Supporting Information

Does the Ruthenium Nitrato Catalyst Work Differently in Z-Selective Olefin Metathesis: A DFT Study

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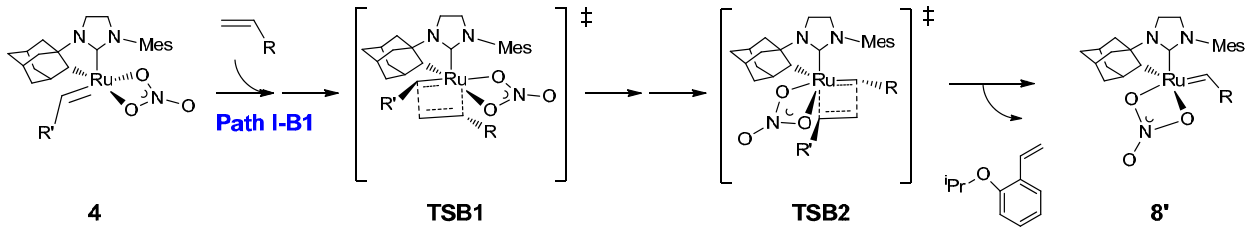
Computational Methods

Geometry optimizations were performed at the B3LYP[1]/BS1 level in the gas phase, BS1 designating a mixed basis set of SDD[2] for Ru and 6-31G(d) for other atoms. When necessary, IRC (intrinsic reaction coordinate) calculations were performed to verify the connections between a transition state and its forward and backward minima.[3] The B3LYP/BS1-optimized geometries were used for solvent-corrected single-point energy calculations at the M06[4,5]/BS2 level with solvation effects modeled by SMD[6] in THF (the solvent used for the reaction), BS2 denoting a mixed basis set of SDD for Ru and 6-311++G(d,p) for other atoms. The gas-phase B3LYP/BS1 harmonic frequencies were used for thermal and entropic corrections to obtain the enthalpies and free energies at 298.15 K and 1 atm. Gibbs free energies (kcal/mol) obtained from the M06 (SMD,THF)/BS2//B3LYP/BS1 calculations were discussed, and enthalpies (kcal/mol) given for reference. All calculations were performed with Gaussian 09.[7]

1. (a) Lee, C. T.; Yang, W. T.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.
2. (a) Andrae, D.; Häussermann, U.; Dolg, M.; Stoll, H.; Preuss, H. *Theor. Chim. Acta* **1990**, *77*, 123. (b) Roy, L. E.; Hay, P. J.; Martin, R. L. *J. Chem. Theory Comput.* **2008**, *4*, 1029.
3. Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363.
4. (a) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157. (b) Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2009**, *5*, 324. (c) Kulkarni, A. D.; Truhlar, D. G. *J. Chem. Theory Comput.* **2011**, *7*, 2325.
5. Recent studies have established that the M06 functional gives more accurate energies for ruthenium complexes in olefin metathesis. See refs (7)–(12) in the main text.
6. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.
7. Gaussian 09, Revision **A.1,** Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

