.u.
Imaginary frequency: -250.5951 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.484729	0.913457	0.335399
O	-1.648571	2.816070	0.408077
O	-0.918197	2.306467	-1.623214
N	-0.683024	-1.937448	-0.140099
N	1.473013	-1.657924	0.087069
C	0.271267	-0.987199	0.041495
C	-0.196398	-3.310636	-0.016494
H	-0.620812	-3.961811	-0.785721
H	-0.457050	-3.728137	0.966363
C	1.310818	-3.108434	-0.173741
H	1.902862	-3.699841	0.529991
H	1.655323	-3.343102	-1.189921
C	-2.098072	-1.564298	-0.123081
C	-2.713784	-1.763717	1.284093
H	-2.109946	-1.227773	2.023640
H	-2.694545	-2.830699	1.551123
C	-4.163491	-1.242569	1.297243
H	-4.587312	-1.374817	2.302079
C	-4.995754	-2.042440	0.274626
H	-5.014858	-3.106625	0.551196
H	-6.037341	-1.693194	0.276765
C	-4.386142	-1.866301	-1.131451
H	-4.971885	-2.439831	-1.862465
C	-2.932083	-2.394678	-1.131455
H	-2.489211	-2.305521	-2.132328
H	-2.932352	-3.462422	-0.864545
C	-4.407273	-0.368698	-1.503238
H	-4.013135	-0.222197	-2.517900
H	-5.445584	-0.005839	-1.507151
C	-3.558262	0.438433	-0.486220
H	-3.591938	1.497134	-0.755495
C	-2.113318	-0.087963	-0.564734
H	-1.798518	-0.061908	-1.617712
C	-4.160180	0.254119	0.921222
H	-3.580199	0.830141	1.651600
H	-5.187641	0.644393	0.942334
C	2.780684	-1.142905	-0.194288
C	3.779217	-1.246666	0.790980
C	5.080875	-0.838741	0.470890
H	5.852702	-0.903224	1.235388
C	5.416062	-0.370036	-0.801229
C	4.408466	-0.319773	-1.772002
H	4.653705	0.026912	-2.773991
C	3.092114	-0.697271	-1.497160
C	3.489435	-1.824025	2.158019
H	4.185025	-1.428658	2.905286
H	3.606492	-2.916708	2.158456
H	2.468243	-1.608160	2.482843
C	6.821066	0.084639	-1.121813
H	7.125365	-0.232401	-2.125699
H	7.545990	-0.315374	-0.405454
H	6.899853	1.179469	-1.092203
C	2.038822	-0.608978	-2.577055
H	1.304440	0.174885	-2.358847
H	1.477059	-1.544317	-2.683047
H	2.498857	-0.384357	-3.544191
C	-0.419983	0.677144	2.201947
H	0.161807	-0.053398	2.777651
C	-1.577889	3.053784	-0.847365
C	-2.333157	4.248994	-1.402003
H	-1.841984	4.627859	-2.301952
H	-3.349384	3.938912	-1.675939
H	-2.414255	5.038562	-0.650158
C	1.212527	2.451436	0.450228
C	1.026412	2.199034	1.838458
H	-1.095021	1.269271	2.834290
H	0.622645	3.275066	0.066811
C	2.536093	2.299744	-0.251265
H	3.142223	1.477837	0.126291
H	2.394095	2.166094	-1.327043
H	3.115477	3.228149	-0.119031
H	0.339937	2.892421	2.318615
C	2.161756	1.708463	2.715509
H	2.910176	2.507270	2.818437
H	1.817368	1.446961	3.720346
H	2.666645	0.841426	2.285336

TS2-s-E

B3LYP SCF energy: -1484.18724075 a.u.
B3LYP enthalpy: -1483.489846 a.u.
B3LYP free energy: -1483.589896 a.u.
M06 SCF energy in solution: -1484.58561278 a.u.
M06 enthalpy in solution: -1483.888218 a.u.
M06 free energy in solution:-1483.988268 a.u.
Imaginary frequency: -205.8370 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.381586	0.891929	-0.543864
O	-1.422165	1.993259	1.291168
O	-1.434799	2.854610	-0.747568
N	-0.724463	-1.969712	-0.142155
N	1.443225	-1.698319	-0.062312
C	0.252072	-1.022608	-0.191020
C	-0.247032	-3.306303	0.215409
H	-0.695425	-4.074332	-0.420788
H	-0.491798	-3.544409	1.260200
C	1.261074	-3.165107	-0.005585
H	1.858408	-3.594321	0.804311
H	1.583206	-3.625540	-0.948411
C	-2.126203	-1.565169	-0.012726
C	-2.528365	-1.485994	1.483119
H	-1.855140	-0.789888	1.996640
H	-2.418555	-2.472935	1.956453
C	-3.986451	-1.003338	1.613047
H	-4.261169	-0.971039	2.676165
C	-4.926087	-1.968273	0.864410
H	-4.871804	-2.976048	1.302006
H	-5.967256	-1.632341	0.965711
C	-4.526169	-2.013190	-0.624413
H	-5.198507	-2.690753	-1.168134
C	-3.079905	-2.548673	-0.733583
H	-2.777759	-2.642714	-1.785405
H	-3.032467	-3.553912	-0.287348
C	-4.625332	-0.591735	-1.223656
H	-4.384734	-0.615590	-2.295418
H	-5.660482	-0.230193	-1.136833
C	-3.655800	0.366503	-0.477328
H	-3.728949	1.367503	-0.917498
C	-2.229735	-0.190602	-0.691664
H	-2.147229	-0.381351	-1.769208
C	-4.088144	0.407708	1.005639
H	-3.455106	1.093922	1.570495
H	-5.125758	0.766916	1.074925
C	2.761604	-1.200784	0.180364
C	3.097322	-0.761336	1.480080
C	4.414129	-0.370896	1.733923
H	4.674122	-0.025002	2.732415
C	5.407946	-0.425970	0.748342
C	5.053906	-0.900800	-0.515575
H	5.813825	-0.965746	-1.291899
C	3.744945	-1.299413	-0.820227
C	2.062760	-0.722130	2.580177
H	2.515725	-0.408512	3.525461
H	1.606378	-1.707483	2.736849
H	1.245909	-0.030619	2.345053
C	6.818029	0.027626	1.046919
H	7.140451	-0.295442	2.043242
H	6.896160	1.122623	1.022579
H	7.530025	-0.367914	0.315407
C	3.429954	-1.841620	-2.195507
H	2.397149	-1.631541	-2.486373
H	3.566970	-2.930819	-2.235367
H	4.096173	-1.407968	-2.948262

C	1.541355	2.090104	0.230459
H	2.251333	1.344410	0.574480
C	-1.782774	2.896247	0.477261
C	-2.665360	4.032210	0.957604
H	-2.396822	4.318755	1.978310
H	-2.591749	4.893032	0.288465
H	-3.708679	3.693473	0.971001
C	0.281409	0.873485	-2.287158
H	1.044196	0.229963	-2.742026
H	-0.127870	1.611751	-2.993376
C	1.589402	2.383502	-1.138322
C	1.205394	3.146105	1.260332
H	2.146251	3.616658	1.585440
H	0.572635	3.933400	0.842811
H	0.707576	2.735153	2.140187
H	1.028237	3.261030	-1.457316
C	2.792220	2.041942	-1.994957
H	3.234544	1.084344	-1.713799
H	2.570502	2.036266	-3.066357
H	3.554670	2.816643	-1.824480

TS2-s-F

B3LYP SCF energy: -1484.19762047 a.u.
B3LYP enthalpy: -1483.499936 a.u.
B3LYP free energy: -1483.598807 a.u.
M06 SCF energy in solution: -1484.59732990 a.u.
M06 enthalpy in solution: -1483.899645 a.u.
M06 free energy in solution:-1483.998516 a.u.
Imaginary frequency: -215.7970 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.408919	0.840201	0.424646
O	-1.368454	2.859730	0.525219
O	-0.648618	2.258846	-1.482514
N	-0.776681	-1.941478	-0.292517
N	1.397867	-1.756495	-0.119283
C	0.215371	-1.055061	-0.021371
C	-0.329009	-3.329161	-0.386234
H	-0.810878	-3.857818	-1.213348
H	-0.548662	-3.874778	0.543048
C	1.175095	-3.140723	-0.598961
H	1.782831	-3.854120	-0.036534
H	1.453640	-3.214796	-1.659351
C	-2.172285	-1.505210	-0.218447
C	-2.787310	-1.809558	1.169337
H	-2.148168	-1.383810	1.949576
H	-2.824660	-2.897518	1.329170
C	-4.205656	-1.213057	1.252238
H	-4.629233	-1.420764	2.244326
C	-5.089125	-1.860042	0.166240
H	-5.166533	-2.943630	0.336688
H	-6.109262	-1.455171	0.216296
C	-4.480782	-1.578940	-1.223338
H	-5.102214	-2.045878	-1.999383
C	-3.058150	-2.184983	-1.292660
H	-2.618060	-2.022875	-2.285523
H	-3.118687	-3.272211	-1.131831
C	-4.426703	-0.052084	-1.445569
H	-4.034255	0.173986	-2.446145
H	-5.444651	0.361901	-1.398819
C	-3.524376	0.602598	-0.366305
H	-3.495820	1.684547	-0.526069
C	-2.114330	0.006106	-0.519976
H	-1.819830	0.108268	-1.572941
C	-4.123117	0.311273	1.025012
H	-3.506901	0.777945	1.802838
H	-5.126977	0.752989	1.100223
C	2.710685	-1.221584	-0.329613
C	3.732873	-1.560138	0.578114
C	5.026859	-1.080872	0.342601
H	5.814463	-1.331964	1.050493
C	5.333016	-0.298337	-0.772697
C	4.305386	-0.015879	-1.679743
H	4.529258	0.568658	-2.569951
C	2.996267	-0.469387	-1.490985
C	3.474090	-2.449895	1.773172
H	4.167900	-2.220977	2.588547
H	3.619464	-3.508905	1.518112
H	2.451758	-2.343660	2.146328
C	6.729243	0.236418	-0.992161
H	6.985305	0.262665	-2.057062
H	7.478548	-0.374318	-0.477693
H	6.826061	1.262001	-0.611485
C	1.936781	-0.142731	-2.517845
H	1.260434	0.648965	-2.174702
H	1.309682	-1.010663	-2.750350
H	2.402974	0.192776	-3.449584
C	-0.500200	0.488567	2.264987
H	-0.082379	-0.345277	2.841952
C	-1.241579	3.083331	-0.723820
C	-1.778094	4.381487	-1.297546
H	-0.964375	5.115777	-1.350451
H	-2.149155	4.223391	-2.313872
H	-2.568645	4.789513	-0.663064
C	1.638099	1.917626	0.655012
H	2.383111	1.221757	0.281357
C	1.278090	1.753959	2.011881
C	1.710430	3.294175	0.032216
H	2.711670	3.713724	0.214489
H	1.550554	3.263140	-1.047525
H	0.977351	3.973205	0.475064
H	-1.083432	1.180549	2.890035
H	0.789307	2.615551	2.466258
C	2.146673	0.932844	2.947713
H	1.660461	0.716724	3.903457
H	2.447939	-0.007657	2.482410
H	3.061321	1.502669	3.164045