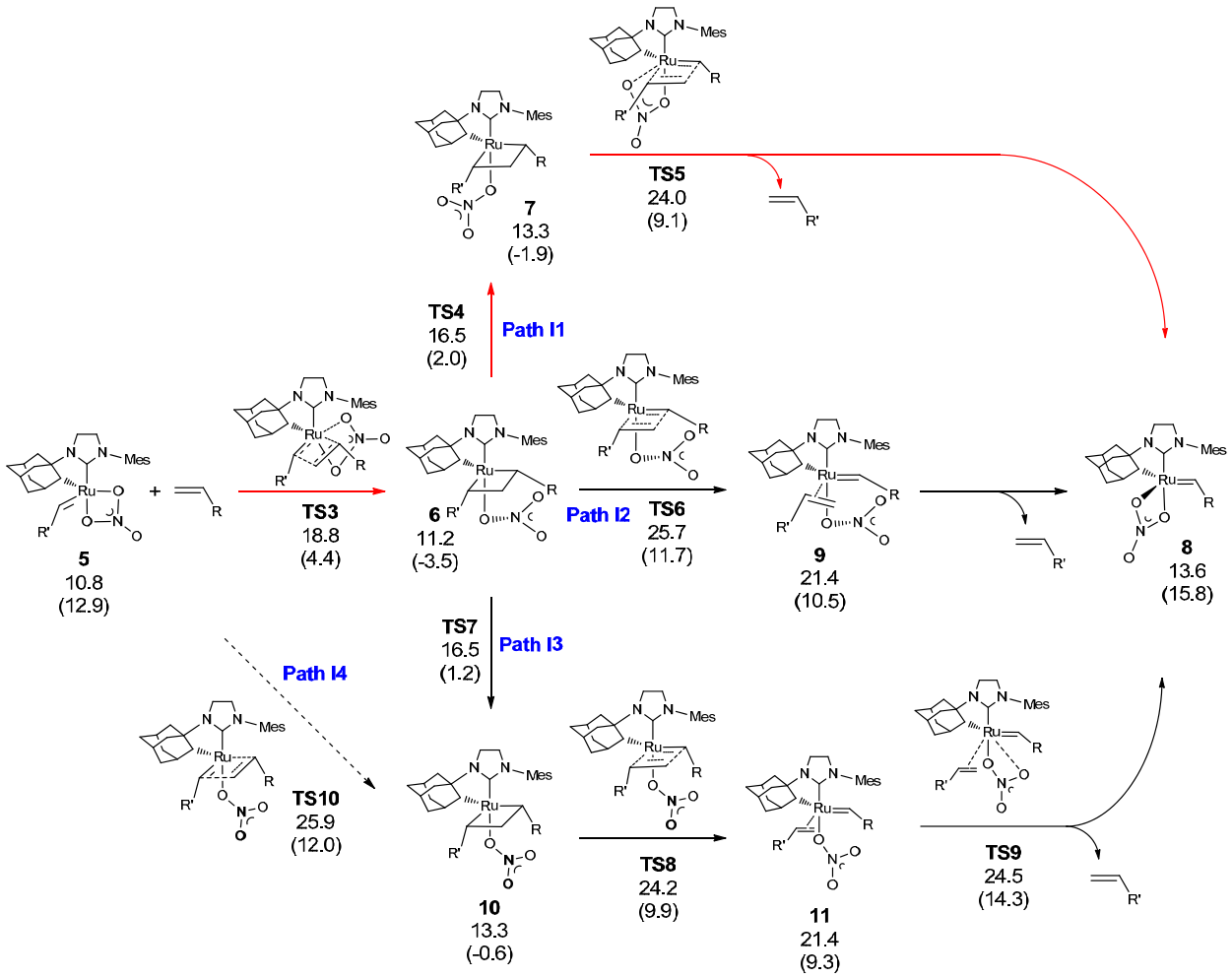
Scheme S1. Key TSs in the Possible Bottom-Bound Pathway of Initiation Metathesis[a,b]