TS2-s-G

B3LYP SCF energy: -1484.18968363 a.u.
B3LYP enthalpy: -1483.491843 a.u.
B3LYP free energy: -1483.590800 a.u.
M06 SCF energy in solution: -1484.58769438 a.u.
M06 enthalpy in solution: -1483.889854 a.u.
M06 free energy in solution:-1483.988811 a.u.
Imaginary frequency: -186.1145 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.353803	0.929691	-0.287942
O	-1.944028	2.074862	1.236672
O	-1.428952	2.808190	-0.790446
N	-0.621354	-1.861934	0.452004
N	1.533087	-1.515278	0.666404
C	0.337082	-0.915977	0.299640
C	-0.163311	-3.067417	1.143478
H	-0.573222	-3.974871	0.693096
H	-0.463516	-3.042841	2.200395
C	1.352383	-2.951922	0.976388
H	1.908900	-3.230348	1.876056
H	1.720211	-3.566319	0.143680
C	-2.024799	-1.570506	0.141558
C	-2.841669	-1.291572	1.426234
H	-2.390936	-0.451903	1.966429
H	-2.815171	-2.173234	2.084361
C	-4.301286	-0.953629	1.054919
H	-4.872730	-0.774661	1.975604
C	-4.933446	-2.118791	0.269336
H	-4.954628	-3.032533	0.881391
H	-5.975659	-1.878810	0.017756
C	-4.119611	-2.361282	-1.017608
H	-4.566702	-3.186342	-1.588838
C	-2.679252	-2.753268	-0.618651

H	-2.078725	-2.989111	-1.507698
H	-2.715582	-3.660142	0.004047
C	-4.115438	-1.076888	-1.877673
H	-3.573368	-1.253316	-2.816993
H	-5.148921	-0.816296	-2.149112
C	-3.456183	0.085812	-1.085693
H	-3.454055	0.993026	-1.701294
C	-1.999249	-0.342744	-0.792487
H	-1.593430	-0.699491	-1.749699
C	-4.302541	0.318441	0.186924
H	-3.906171	1.149108	0.770610
H	-5.334027	0.567942	-0.102821
C	2.849379	-1.128462	0.239061
C	3.815820	-0.766524	1.198353
C	5.093458	-0.393572	0.759587
H	5.832285	-0.096231	1.501707
C	5.448292	-0.405543	-0.589704
C	4.498260	-0.861984	-1.510798
H	4.771321	-0.937748	-2.561587
C	3.213920	-1.253021	-1.122760
C	3.558689	-0.835915	2.687855
H	3.808027	0.109130	3.183009
H	4.190973	-1.610491	3.141123
H	2.518962	-1.074162	2.916909
C	6.816415	0.046969	-1.043788
H	6.805676	1.104146	-1.340905
H	7.162250	-0.528307	-1.909537
H	7.559117	-0.059296	-0.246169
C	2.301453	-1.891133	-2.149960
H	1.247831	-1.653354	-1.994790
H	2.402695	-2.984935	-2.120386
H	2.575408	-1.574396	-3.161316
C	0.870312	2.347146	1.039757
C	-2.088852	2.908911	0.296491
C	-3.089125	4.041991	0.437647
H	-3.163580	4.360618	1.480893
H	-2.814680	4.885859	-0.200536
H	-4.078445	3.685433	0.124727
C	0.754231	1.099280	-1.774123
H	1.682808	0.589877	-2.042598
H	0.460054	1.880800	-2.488296
C	1.759377	2.295129	-0.039246
H	2.584660	1.589264	0.013495
C	1.970275	3.514883	-0.915066
H	2.639346	4.215557	-0.394126
H	2.434416	3.270837	-1.875222
H	1.021476	4.026008	-1.101944
H	0.246144	3.236562	1.072164
C	1.085045	1.709557	2.388502
H	0.123169	1.527421	2.876565
H	1.628001	0.769733	2.316045
H	1.661067	2.389699	3.035543

TS1-b-A

B3LYP SCF energy: -1484.19109104 a.u.
B3LYP enthalpy: -1483.492803 a.u.
B3LYP free energy: -1483.592168 a.u.
M06 SCF energy in solution: -1484.59364936 a.u.
M06 enthalpy in solution: -1483.895361 a.u.
M06 free energy in solution:-1483.994726 a.u.
Imaginary frequency: -172.5915 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.381378	1.027960	-0.128621
O	1.094024	0.786946	-2.045389
O	1.739862	1.911356	-0.244027
N	-0.959999	-1.870541	-0.099386
N	1.215692	-1.771338	0.078262
C	0.084891	-1.035452	-0.041778
C	-0.589559	-3.290673	-0.032727
H	-0.828393	-3.793877	-0.976539
H	-1.131249	-3.801717	0.769644
C	0.924652	-3.215686	0.228762
H	1.197373	-3.545416	1.238892
H	1.507919	-3.803462	-0.484913
C	-2.336841	-1.366114	-0.075525
C	-2.886937	-1.445964	1.371104
H	-2.232649	-0.862941	2.030015
H	-2.870670	-2.487372	1.725399
C	-4.325798	-0.897969	1.420380
H	-4.708595	-0.970808	2.447402
C	-5.226889	-1.712370	0.471193
H	-5.261946	-2.764878	0.787449
H	-6.256601	-1.331918	0.512157
C	-4.678647	-1.607036	-0.966275
H	-5.321496	-2.178317	-1.649258
C	-3.253509	-2.201812	-1.002222
H	-2.852058	-2.182604	-2.023909
H	-3.292547	-3.255040	-0.684035
C	-4.649144	-0.123735	-1.397264
H	-4.300061	-0.038260	-2.434784
H	-5.669208	0.287375	-1.366734
C	-3.712070	0.677762	-0.452558
H	-3.721866	1.730483	-0.765583
C	-2.280147	0.091228	-0.585260
H	-2.103543	0.007533	-1.671979
C	-4.304465	0.574720	0.971126
H	-3.732570	1.171674	1.688061
H	-5.327217	0.978960	0.972006
C	2.577663	-1.342466	0.223503
C	3.038952	-0.922213	1.483491
C	4.393997	-0.610738	1.626148
H	4.755871	-0.280180	2.597545
C	5.293764	-0.723695	0.561894
C	4.805035	-1.164606	-0.671617
H	5.491042	-1.266450	-1.510201
C	3.454936	-1.476238	-0.868721
C	2.106628	-0.826724	2.667056
H	2.640536	-0.465486	3.551139
H	1.667784	-1.800942	2.919889
H	1.277936	-0.141500	2.467598
C	6.750070	-0.358283	0.734376
H	6.918455	0.706235	0.523435
H	7.390583	-0.929502	0.053777
H	7.092036	-0.543225	1.758476
C	2.964886	-1.913990	-2.228899
H	2.537755	-2.924905	-2.214210
H	3.789271	-1.920600	-2.948780
H	2.190481	-1.228244	-2.588399
C	-0.986795	1.910154	1.469773
H	-2.008446	1.860660	1.854765
C	1.939982	1.507414	-1.434384
C	3.217863	1.935631	-2.137259
H	3.267505	1.523790	-3.147706
H	3.254104	3.029881	-2.189137
H	4.087431	1.605887	-1.560615
C	-1.063699	2.599295	-1.276171
C	-1.174264	3.189061	0.074849
H	-0.261464	2.987582	-1.902249
H	-1.982849	2.399911	-1.822218
H	-2.218003	3.364289	0.337887
C	-0.027381	2.379977	2.543737
H	-0.347249	3.320449	3.014599
H	-0.024170	1.623219	3.340866
H	0.994696	2.495625	2.173583
C	-0.257137	4.378066	0.342236
H	-0.527981	5.198213	-0.334402
H	-0.344384	4.754480	1.365153
H	0.783915	4.102612	0.154650

TS1-b-B

B3LYP SCF energy: -1484.19347453 a.u.
B3LYP enthalpy: -1483.495250 a.u.