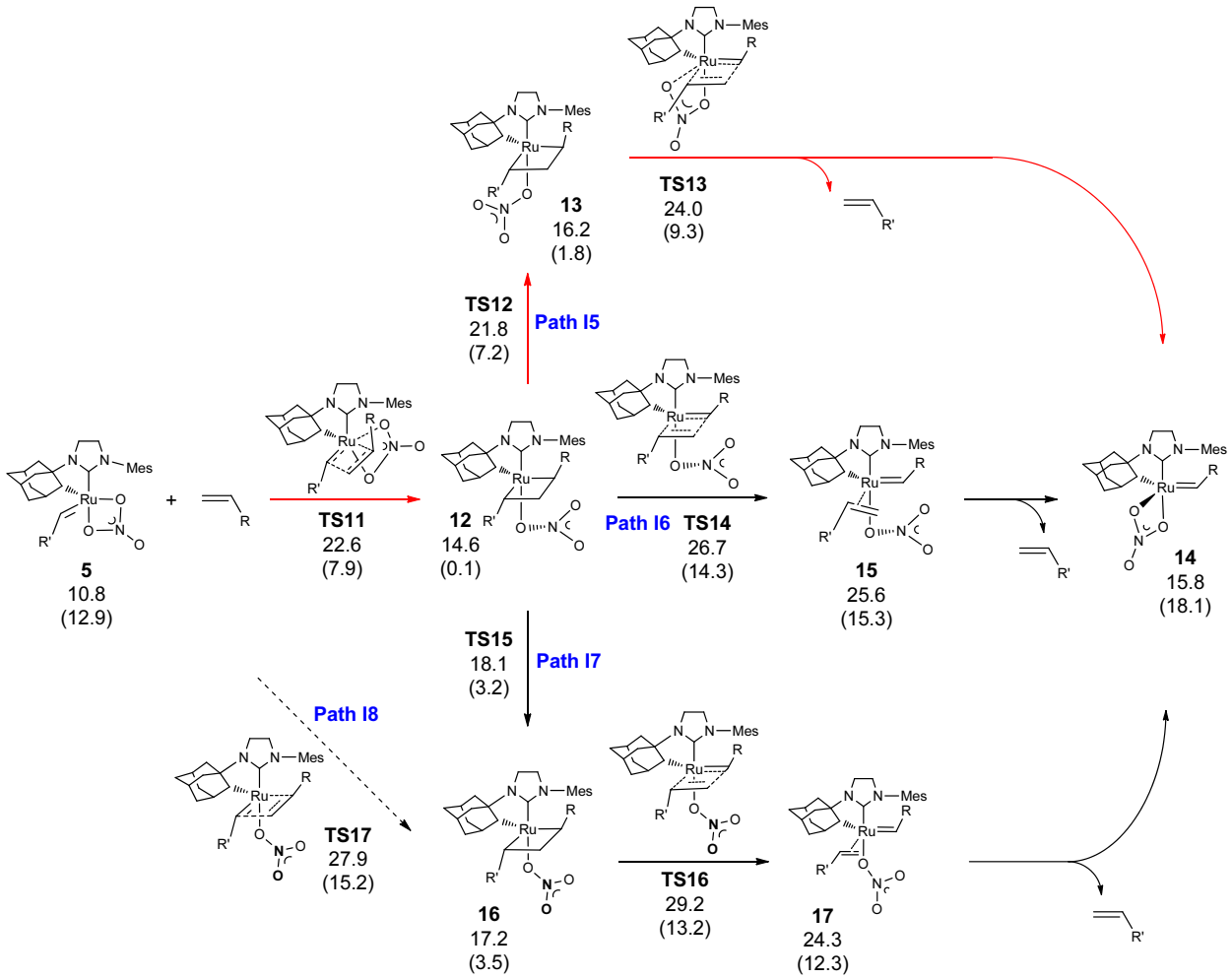
[a] We considered several possible orientations of olefin binding to the open bottom site in complex **4**, and Path I-B1 was the only pathway located that would lead to a new Ru-alkylidene complex (**8'**) that could enter the subsequent metathesis homodimerization. The highest activation barrier **TSB1** is 3.3 kcal/mol higher than those (**TS5** and **TS13**) in the most favorable side-bound pathways leading to **8** and **14**.

[b] Complex **8'** could metathesize with phenylpropene via the bottom-bound mechanism to afford the (*Z*)- and (*E*)-olefin homodimers, but this proved to be a high-energy and disfavored path (see Scheme S9) as compared with Path C2 and Path C3 for complex **8** (see Figure 4).