B3LYP free energy: -1483.594698 a.u.
M06 SCF energy in solution: -1484.59673930 a.u.
M06 enthalpy in solution: -1483.898515 a.u.
M06 free energy in solution:-1483.997963 a.u.
Imaginary frequency: -179.1259 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.362601	1.020473	-0.072354
O	0.384274	0.498058	2.156714
O	1.631874	1.755427	0.819292
N	-0.987253	-1.854721	-0.377446
N	1.196899	-1.787214	-0.309655
C	0.069097	-1.038236	-0.256429
C	-0.618694	-3.276494	-0.333361
H	-1.155788	-3.852268	-1.090931
H	-0.847537	-3.702812	0.652510
C	0.891882	-3.206178	-0.599026
H	1.476035	-3.869927	0.043151
H	1.138337	-3.434616	-1.644445
C	-2.339601	-1.322178	-0.166021
C	-2.731949	-1.464227	1.325694
H	-1.990312	-0.940384	1.939731
H	-2.717842	-2.524861	1.617816
C	-4.136596	-0.875614	1.554152
H	-4.410725	-0.989947	2.611483
C	-5.165586	-1.604957	0.669115
H	-5.211317	-2.671045	0.934497
H	-6.168914	-1.190173	0.838424
C	-4.768668	-1.440881	-0.811764
H	-5.500418	-1.953406	-1.450692
C	-3.377806	-2.077282	-1.028714
H	-3.085931	-2.021658	-2.085948
H	-3.424074	-3.143008	-0.756133
C	-4.731377	0.062281	-1.165439
H	-4.493255	0.194626	-2.229409
H	-5.726878	0.501389	-1.002577
C	-3.669346	0.782845	-0.292018
H	-3.673041	1.850547	-0.555384
C	-2.281252	0.164148	-0.608354
H	-2.224166	0.130091	-1.708806
C	-4.094858	0.618156	1.186433
H	-3.401605	1.126099	1.863718
H	-5.084973	1.071966	1.338987
C	2.563209	-1.349453	-0.295328
C	3.305268	-1.497999	0.891472
C	4.651426	-1.120152	0.880582
H	5.232385	-1.228626	1.794386
C	5.268286	-0.606568	-0.265011
C	4.509462	-0.504854	-1.433927
H	4.977466	-0.129580	-2.341852
C	3.163097	-0.881929	-1.477092
C	2.678057	-2.059251	2.146908
H	3.379620	-2.002882	2.984872
H	2.403565	-3.115816	2.025827
H	1.769757	-1.511696	2.416361
C	6.711295	-0.159469	-0.233478
H	7.179331	-0.241051	-1.220373
H	7.300881	-0.754426	0.472594
H	6.791897	0.890090	0.079375
C	2.404133	-0.832882	-2.782534
H	2.321775	-1.832467	-3.231669
H	2.919876	-0.195133	-3.506785
H	1.388915	-0.450602	-2.651554
C	-1.277206	2.617015	0.896519
H	-2.333092	2.506080	1.104336
C	1.414426	1.210293	1.946858
H	-0.682415	2.907519	1.761836
C	2.416848	1.438123	3.066532
H	2.090894	0.956843	3.991206
H	3.395231	1.045536	2.769689
H	2.537268	2.513864	3.235855
C	-0.422509	1.978613	-1.735451
C	-0.907263	3.246456	-0.380561
H	-1.314728	1.963702	-2.379533
H	-1.794826	3.519682	-0.953751
C	0.794337	2.453386	-2.496561
H	0.978846	1.732515	-3.303973
H	0.637357	3.426460	-2.983083
H	1.689848	2.504979	-1.871263
C	0.145852	4.345167	-0.294713
H	0.427713	4.740092	-1.274266
H	-0.261996	5.179208	0.290136
H	1.040807	3.972664	0.209979

TS1-b-C
B3LYP SCF energy: -1484.17977286 a.u.
B3LYP enthalpy: -1483.481653 a.u.
B3LYP free energy: -1483.581983 a.u.
M06 SCF energy in solution: -1484.58491236 a.u.
M06 enthalpy in solution: -1483.886793 a.u.
M06 free energy in solution:-1483.987123 a.u.
Imaginary frequency: -108.9849 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.291932	1.037731	-0.175013
O	0.954780	0.648430	-2.238621
O	1.765971	1.914450	-0.599992
N	-0.805704	-1.875938	-0.051949
N	1.358564	-1.685744	0.196606
C	0.204880	-1.001456	0.006829
C	-0.379257	-3.277414	0.061835
H	-0.546647	-3.807325	-0.883055
H	-0.938009	-3.798087	0.845748
C	1.116282	-3.132437	0.396477
H	1.347281	-3.408689	1.433160
H	1.756408	-3.726911	-0.260419
C	-2.200029	-1.423580	-0.085125
C	-2.809666	-1.529223	1.334705
H	-2.210312	-0.921718	2.022531
H	-2.769867	-2.569820	1.689313
C	-4.270028	-1.037707	1.317169
H	-4.695299	-1.123047	2.326397
C	-5.094147	-1.890651	0.332358
H	-5.101008	-2.942679	0.652277
H	-6.139412	-1.552666	0.325241
C	-4.488045	-1.767916	-1.080360
H	-5.075139	-2.368815	-1.787752
C	-3.037856	-2.296781	-1.052355
H	-2.591982	-2.256538	-2.054806
H	-3.040543	-3.351227	-0.735757
C	-4.500070	-0.287425	-1.516969
H	-4.105218	-0.190237	-2.536934
H	-5.536243	0.081982	-1.537278
C	-3.644527	0.556314	-0.533633
H	-3.685211	1.603831	-0.856601
C	-2.183232	0.038913	-0.585328
H	-1.947979	-0.034348	-1.663493
C	-4.286755	0.433985	0.862734
H	-3.752781	1.051376	1.590237
H	-5.321740	0.804017	0.831124
C	2.693832	-1.182991	0.352043
C	3.101551	-0.665755	1.594927
C	4.430840	-0.261142	1.743109
H	4.750865	0.143898	2.701041
C	5.357836	-0.370702	0.702163
C	4.925326	-0.912540	-0.511504
H	5.634608	-1.017681	-1.330144
C	3.602750	-1.324212	-0.712784
C	2.140510	-0.552905	2.754073
H	2.663119	-0.226076	3.658239
H	1.652498	-1.509817	2.977273
H	1.346573	0.169208	2.539465
C	6.782064	0.101732	0.881002
H	6.869027	1.178027	0.681119

H	7.465134	-0.413233	0.197190
H	7.135302	-0.066211	1.904466
C	3.176233	-1.888548	-2.048351
H	2.922158	-2.955038	-1.984593
H	3.986179	-1.795114	-2.778413
H	2.299800	-1.356949	-2.432500
C	-0.410825	2.010809	1.487492
C	1.848362	1.417257	-1.769471
C	3.054313	1.781597	-2.620445
H	3.970749	1.446955	-2.123515
H	2.985636	1.328650	-3.612023
H	3.116438	2.871106	-2.719002
C	-0.975836	2.675484	-1.200336
C	-0.917661	3.210871	0.198318
H	-0.219549	3.053065	-1.885774
H	-1.968109	2.595173	-1.641156
H	0.595435	2.381429	1.736220
C	-1.264521	1.991294	2.733697
H	-1.218375	2.938280	3.291801
H	-2.310018	1.743685	2.554018
H	-0.850100	1.219407	3.397076
H	-0.060224	3.878671	0.288979
C	-2.226523	3.851007	0.667414
H	-2.153610	4.242062	1.686091
H	-2.467841	4.690929	0.005629
H	-3.057835	3.143761	0.627356

TS1-b-D

B3LYP SCF energy: -1484.18846305 a.u.
B3LYP enthalpy: -1483.490225 a.u.
B3LYP free energy: -1483.589033 a.u.
M06 SCF energy in solution: -1484.59213648 a.u.
M06 enthalpy in solution: -1483.893898 a.u.
M06 free energy in solution:-1483.992706 a.u.
Imaginary frequency: -201.6514 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.314466	0.992469	0.072658
O	0.466156	0.264726	2.238262
O	1.629448	1.725488	1.035172
N	-0.795262	-1.862815	-0.510994
N	1.382333	-1.652586	-0.513824
C	0.211147	-0.994042	-0.344443
C	-0.334951	-3.253545	-0.611270
H	-0.866008	-3.796324	-1.397051
H	-0.490126	-3.780917	0.339715
C	1.155667	-3.056214	-0.927322
H	1.808514	-3.736067	-0.375001
H	1.369630	-3.168533	-1.998626
C	-2.164278	-1.428124	-0.204396
C	-2.484180	-1.704947	1.285896
H	-1.742765	-1.196835	1.912519
H	-2.411148	-2.783621	1.490938
C	-3.902672	-1.202412	1.612708
H	-4.125909	-1.403566	2.669025
C	-4.932854	-1.918804	0.718166
H	-4.915332	-3.001756	0.907998
H	-5.947141	-1.568962	0.955093
C	-4.608750	-1.632606	-0.761848
H	-5.340439	-2.138666	-1.406070
C	-3.196924	-2.173988	-1.080515
H	-2.955166	-2.023500	-2.141364
H	-3.173154	-3.257936	-0.888056
C	-4.662100	-0.109532	-1.008088
H	-4.477804	0.108497	-2.068971
H	-5.670633	0.263338	-0.774731
C	-3.601443	0.603807	-0.127781
H	-3.674247	1.684649	-0.310640
C	-2.196258	0.089817	-0.534875
H	-2.166939	0.131249	-1.633383
C	-3.944421	0.314517	1.352125
H	-3.236113	0.807776	2.024874
H	-4.944209	0.709062	1.585359
C	2.716433	-1.125808	-0.473486
C	3.506911	-1.381417	0.661885
C	4.824361	-0.911405	0.669677
H	5.441924	-1.101209	1.545407
C	5.365177	-0.203999	-0.408102
C	4.557721	0.010254	-1.529177
H	4.966136	0.543155	-2.385491
C	3.237522	-0.445912	-1.588057
C	2.958462	-2.138064	1.849951
H	3.660516	-2.096783	2.688361
H	2.794748	-3.199610	1.619468
H	2.002350	-1.718685	2.178139
C	6.776601	0.332942	-0.354657
H	7.415844	-0.280078	0.289773
H	6.793801	1.355058	0.046433
H	7.231574	0.367719	-1.350538
C	2.408239	-0.221840	-2.830511
H	2.069051	-1.168768	-3.269619
H	2.989752	0.306294	-3.592314
H	1.513883	0.369838	-2.612309
C	-1.236916	2.494898	1.185120
H	-2.312951	2.453181	1.323341
C	1.457761	1.046746	2.096016
H	-0.672397	2.613523	2.106975
C	2.468323	1.195343	3.221556
H	2.196086	0.575984	4.078968
H	3.463867	0.915250	2.861410
H	2.519373	2.245427	3.530348
C	-0.240746	2.143176	-1.461699
C	-0.765649	3.257452	0.015620
H	0.770889	2.550698	-1.614087
H	0.192337	3.740992	0.200072
C	-1.078895	2.295464	-2.709096
H	-2.136986	2.072830	-2.557657
H	-0.988149	3.287732	-3.170804
H	-0.694744	1.573369	-3.444129
C	-1.806015	4.191498	-0.604474
H	-1.432984	4.696850	-1.499408
H	-2.728836	3.664828	-0.861771
H	-2.057545	4.962425	0.133572