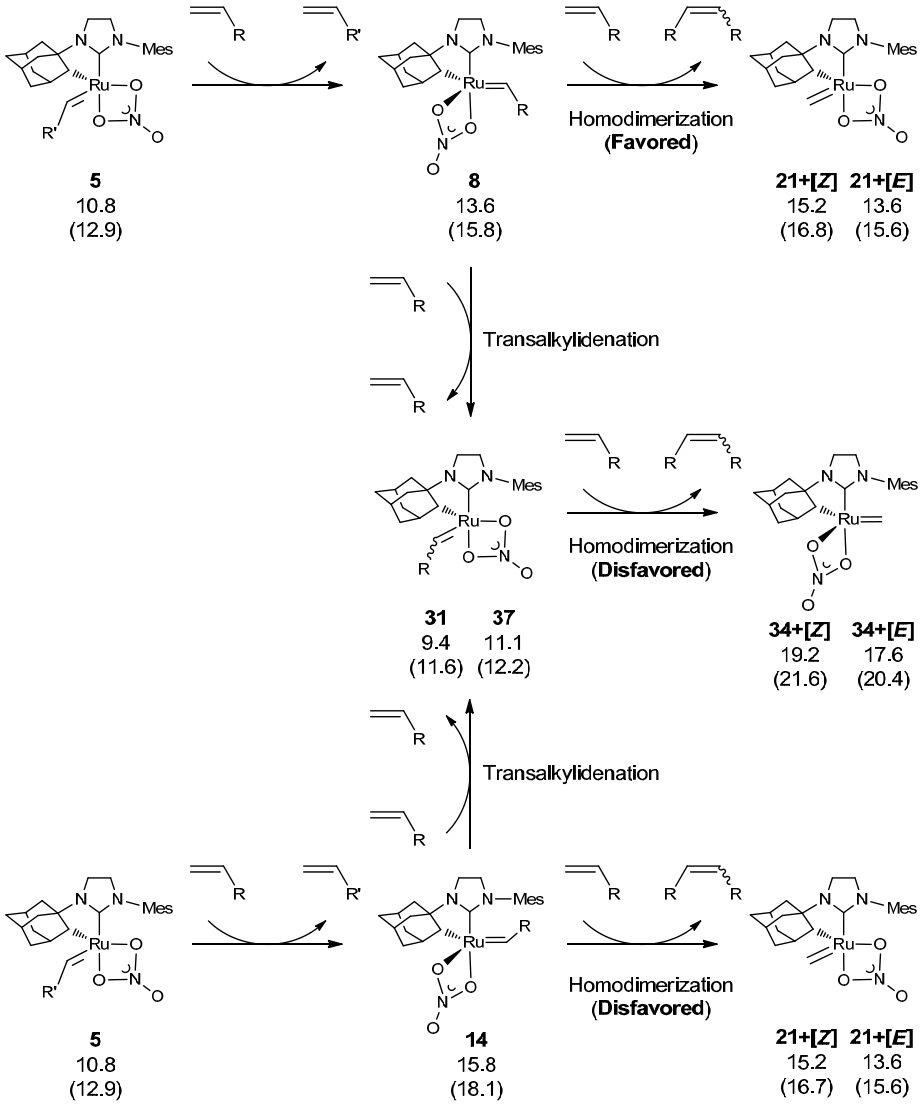
Scheme S2. Possible Side-Bound Pathways Leading to Complex **8**