TS1-b-E

B3LYP SCF energy: -1484.18998354 a.u.
B3LYP enthalpy: -1483.491652 a.u.
B3LYP free energy: -1483.590833 a.u.
M06 SCF energy in solution: -1484.59341632 a.u.
M06 enthalpy in solution: -1483.895085 a.u.
M06 free energy in solution:-1483.994266 a.u.
Imaginary frequency: -190.1498 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.359751	1.014632	-0.154799
O	1.071368	0.794828	-2.098955
O	1.729587	1.958173	-0.325607
N	-0.844606	-1.900029	-0.089570
N	1.325827	-1.724272	0.097308
C	0.170768	-1.030749	-0.038871
C	-0.428073	-3.305569	0.008221
H	-0.657875	-3.839817	-0.920363
H	-0.946978	-3.813541	0.827697
C	1.086198	-3.177165	0.255108
H	1.380496	-3.495018	1.262796
H	1.681596	-3.746687	-0.463620
C	-2.236635	-1.437066	-0.073829
C	-2.781702	-1.502669	1.375713
H	-2.143017	-0.889104	2.021906
H	-2.737321	-2.536014	1.750794
C	-4.235138	-0.993892	1.414939
H	-4.613612	-1.050663	2.444600

C	-5.112905	-1.861015	0.490638
H	-5.116312	-2.904462	0.837500
H	-6.153627	-1.510702	0.522494
C	-4.570870	-1.780901	-0.950955
H	-5.196233	-2.392460	-1.615091
C	-3.126185	-2.325731	-0.977184
H	-2.729101	-2.316738	-2.000795
H	-3.125711	-3.371582	-0.633393
C	-4.588372	-0.311439	-1.422987
H	-4.240827	-0.243563	-2.462390
H	-5.620749	0.068536	-1.404098
C	-3.678626	0.546779	-0.502536
H	-3.725769	1.585292	-0.852191
C	-2.225759	0.013525	-0.610794
H	-2.031515	-0.080559	-1.694434
C	-4.257568	0.466930	0.927118
H	-3.690563	1.096619	1.620162
H	-5.290633	0.844375	0.930130
C	2.667695	-1.238556	0.250572
C	3.097395	-0.785760	1.510772
C	4.433633	-0.405923	1.661243
H	4.770523	-0.048892	2.632330
C	5.346673	-0.482357	0.604815
C	4.891552	-0.960500	-0.627387
H	5.589031	-1.036324	-1.459224
C	3.560189	-1.341543	-0.832096
C	2.152020	-0.729927	2.686649
H	2.655265	-0.319968	3.567515
H	1.776490	-1.726609	2.953961
H	1.281687	-0.104444	2.470139
C	6.780099	-0.039126	0.785877
H	7.134934	-0.233021	1.804065
H	6.885998	1.039039	0.605916
H	7.450559	-0.552929	0.088735
C	3.105167	-1.823056	-2.189793
H	2.766316	-2.866986	-2.169281
H	3.925969	-1.763666	-2.911295
H	2.275731	-1.207408	-2.552940
C	-0.909140	1.871390	1.464189
H	-1.931698	1.859029	1.854916
C	1.914293	1.541707	-1.513246
C	3.167597	1.986936	-2.249501
H	3.207149	1.557061	-3.252917
H	3.176392	3.080506	-2.322849
H	4.055785	1.689535	-1.683745
C	-1.051660	2.644822	-1.274737
C	-1.038026	3.220660	0.065888
H	-0.247803	2.928074	-1.948262
H	-2.015960	2.514609	-1.762478
C	0.065064	2.419963	2.486199
H	-0.231431	3.419856	2.839301
H	0.055292	1.764298	3.368244
H	1.086176	2.470708	2.097578
H	-0.124660	3.774679	0.279013
C	-2.306044	3.932765	0.535586
H	-2.252595	4.222339	1.590243
H	-2.432582	4.848450	-0.055711
H	-3.195828	3.315259	0.390819

TS1-b-F
B3LYP SCF energy: -1484.19327628 a.u.
B3LYP enthalpy: -1483.495016 a.u.
B3LYP free energy: -1483.593584 a.u.
M06 SCF energy in solution: -1484.59689172 a.u.
M06 enthalpy in solution: -1483.898631 a.u.
M06 free energy in solution:-1483.997199 a.u.
Imaginary frequency: -186.9120 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.358638	1.005639	0.013551
O	0.392273	0.359088	2.209916
O	1.591395	1.761615	0.974121
N	-0.862756	-1.854257	-0.533353
N	1.317134	-1.701534	-0.452573
C	0.159090	-1.008354	-0.340382
C	-0.435747	-3.258421	-0.597654
H	-0.948258	-3.796564	-1.398734
H	-0.646242	-3.768516	0.351944
C	1.071055	-3.105871	-0.851656
H	1.682284	-3.791295	-0.259446
H	1.327404	-3.242966	-1.910428
C	-2.229981	-1.395818	-0.250353
C	-2.564094	-1.663143	1.239538
H	-1.822947	-1.156553	1.868100
H	-2.499259	-2.741255	1.449470
C	-3.980155	-1.150792	1.557263
H	-4.211512	-1.349100	2.612394
C	-5.009172	-1.861181	0.656563
H	-5.001801	-2.943687	0.849716
H	-6.022366	-1.502518	0.884841
C	-4.671991	-1.581342	-0.821847
H	-5.403843	-2.082128	-1.469947
C	-3.262895	-2.135532	-1.130927
H	-3.013480	-1.990310	-2.190590
H	-3.249848	-3.219024	-0.934904
C	-4.709702	-0.058586	-1.070618
H	-4.515448	0.157077	-2.129906
H	-5.716156	0.323877	-0.844033
C	-3.649191	0.646678	-0.183882
H	-3.713740	1.726255	-0.370064
C	-2.244364	0.121139	-0.583261
H	-2.210702	0.174522	-1.684669
C	-4.005627	0.365301	1.293872
H	-3.296690	0.853088	1.970460
H	-5.002851	0.770900	1.518932
C	2.663880	-1.210323	-0.389065
C	3.400576	-1.413842	0.792197
C	4.729768	-0.979666	0.824354
H	5.306668	-1.129099	1.734932
C	5.334258	-0.359988	-0.273856
C	4.581460	-0.204305	-1.441404
H	5.040896	0.254962	-2.314412
C	3.252436	-0.630824	-1.526268
C	2.785863	-2.089197	1.996580
H	3.470520	-2.050347	2.849405
H	2.570960	-3.148805	1.802528
H	1.845853	-1.608352	2.283712
C	6.756715	0.143541	-0.194809
H	7.252043	0.104508	-1.171078
H	7.352147	-0.444037	0.512275
H	6.786387	1.187882	0.143398
C	2.494750	-0.507463	-2.827413
H	2.380244	-1.484304	-3.317051
H	3.027864	0.144775	-3.525670
H	1.491550	-0.100928	-2.676550
C	-1.294233	2.554200	1.084308
H	-2.363687	2.481773	1.252282
C	1.394079	1.125858	2.056458
H	-0.708007	2.711868	1.985994
C	2.385292	1.308637	3.194373
H	2.084173	0.736709	4.074762
H	3.381416	0.991091	2.868299
H	2.452901	2.371118	3.453301
C	-0.379935	2.084849	-1.564267
C	-0.861252	3.259220	-0.121029
H	-1.251596	2.130197	-2.233490
C	0.850100	2.701059	-2.195601
H	1.070469	2.167596	-3.129481
H	0.687165	3.754717	-2.469694
H	1.723871	2.636060	-1.540773
H	0.091528	3.771517	0.005428
C	-1.916952	4.102537	-0.839065
H	-1.549917	4.505110	-1.788843
H	-2.827635	3.530096	-1.035596
H	-2.184495	4.950657	-0.196766

TS1-b-G
B3LYP SCF energy: -1484.18508626 a.u.
B3LYP enthalpy: -1483.487110 a.u.
B3LYP free energy: -1483.587545 a.u.
M06 SCF energy in solution: -1484.58855346 a.u.
M06 enthalpy in solution: -1483.890577 a.u.
M06 free energy in solution: -1483.991012 a.u.
Imaginary frequency: -113.2559 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.306373	1.029624	-0.148882
O	0.885574	0.665855	-2.201365
O	1.786880	1.874858	-0.569136
N	-0.921080	-1.860757	-0.036097
N	1.249420	-1.752538	0.202330
C	0.122818	-1.024277	0.016495
C	-0.548425	-3.277035	0.082382
H	-0.742772	-3.805492	-0.858208
H	-1.121501	-3.771482	0.873051
C	0.953924	-3.188565	0.406675
H	1.180894	-3.471684	1.442337
H	1.566962	-3.808300	-0.252926
C	-2.297752	-1.357271	-0.076877
C	-2.921454	-1.437820	1.338570
H	-2.303776	-0.854859	2.031255
H	-2.923800	-2.479015	1.693656
C	-4.362851	-0.892533	1.311030
H	-4.798614	-0.963951	2.316915
C	-5.210637	-1.712759	0.318361
H	-5.258073	-2.764769	0.634891
H	-6.242632	-1.336402	0.305241
C	-4.589836	-1.608920	-1.089701
H	-5.194642	-2.184583	-1.803134
C	-3.162448	-2.196124	-1.050672
H	-2.707334	-2.174236	-2.049495
H	-3.211240	-3.249517	-0.734131
C	-4.541318	-0.127526	-1.523875
H	-4.134908	-0.044704	-2.540466
H	-5.562429	0.281133	-1.551511
C	-3.662348	0.680636	-0.530553
H	-3.659958	1.732269	-0.845839
C	-2.222321	0.101858	-0.578885
H	-1.989638	0.019715	-1.656267
C	-4.327582	0.578618	0.856459
H	-3.793555	1.187230	1.590151
H	-5.351203	0.977052	0.805456
C	2.604996	-1.300798	0.333565
C	3.058536	-0.808831	1.570408
C	4.406461	-0.459459	1.692519
H	4.763064	-0.074737	2.645851
C	5.305899	-0.598968	0.631458
C	4.825854	-1.110898	-0.577681
H	5.512817	-1.237717	-1.412184
C	3.483712	-1.465985	-0.753136
C	2.126745	-0.663739	2.749911
H	2.678725	-0.349967	3.641152
H	1.615900	-1.605208	2.987653
H	1.349334	0.080681	2.550260
C	6.752527	-0.188721	0.782270
H	6.888165	0.874996	0.545521
H	7.403537	-0.757412	0.109639
H	7.107932	-0.339925	1.807420
C	3.001993	-1.994083	-2.084778
H	2.665570	-3.037189	-2.019741
H	3.808445	-1.961133	-2.823868
H	2.163666	-1.396582	-2.457771
C	-0.451813	1.940650	1.540097
C	1.821842	1.394391	-1.746296
C	3.021141	1.711442	-2.623949
H	2.862039	1.360705	-3.646147
H	3.201646	2.791592	-2.625837
H	3.914278	1.232119	-2.208699
C	-0.996070	2.713136	-1.134962
C	-1.026585	3.166814	0.277542
H	-0.226744	3.160712	-1.763742
H	-1.950539	2.576516	-1.635683
H	-2.049791	3.260039	0.643433
C	-0.141945	4.384721	0.563921
H	-0.522729	5.253889	0.013523
H	-0.126425	4.641225	1.628651
H	0.881626	4.184931	0.234153
H	0.547570	2.329688	1.792593
C	-1.329571	1.981683	2.768602
H	-1.361922	2.986051	3.218291
H	-2.351031	1.647399	2.589667
H	-0.885458	1.316997	3.522669

TS1-b-H
B3LYP SCF energy: -1484.19433746 a.u.
B3LYP enthalpy: -1483.496306 a.u.
B3LYP free energy: -1483.595897 a.u.
M06 SCF energy in solution: -1484.59714581 a.u.
M06 enthalpy in solution: -1483.899114 a.u.
M06 free energy in solution: -1483.998705 a.u.
Imaginary frequency: -178.2185 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.327475	1.008113	-0.009343
O	0.346349	0.369963	2.183771
O	1.651418	1.695041	0.971417
N	-0.914719	-1.852166	-0.439160
N	1.269469	-1.735296	-0.445881
C	0.128004	-1.019341	-0.315258
C	-0.515157	-3.264998	-0.472375
H	-1.063554	-3.818361	-1.238699
H	-0.702374	-3.742079	0.499255
C	0.985823	-3.148638	-0.782889
H	1.604046	-3.824333	-0.187121
H	1.203707	-3.329849	-1.843850
C	-2.265952	-1.346933	-0.158640
C	-2.600636	-1.533367	1.341860
H	-1.841173	-1.023791	1.945018
H	-2.571676	-2.602306	1.601622
C	-3.999046	-0.957943	1.635388
H	-4.233533	-1.097433	2.699195
C	-5.055823	-1.673995	0.772342
H	-5.084366	-2.746081	1.015034
H	-6.055105	-1.270503	0.987011
C	-4.715421	-1.473951	-0.718166
H	-5.465908	-1.979209	-1.341014
C	-3.327399	-2.091092	-1.001356
H	-3.075727	-2.007061	-2.067122
H	-3.352645	-3.163640	-0.753272
C	-4.705302	0.037037	-1.038216
H	-4.509825	0.194907	-2.107682
H	-5.698151	0.461574	-0.827567
C	-3.617593	0.748160	-0.189225
H	-3.640710	1.822199	-0.425062
C	-2.236811	0.151678	-0.566534
H	-2.207712	0.134966	-1.665719
C	-3.978213	0.544759	1.301412
H	-3.255100	1.040411	1.956405
H	-4.962158	0.990391	1.508520
C	2.624513	-1.264325	-0.414166
C	3.387263	-1.488602	0.746589
C	4.722936	-1.073770	0.751242
H	5.319080	-1.239613	1.646451
C	5.308808	-0.450925	-0.354776
C	4.527860	-0.267542	-1.499790
H	4.971329	0.198141	-2.377617
C	3.190288	-0.670859	-1.555926

C	2.790905	-2.158796	1.963331
H	3.478930	-2.096836	2.811986
H	2.593226	-3.224879	1.786718
H	1.844335	-1.690798	2.250334
C	6.740618	0.029548	-0.307218
H	7.344135	-0.572681	0.380402
H	6.795182	1.070739	0.037597
H	7.211017	-0.009486	-1.295776
C	2.390799	-0.481794	-2.823572
H	1.997337	-1.433372	-3.202908
H	3.012940	-0.043674	-3.609991
H	1.532668	0.177435	-2.659999
C	-1.192395	2.640507	0.996332
H	-2.248269	2.536920	1.212561
C	1.392392	1.082119	2.052501
H	-0.578658	2.903081	1.856703
C	2.356832	1.222813	3.218498
H	2.022797	0.639018	4.078983
H	3.356403	0.897361	2.911799
H	2.433182	2.278590	3.502237
C	-0.218183	2.020774	-1.633460
C	-0.831369	3.257826	-0.278257
H	-1.712134	3.518272	-0.864838
C	0.254458	4.329352	-0.246425
H	0.525079	4.673983	-1.250068
H	-0.107335	5.197789	0.318837
H	1.148048	3.939519	0.248320
H	0.802210	2.401115	-1.797249
C	-1.060277	2.198587	-2.876201
H	-0.692520	1.501726	-3.642927
H	-2.120017	1.985841	-2.715247
H	-0.965001	3.209482	-3.298665

TS2-b-A

B3LYP SCF energy: -1484.18983032 a.u.
B3LYP enthalpy: -1483.492218 a.u.
B3LYP free energy: -1483.591864 a.u.
M06 SCF energy in solution: -1484.59068430 a.u.
M06 enthalpy in solution: -1483.893072 a.u.
M06 free energy in solution:-1483.992718 a.u.
Imaginary frequency: -204.9353 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.347959	0.925026	-0.350919
O	0.217988	0.831113	1.918610
O	1.641269	1.780286	0.505187
N	-0.890846	-1.963941	-0.230301
N	1.291096	-1.823207	-0.185627
C	0.142716	-1.108120	-0.229110
C	-0.480796	-3.352334	0.017216
H	-0.999604	-4.048299	-0.646632
H	-0.695689	-3.639185	1.055560
C	1.028665	-3.277893	-0.260908
H	1.630804	-3.821888	0.470954
H	1.284139	-3.651904	-1.261262
C	-2.249758	-1.431410	-0.060142
C	-2.584363	-1.328594	1.450419
H	-1.828718	-0.709770	1.946675
H	-2.550718	-2.328246	1.909701
C	-3.985830	-0.719174	1.633069
H	-4.216093	-0.651599	2.704835
C	-5.034087	-1.604973	0.931794
H	-5.046974	-2.607737	1.382923
H	-6.039185	-1.181706	1.066160
C	-4.698182	-1.699344	-0.570402
H	-5.442688	-2.327406	-1.078008
C	-3.301049	-2.337941	-0.739479
H	-3.055764	-2.452320	-1.803983
H	-3.307331	-3.344558	-0.293641
C	-4.709986	-0.281336	-1.179361
H	-4.516248	-0.331043	-2.259355
H	-5.708003	0.164424	-1.053174
C	-3.633649	0.598405	-0.490149
H	-3.677398	1.600134	-0.940856
C	-2.240794	-0.036002	-0.743682
H	-2.209474	-0.247458	-1.826662
C	-3.984837	0.690976	1.012670
H	-3.261354	1.315267	1.549007
H	-4.972727	1.158150	1.136900
C	2.642196	-1.341035	-0.207225
C	3.360588	-1.305680	1.001542
C	4.695534	-0.890240	0.967568
H	5.257520	-0.857633	1.898929
C	5.322848	-0.514500	-0.223906
C	4.585293	-0.585624	-1.409628
H	5.061910	-0.314703	-2.349672
C	3.251435	-1.004169	-1.428415
C	2.719894	-1.711940	2.309071
H	3.374038	-1.465027	3.150751
H	2.533474	-2.793793	2.351900
H	1.759867	-1.208556	2.458460
C	6.753058	-0.026805	-0.228414
H	7.268842	-0.301568	-1.155091
H	7.321010	-0.440655	0.611694
H	6.797006	1.067268	-0.144665
C	2.507800	-1.120115	-2.738208
H	2.301096	-2.168433	-2.992719
H	3.097735	-0.695776	-3.556404
H	1.546007	-0.600738	-2.702535
C	-1.321001	2.864253	0.119094
H	-2.365106	2.619639	0.268729
C	1.313365	1.439903	1.680131
C	2.229051	1.804583	2.836069
H	1.928980	1.292687	3.753193
H	3.265527	1.559514	2.586151
H	2.178881	2.887060	3.005324
C	-0.232055	1.316687	-2.189705
C	-0.936533	3.046813	-1.249915
H	-0.979358	1.096020	-2.970802
H	-1.763736	2.983710	-1.956707
C	0.160304	4.035154	-1.611422
H	0.336311	4.065177	-2.690571
H	-0.133045	5.044301	-1.291822
H	1.099124	3.780446	-1.111714
C	-0.738668	3.705469	1.232195
H	-1.258805	4.675166	1.274374
H	-0.880849	3.210917	2.197054
H	0.326943	3.898019	1.101053
H	0.687104	1.739693	-2.617121