Scheme S3. Possible Side-Bound Pathways Leading to Complex **14**

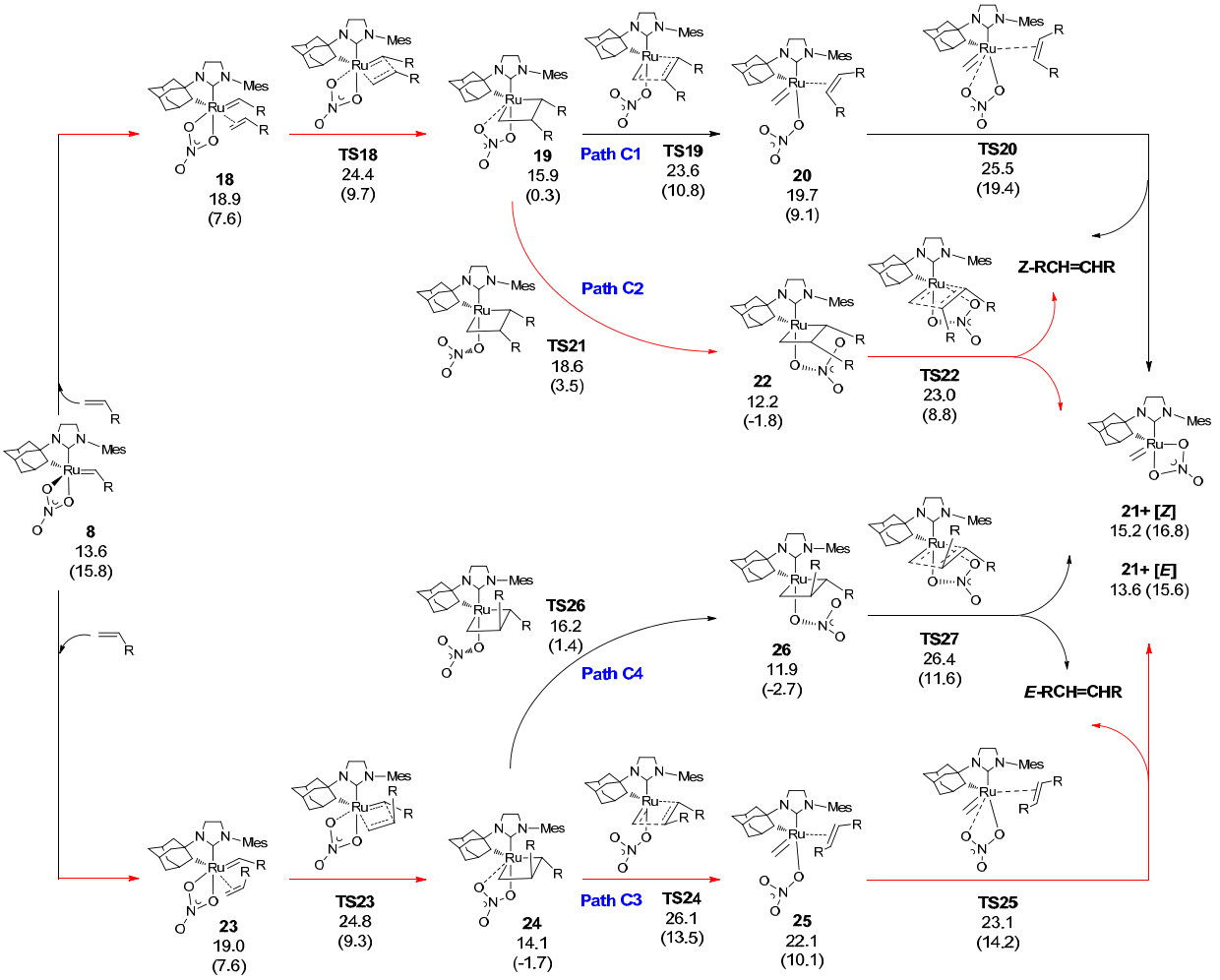


Scheme S4. Possible Reactions Involving Complex **8** or **14**[a]

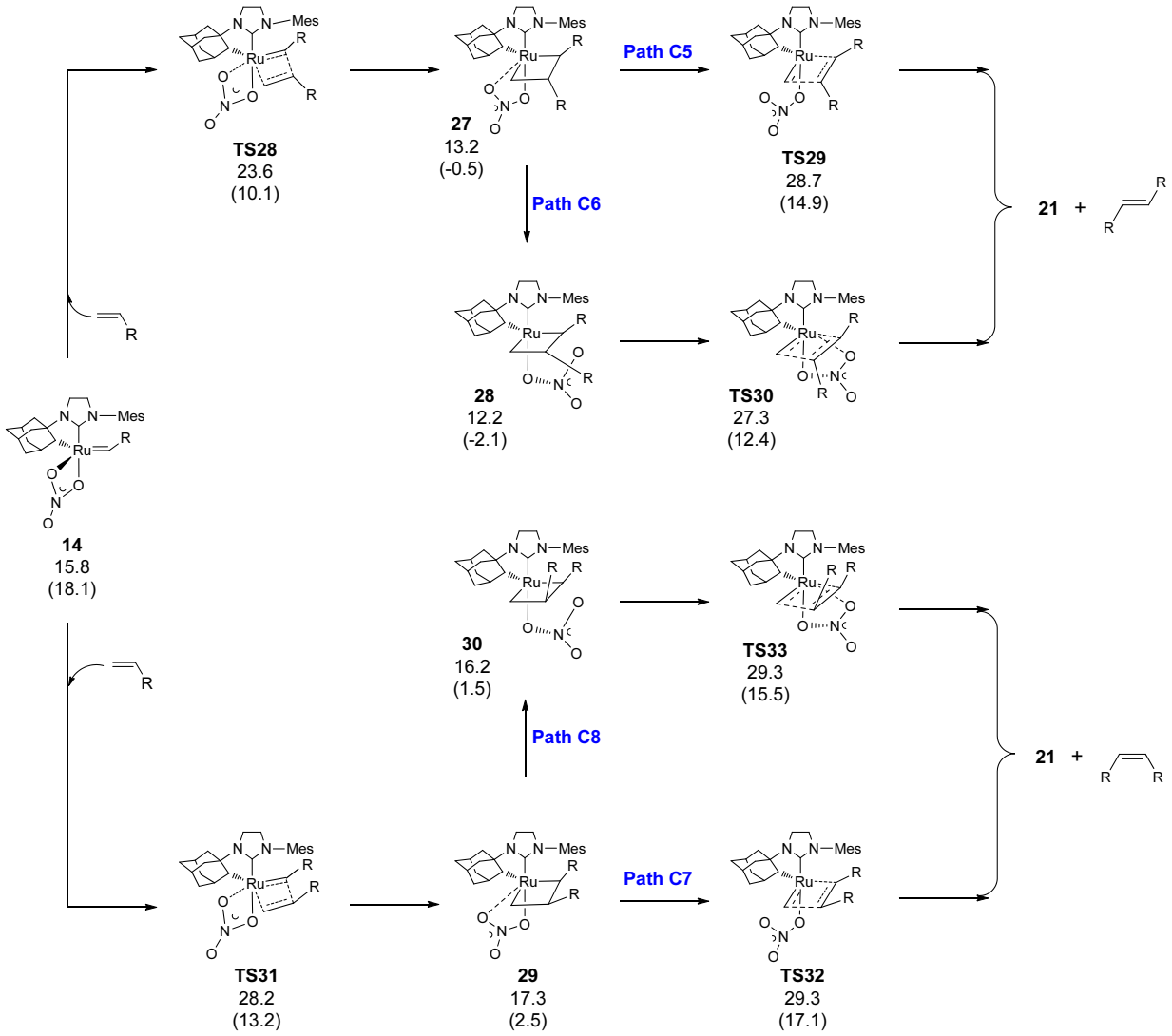


[a] [*Z*] = *Z*-RCH=CHR; [*E*] = *E*-RCH=CHR.

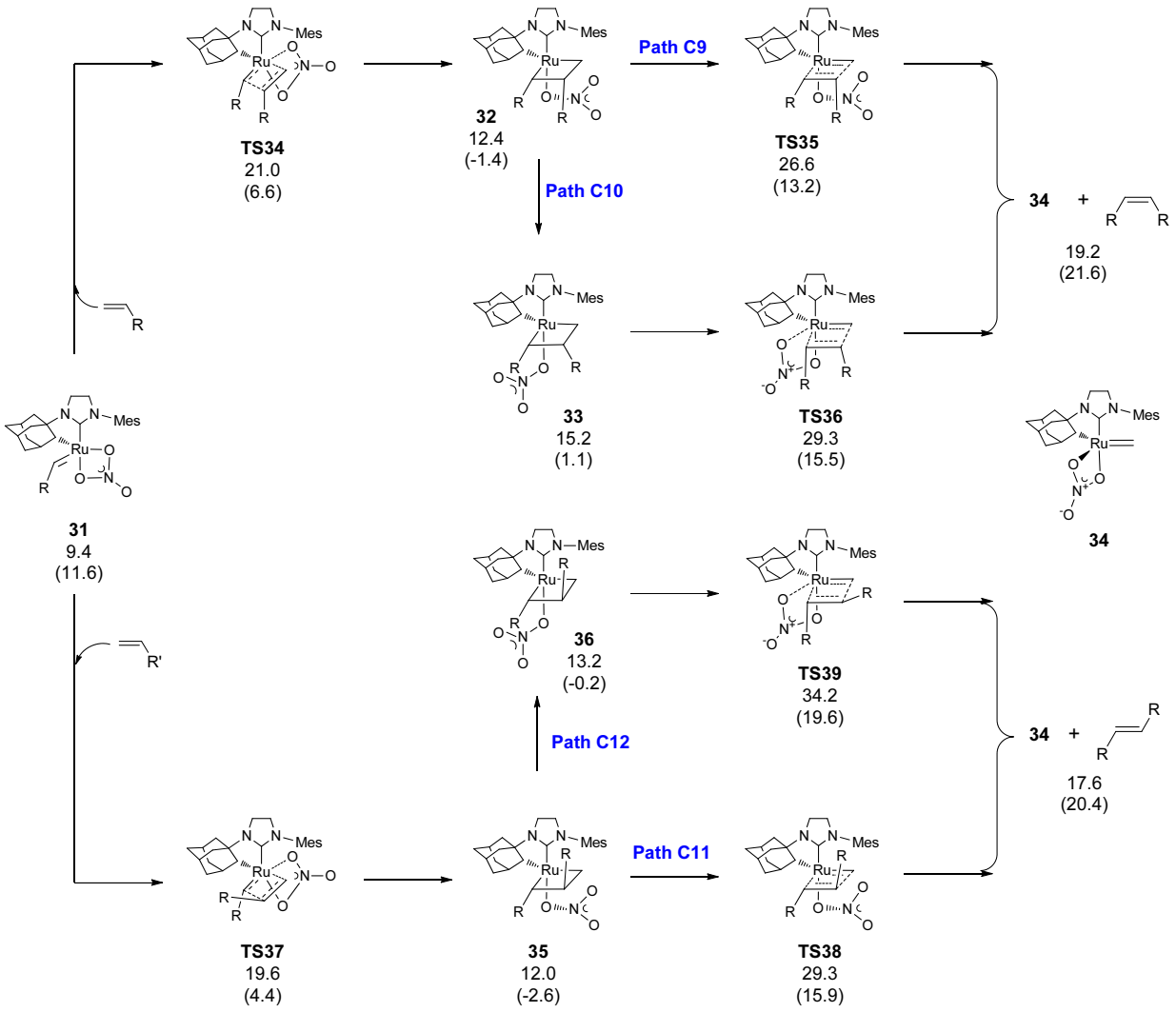
Scheme S5. Possible Side-Bound Pathways for Phenylpropene Homodimerization with Complex **8**