TS2-b-B

B3LYP SCF energy: -1484.18669742 a.u.
B3LYP enthalpy: -1483.489235 a.u.
B3LYP free energy: -1483.589548 a.u.
M06 SCF energy in solution: -1484.58806702 a.u.
M06 enthalpy in solution: -1483.890605 a.u.
M06 free energy in solution:-1483.990918 a.u.
Imaginary frequency: -180.3273 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.379958	0.967109	0.122473
O	0.971309	1.044659	-1.799901
O	1.775294	1.842463	0.110195
N	-0.917525	-1.908631	-0.194246
N	1.256105	-1.803636	0.005864
C	0.117835	-1.072422	-0.032155
C	-0.533655	-3.324356	-0.265205
H	-0.792891	-3.745829	-1.242817
H	-1.049357	-3.910769	0.502904
C	0.987548	-3.259379	-0.035698
H	1.294534	-3.719751	0.911234
H	1.556279	-3.734940	-0.839518

C	-2.299646	-1.418300	-0.150291
C	-2.891651	-1.659118	1.262774
H	-2.253483	-1.175719	2.010209
H	-2.898983	-2.736455	1.486117
C	-4.326315	-1.102649	1.336326
H	-4.734748	-1.279620	2.340590
C	-5.205876	-1.810063	0.286173
H	-5.254837	-2.888198	0.496007
H	-6.234630	-1.427744	0.336520
C	-4.619517	-1.565864	-1.119546
H	-5.244067	-2.066309	-1.871619
C	-3.191148	-2.152972	-1.181821
H	-2.765932	-2.028110	-2.186315
H	-3.234667	-3.233506	-0.975538
C	-4.584226	-0.047718	-1.396857
H	-4.207352	0.144091	-2.410264
H	-5.605744	0.358439	-1.352067
C	-3.674011	0.653244	-0.352703
H	-3.684427	1.731833	-0.558476
C	-2.237328	0.086898	-0.503477
H	-2.023881	0.120970	-1.587139
C	-4.287641	0.409483	1.043421
H	-3.716006	0.926945	1.821900
H	-5.307336	0.820135	1.075868
C	2.613991	-1.368985	0.168280
C	3.097451	-1.063566	1.453695
C	4.450205	-0.746203	1.595809
H	4.829496	-0.506032	2.587126
C	5.326594	-0.734274	0.505156
C	4.814478	-1.049535	-0.755781
H	5.479182	-1.043406	-1.617180
C	3.464825	-1.366404	-0.951638
C	2.186044	-1.071982	2.656601
H	2.757919	-0.914534	3.576222
H	1.645133	-2.021392	2.755724
H	1.434092	-0.279906	2.579542
C	6.782499	-0.372304	0.689234
H	6.905264	0.705386	0.859072
H	7.375656	-0.636306	-0.192292
H	7.217235	-0.885134	1.555262
C	2.945993	-1.662152	-2.339917
H	2.612177	-2.702279	-2.448937
H	3.731032	-1.496667	-3.084445
H	2.098666	-1.010949	-2.578672
C	-0.869286	1.287545	1.911368
H	-1.811250	1.112764	2.448692
C	1.896098	1.613269	-1.130730
C	3.147441	2.086568	-1.849692
H	3.260439	1.585992	-2.814248
H	3.065898	3.166032	-2.029369
H	4.030472	1.915627	-1.229189
C	-1.126863	2.915047	-0.606546
C	-1.344051	3.033540	0.803864
H	-1.996711	2.626803	-1.191053
H	-2.373365	2.876078	1.119477
C	-0.560645	4.054911	1.612558
H	-0.798160	5.066645	1.255707
H	-0.813222	4.007666	2.675734
H	0.516787	3.902586	1.505450
C	-0.188442	3.837815	-1.349877
H	0.066002	3.414381	-2.324545
H	-0.683924	4.805937	-1.522666
H	0.737212	4.024552	-0.803111
H	-0.097469	1.686327	2.587673

TS2-b-C

B3LYP SCF energy: -1484.18011165 a.u.

B3LYP enthalpy: -1483.482150 a.u.

B3LYP free energy: -1483.582710 a.u.

M06 SCF energy in solution: -1484.58274981 a.u.

M06 enthalpy in solution: -1483.884788 a.u.

M06 free energy in solution: -1483.985348 a.u.

Imaginary frequency: -211.2876 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.317113	0.959906	-0.260456
O	0.231128	0.737207	2.008362
O	1.679407	1.774622	0.679879
N	-0.692562	-1.964403	-0.337332
N	1.477667	-1.700684	-0.274732
C	0.288431	-1.054915	-0.268927
C	-0.204110	-3.343700	-0.202962
H	-0.674750	-4.007616	-0.932373
H	-0.415800	-3.729846	0.802921
C	1.302003	-3.160411	-0.449232
H	1.926032	-3.715089	0.255932
H	1.593400	-3.451527	-1.466857
C	-2.078098	-1.527598	-0.110711
C	-2.390630	-1.578341	1.406897
H	-1.667958	-0.953243	1.943102
H	-2.278849	-2.609682	1.774132
C	-3.826091	-1.083477	1.659590
H	-4.040951	-1.122774	2.735996
C	-4.827892	-1.971165	0.896354
H	-4.771835	-3.008063	1.258131
H	-5.854823	-1.624636	1.077628
C	-4.513080	-1.914880	-0.612113
H	-5.223812	-2.545791	-1.162934
C	-3.080494	-2.442124	-0.851766
H	-2.846691	-2.452450	-1.924926
H	-3.011861	-3.479964	-0.490411
C	-4.625297	-0.454669	-1.096658
H	-4.447435	-0.399580	-2.179337
H	-5.647209	-0.087021	-0.920147
C	-3.594589	0.430085	-0.345978
H	-3.714485	1.460636	-0.700611
C	-2.168449	-0.080236	-0.677570
H	-2.150298	-0.204281	-1.773669
C	-3.916833	0.369950	1.162841
H	-3.213036	0.982363	1.732183
H	-4.924584	0.770758	1.346926
C	2.799303	-1.141364	-0.288938
C	3.541354	-1.141857	0.905939
C	4.845795	-0.639592	0.876799
H	5.424351	-0.630946	1.798509
C	5.421233	-0.144409	-0.297330
C	4.665389	-0.188386	-1.472248
H	5.103490	0.173282	-2.400410
C	3.360383	-0.690177	-1.495897
C	2.957292	-1.676874	2.193529
H	3.596889	-1.418712	3.042909
H	2.871676	-2.772187	2.176045
H	1.957383	-1.273864	2.379737
C	6.814059	0.441307	-0.291564
H	7.300596	0.331944	-1.266859
H	7.449263	-0.038779	0.460849
H	6.788526	1.514279	-0.059050
C	2.601479	-0.769750	-2.799826
H	2.450465	-1.810854	-3.115754
H	3.153147	-0.264081	-3.598362
H	1.613076	-0.309051	-2.721560
C	-0.935137	2.982370	0.358625
C	1.320741	1.375342	1.827154
C	2.191738	1.707548	3.028175
H	1.899873	1.119961	3.901628
H	3.244697	1.535140	2.787091
H	2.080298	2.771847	3.268902
C	-0.246160	1.476646	-2.078878
C	-0.800029	3.126904	-1.074428
H	-1.033722	1.322985	-2.833062
H	0.677261	1.857588	-2.536945
H	-0.041046	3.278555	0.901093
H	0.146740	3.591012	-1.348093
C	-1.983056	3.594331	-1.911268
H	-1.716942	3.683254	-2.968437

H	-2.837321	2.918504	-1.832111
H	-2.305506	4.584376	-1.561852
C	-2.204726	3.332830	1.092624
H	-3.112763	2.995707	0.592408
H	-2.186154	2.914657	2.103312
H	-2.273597	4.427969	1.199517