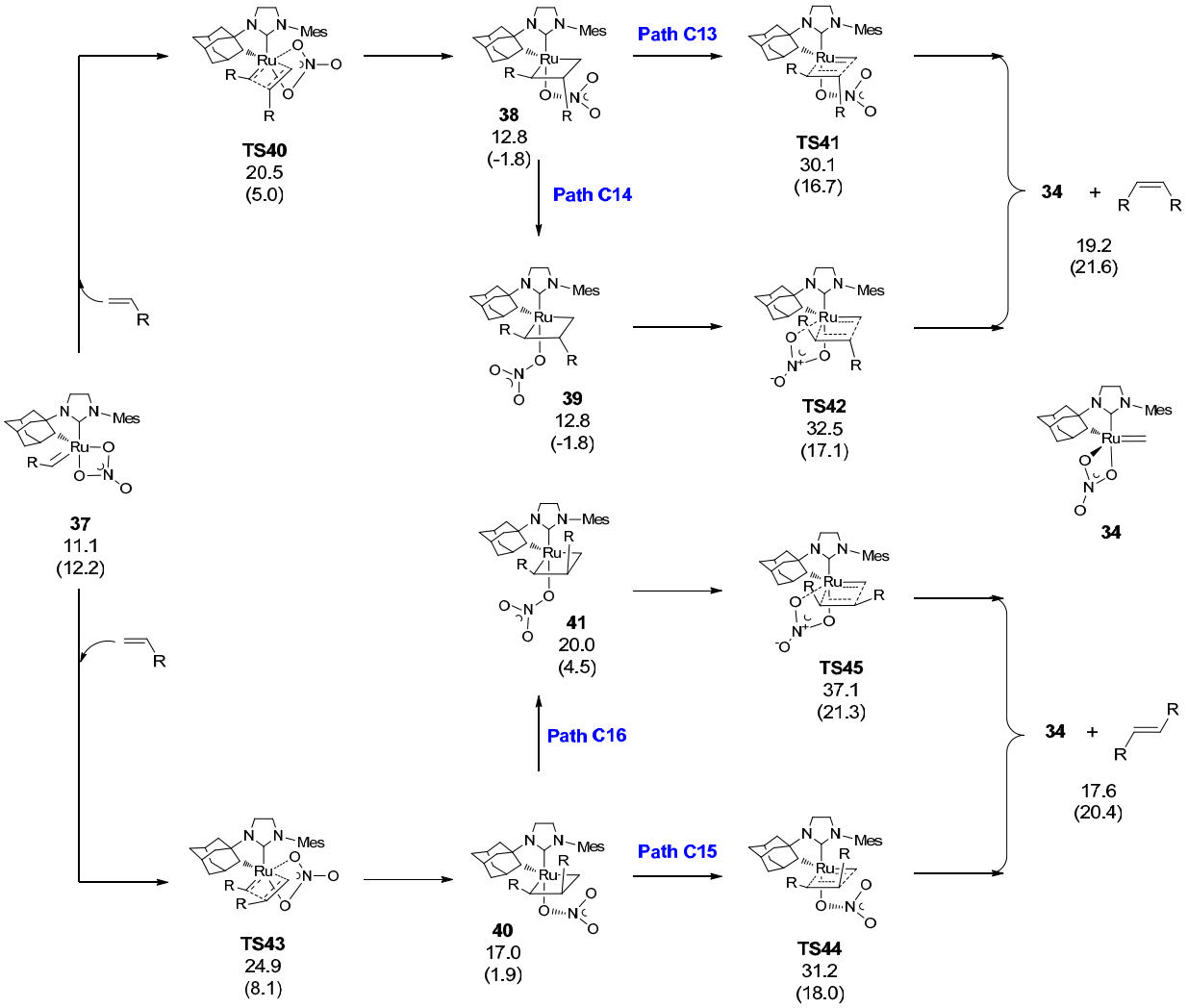
Scheme S6. Possible Side-Bound Pathways for Phenylpropene Homodimerization with Complex **14**