TS2-b-D

B3LYP SCF energy: -1484.18063689 a.u.
B3LYP enthalpy: -1483.483014 a.u.
B3LYP free energy: -1483.583709 a.u.
M06 SCF energy in solution: -1484.58342592 a.u.
M06 enthalpy in solution: -1483.885803 a.u.
M06 free energy in solution: -1483.986498 a.u.
Imaginary frequency: -204.6708 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.361079	0.989410	0.174451
O	1.026374	1.126680	-1.758626
O	1.794606	1.887884	0.182975
N	-0.737033	-1.910465	-0.151675
N	1.430542	-1.684106	0.004337
C	0.250624	-1.019219	-0.011416
C	-0.272584	-3.300346	-0.257258
H	-0.491017	-3.701343	-1.253468
H	-0.766022	-3.939668	0.481893
C	1.236577	-3.152353	-0.000894
H	1.543913	-3.567115	0.967325
H	1.846737	-3.622480	-0.776508
C	-2.144824	-1.498728	-0.134808
C	-2.745233	-1.785118	1.266009
H	-2.160171	-1.251252	2.023245
H	-2.670769	-2.859586	1.490947
C	-4.219378	-1.341066	1.310007
H	-4.634364	-1.551017	2.305180
C	-5.022236	-2.108033	0.240357
H	-4.994905	-3.187837	0.445959
H	-6.077490	-1.803735	0.271258
C	-4.427920	-1.815221	-1.152595
H	-4.998696	-2.356741	-1.918906
C	-2.960480	-2.293460	-1.185839
H	-2.525115	-2.135360	-2.181319
H	-2.927344	-3.374490	-0.980441
C	-4.491694	-0.298886	-1.425712
H	-4.106636	-0.078616	-2.430193
H	-5.539460	0.035905	-1.402466
C	-3.656851	0.461605	-0.360351
H	-3.745794	1.532252	-0.567212
C	-2.174766	0.014294	-0.481176
H	-1.939563	0.070682	-1.558695
C	-4.283389	0.169160	1.020480
H	-3.768424	0.722246	1.812712
H	-5.330564	0.505711	1.030061
C	2.768681	-1.188738	0.160055
C	3.242697	-0.843435	1.438581
C	4.583560	-0.475786	1.571623
H	4.955463	-0.204319	2.557653
C	5.457086	-0.450906	0.478921
C	4.954026	-0.804429	-0.775510
H	5.616011	-0.787230	-1.638860
C	3.616398	-1.173152	-0.962124
C	2.332549	-0.854098	2.641791
H	2.902065	-0.678148	3.559538
H	1.804361	-1.809355	2.751483
H	1.571111	-0.072439	2.553901
C	6.899195	-0.033011	0.653142
H	6.983567	1.052160	0.797149
H	7.501408	-0.296428	-0.222433
H	7.352010	-0.509100	1.530773
C	3.103051	-1.504843	-2.344265
H	2.797340	-2.555121	-2.437321
H	3.881030	-1.328224	-3.093646
H	2.236560	-0.881344	-2.588742
C	-0.932191	1.341851	1.938481
H	-1.930551	1.240530	2.378400
C	1.926906	1.701715	-1.065622
C	3.160109	2.250683	-1.764269
H	3.331882	1.742215	-2.716004
H	3.003916	3.317393	-1.970501
H	4.037901	2.157656	-1.120728
C	-0.776231	3.024914	-0.487048
C	-1.110394	3.123180	0.911108
H	-0.191512	1.632650	2.700386
H	-0.299651	3.546610	1.501862
H	0.228242	3.372934	-0.708283
C	-2.495705	3.565525	1.354289
H	-3.286847	2.948092	0.926831
H	-2.597597	3.546943	2.443250
H	-2.661882	4.599216	1.021325
C	-1.742530	3.279738	-1.617960
H	-1.372930	2.807617	-2.533680
H	-2.753074	2.918371	-1.426941
H	-1.808375	4.362159	-1.812029

TS2-b-E

B3LYP SCF energy: -1484.18627599 a.u.
B3LYP enthalpy: -1483.488570 a.u.
B3LYP free energy: -1483.588014 a.u.
M06 SCF energy in solution: -1484.58664112 a.u.
M06 enthalpy in solution: -1483.888935 a.u.
M06 free energy in solution: -1483.988379 a.u.
Imaginary frequency: -209.5802 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.331899	0.937644	-0.284064
O	0.210969	0.776132	1.988332
O	1.624329	1.804547	0.619523
N	-0.760351	-1.972655	-0.243406
N	1.415376	-1.750997	-0.224183
C	0.239762	-1.079385	-0.232323
C	-0.296015	-3.350621	-0.036369
H	-0.796713	-4.048227	-0.712238
H	-0.488018	-3.671080	0.996537
C	1.206601	-3.212459	-0.329505
H	1.837200	-3.749269	0.383565
H	1.463687	-3.555117	-1.340548
C	-2.135206	-1.492835	-0.045156
C	-2.447988	-1.427420	1.472405
H	-1.705635	-0.792012	1.966741
H	-2.371569	-2.433803	1.911499
C	-3.866681	-0.871384	1.688866
H	-4.080301	-0.828489	2.765338
C	-4.893490	-1.785396	0.991705
H	-4.863120	-2.793661	1.429529
H	-5.911162	-1.400986	1.147275
C	-4.579688	-1.847730	-0.517105
H	-5.308668	-2.496941	-1.020705
C	-3.162310	-2.428893	-0.720910
H	-2.932921	-2.517566	-1.791446
H	-3.120652	-3.441577	-0.290901
C	-4.653957	-0.423827	-1.105318
H	-4.474694	-0.451599	-2.188801
H	-5.665921	-0.017746	-0.958274
C	-3.601456	0.486204	-0.419370
H	-3.697266	1.491234	-0.848607
C	-2.187036	-0.084496	-0.704387
H	-2.154518	-0.270641	-1.792573
C	-3.927087	0.546044	1.089502
H	-3.214493	1.190376	1.616531
H	-4.928607	0.975440	1.238839
C	2.744930	-1.213933	-0.274182
C	3.496156	-1.167014	0.914038

C	4.805799	-0.680988	0.851954
H	5.391602	-0.635949	1.767982
C	5.378018	-0.248704	-0.348122
C	4.613094	-0.339760	-1.514784
H	5.048498	-0.028424	-2.462268
C	3.302658	-0.827123	-1.505264
C	2.917820	-1.638785	2.228554
H	3.568099	-1.351888	3.060429
H	2.820001	-2.732816	2.258418
H	1.924166	-1.216928	2.405787
C	6.777748	0.319410	-0.380774
H	7.269624	0.122462	-1.339593
H	7.401761	-0.102974	0.414212
H	6.763891	1.408461	-0.240268
C	2.533139	-0.962406	-2.798376
H	2.367654	-2.016110	-3.060322
H	3.083730	-0.503475	-3.625323
H	1.550005	-0.487260	-2.735732
C	-1.349208	2.869070	0.208841
H	-2.413930	2.675163	0.305751
C	1.294821	1.417424	1.778708
C	2.188987	1.768911	2.955202
H	1.924945	1.184661	3.839682
H	3.238674	1.609477	2.692288
H	2.065785	2.833159	3.190612
C	-0.157997	1.369646	-2.102185
C	-0.895924	3.100785	-1.124067
H	-0.869437	1.144951	-2.913258
C	-0.764749	3.646034	1.368798
H	-1.313622	4.592630	1.487791
H	-0.855309	3.089800	2.306010
H	0.289506	3.880955	1.204335
H	0.761922	1.837937	-2.483809
H	0.050166	3.638940	-1.188936
C	-1.891104	3.450481	-2.224085
H	-1.439027	3.452657	-3.220256
H	-2.747327	2.771565	-2.233291
H	-2.269819	4.463351	-2.030644

TS2-b-F

B3LYP SCF energy: -1484.18131458 a.u.
B3LYP enthalpy: -1483.484008 a.u.
B3LYP free energy: -1483.583494 a.u.
M06 SCF energy in solution: -1484.58172474 a.u.
M06 enthalpy in solution: -1483.884418 a.u.
M06 free energy in solution:-1483.983904 a.u.
Imaginary frequency: -159.6689 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.370798	0.986739	0.148813
O	0.984846	1.091385	-1.779600
O	1.770484	1.887025	0.139868
N	-0.806533	-1.907069	-0.199872
N	1.358730	-1.732287	0.028814
C	0.196485	-1.038142	-0.018066
C	-0.370646	-3.305603	-0.306152
H	-0.570159	-3.693697	-1.311578
H	-0.898669	-3.939853	0.413281
C	1.133820	-3.195746	-0.005544
H	1.405685	-3.633809	0.962994
H	1.754564	-3.666053	-0.772622
C	-2.205585	-1.467438	-0.184252
C	-2.822293	-1.762757	1.207427
H	-2.225352	-1.265846	1.980213
H	-2.785796	-2.843584	1.410283
C	-4.280762	-1.270186	1.252487
H	-4.707760	-1.483486	2.241870
C	-5.102908	-1.990834	0.165800
H	-5.112659	-3.074265	0.352851
H	-6.147547	-1.651852	0.196952
C	-4.491824	-1.693128	-1.218591
H	-5.074920	-2.203423	-1.996916
C	-3.038911	-2.218008	-1.253471
H	-2.593347	-2.055608	-2.243620
H	-3.041683	-3.303258	-1.068319
C	-4.511938	-0.170007	-1.464216
H	-4.118667	0.058158	-2.463695
H	-5.550198	0.192990	-1.436699
C	-3.657016	0.545831	-0.384276
H	-3.707151	1.624865	-0.574283
C	-2.193652	0.047403	-0.507463
H	-1.956361	0.110301	-1.585021
C	-4.291310	0.247407	0.992220
H	-3.751137	0.761012	1.794498
H	-5.325211	0.622122	1.014477
C	2.704262	-1.261857	0.195486
C	3.179491	-0.947031	1.481368
C	4.523775	-0.595657	1.624586
H	4.896422	-0.347273	2.616380
C	5.400215	-0.560775	0.534571
C	4.897457	-0.890000	-0.726606
H	5.562884	-0.868509	-1.587215
C	3.556499	-1.240669	-0.923409
C	2.268719	-0.984039	2.684053
H	2.834045	-0.802322	3.603219
H	1.763377	-1.952541	2.786855
H	1.488347	-0.220843	2.604016
C	6.845811	-0.159688	0.718564
H	6.942375	0.925507	0.854767
H	7.452308	-0.437065	-0.149757
H	7.284821	-0.634582	1.603704
C	3.047421	-1.555622	-2.311181
H	2.743089	-2.605248	-2.416311
H	3.828412	-1.371477	-3.055605
H	2.181960	-0.930161	-2.553717
C	-0.847336	1.246333	1.941464
H	-1.806930	1.087934	2.451375
C	1.900242	1.664980	-1.101357
C	3.145674	2.162982	-1.813782
H	3.307779	1.620305	-2.748202
H	3.010850	3.224821	-2.056516
H	4.020621	2.072711	-1.165985
C	-1.153645	2.981057	-0.538181
C	-1.155959	3.148050	0.870588
H	-2.123919	2.788282	-0.994312
C	-0.223886	3.792868	-1.413251
H	-0.000035	3.277907	-2.350251
H	-0.712119	4.748336	-1.658418
H	0.715064	4.015897	-0.900643
H	-0.079721	1.610264	2.646038
H	-0.262374	3.623195	1.275247
C	-2.439454	3.481336	1.613467
H	-3.284508	2.890013	1.255236
H	-2.355935	3.356495	2.697015
H	-2.669833	4.538959	1.422179

TS2-b-G

B3LYP SCF energy: -1484.18174398 a.u.
B3LYP enthalpy: -1483.483727 a.u.
B3LYP free energy: -1483.584407 a.u.
M06 SCF energy in solution: -1484.58147743 a.u.
M06 enthalpy in solution: -1483.883460 a.u.
M06 free energy in solution:-1483.984140 a.u.
Imaginary frequency: -200.8195 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.329131	0.965487	-0.289465
O	0.255878	0.802240	1.975833
O	1.718788	1.730366	0.584947
N	-0.840025	-1.941421	-0.314081
N	1.338535	-1.775738	-0.220311
C	0.180899	-1.075816	-0.247811

C	-0.416567	-3.340092	-0.156496
H	-0.902427	-3.989538	-0.889016
H	-0.665270	-3.706414	0.848154
C	1.100709	-3.228528	-0.373768
H	1.684537	-3.798314	0.353520
H	1.400053	-3.550043	-1.379862
C	-2.211141	-1.446414	-0.124321
C	-2.573438	-1.488594	1.381846
H	-1.844762	-0.891832	1.942327
H	-2.513864	-2.522987	1.752204
C	-3.995994	-0.938294	1.591162
H	-4.246601	-0.975622	2.659909
C	-5.008918	-1.778224	0.790177
H	-5.007194	-2.819546	1.143561
H	-6.025510	-1.390540	0.944326
C	-4.644678	-1.722265	-0.706791
H	-5.363575	-2.317561	-1.285881
C	-3.229754	-2.311734	-0.902503
H	-2.960408	-2.327324	-1.967120
H	-3.220986	-3.353501	-0.546272
C	-4.680862	-0.253772	-1.181632
H	-4.469474	-0.198078	-2.258072
H	-5.691292	0.155026	-1.031840
C	-3.635912	0.580715	-0.392580
H	-3.691825	1.619232	-0.745064
C	-2.227238	0.002975	-0.688382
H	-2.201928	-0.128151	-1.782950
C	-4.014701	0.520852	1.103690
H	-3.313541	1.101163	1.706896
H	-5.013246	0.957397	1.253973
C	2.685841	-1.281103	-0.223921
C	3.409095	-1.297796	0.982038
C	4.741313	-0.873354	0.962114
H	5.307029	-0.880316	1.891787
C	5.360872	-0.437610	-0.213032
C	4.618487	-0.457647	-1.397337
H	5.088854	-0.138545	-2.325349
C	3.287205	-0.883631	-1.430423
C	2.775199	-1.765465	2.272236
H	3.427503	-1.545794	3.122843
H	2.601295	-2.850275	2.270745
H	1.809588	-1.279973	2.443431
C	6.787224	0.061071	-0.200108
H	7.291158	-0.136807	-1.152492
H	7.370958	-0.411195	0.597403
H	6.824080	1.145742	-0.032389
C	2.540421	-0.942755	-2.742220
H	2.362257	-1.979676	-3.058418
H	3.114954	-0.455002	-3.535738
H	1.565296	-0.453023	-2.673641
C	-0.863420	3.031526	0.318966
C	1.366147	1.389701	1.752457
C	2.271241	1.731725	2.925160
H	1.962179	1.202453	3.829381
H	3.309825	1.491574	2.679710
H	2.220286	2.810789	3.115294
C	-0.278623	1.405212	-2.118229
C	-0.891172	3.138707	-1.105642
H	-1.077010	1.252387	-2.864067
H	-1.884613	3.156130	-1.554071
C	0.140219	4.055844	-1.757819
H	0.148202	3.985053	-2.849412
H	-0.101455	5.093933	-1.492579
H	1.142806	3.835128	-1.378701
H	0.638382	1.787839	-2.584570
H	0.069701	3.376472	0.762821
C	-2.066876	3.306128	1.184390
H	-3.007930	3.042680	0.699401
H	-1.992046	2.774326	2.137362
H	-2.102575	4.382404	1.416094

TS2-b-H

B3LYP SCF energy: -1484.18455151 a.u.
B3LYP enthalpy: -1483.487082 a.u.
B3LYP free energy: -1483.588211 a.u.
M06 SCF energy in solution: -1484.58511523 a.u.
M06 enthalpy in solution: -1483.887646 a.u.
M06 free energy in solution:-1483.988775 a.u.
Imaginary frequency: -185.3484 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ru	-0.374498	0.991001	0.142874
O	1.027303	1.080588	-1.774552
O	1.790453	1.867829	0.157494
N	-0.845269	-1.899532	-0.129036
N	1.330165	-1.742477	0.006123
C	0.173641	-1.039333	-0.003966
C	-0.428599	-3.305861	-0.213671
H	-0.684152	-3.722919	-1.194241
H	-0.924705	-3.911807	0.551754
C	1.091126	-3.204033	0.004810
H	1.410679	-3.630030	0.963940
H	1.666558	-3.691126	-0.786938
C	-2.238909	-1.441538	-0.094334
C	-2.825163	-1.687066	1.320469
H	-2.207318	-1.168773	2.062092
H	-2.788611	-2.760993	1.556994
C	-4.280400	-1.186424	1.386196
H	-4.684572	-1.370752	2.390853
C	-5.131416	-1.932376	0.339196
H	-5.141986	-3.010364	0.555281
H	-6.173332	-1.586975	0.385648
C	-4.551014	-1.675988	-1.066863
H	-5.156164	-2.202095	-1.817307
C	-3.104360	-2.215367	-1.120162
H	-2.680794	-2.087411	-2.125000
H	-3.113338	-3.294422	-0.902284
C	-4.564725	-0.159682	-1.354585
H	-4.192976	0.036786	-2.369070
H	-5.599182	0.212646	-1.313904
C	-3.680532	0.577772	-0.312853
H	-3.731961	1.652812	-0.518625
C	-2.221508	0.064065	-0.466419
H	-2.016936	0.090616	-1.550909
C	-4.295669	0.322068	1.080334
H	-3.755110	0.869478	1.859505
H	-5.330665	0.693695	1.097458
C	2.682788	-1.284991	0.150354
C	3.172531	-0.942325	1.424001
C	4.524815	-0.615990	1.548562
H	4.909056	-0.347609	2.530714
C	5.394577	-0.629546	0.452428
C	4.874807	-0.974985	-0.797354
H	5.532945	-0.984568	-1.663733
C	3.524990	-1.301610	-0.975848
C	2.267278	-0.912545	2.630719
H	2.846272	-0.749545	3.544928
H	1.706952	-1.848173	2.749320
H	1.532614	-0.105643	2.539721
C	6.851614	-0.263686	0.619732
H	6.971736	0.808664	0.821379
H	7.429149	-0.497072	-0.280530
H	7.306114	-0.800831	1.460797
C	2.994323	-1.619602	-2.354563
H	2.637882	-2.654311	-2.439494
H	3.778394	-1.485434	-3.106359
H	2.158505	-0.956287	-2.601349
C	-0.945043	1.378721	1.892374
H	-1.927534	1.268518	2.367122
C	1.928987	1.661062	-1.085954
C	3.178170	2.175996	-1.781902
H	3.281459	1.741280	-2.778793
H	3.106972	3.266351	-1.882014
H	4.063480	1.955002	-1.180376
C	-0.795123	2.994121	-0.605561

C	-1.334121	3.084275	0.717727
H	-2.415707	2.990417	0.796673
C	-0.692023	4.081927	1.676150
H	-0.950282	5.099113	1.351333
H	-1.038591	3.964487	2.707200
H	0.397882	3.986227	1.657021
H	-0.198073	1.752813	2.608824
H	0.186029	3.457818	-0.706671
C	-1.611408	3.059996	-1.875260
H	-1.743584	4.111720	-2.173282
H	-1.080428	2.552435	-2.686321
H	-2.602886	2.616608	-1.773514