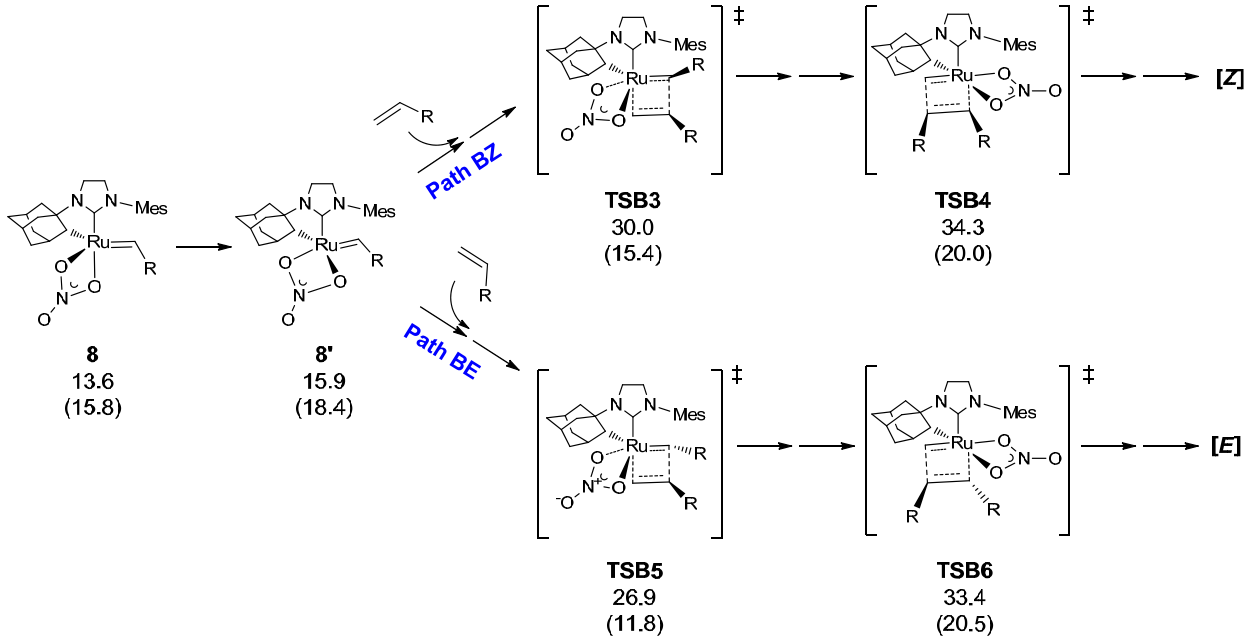
Scheme S7. Possible Side-Bound Pathways for Phenylpropene Homodimerization with Complex **31**

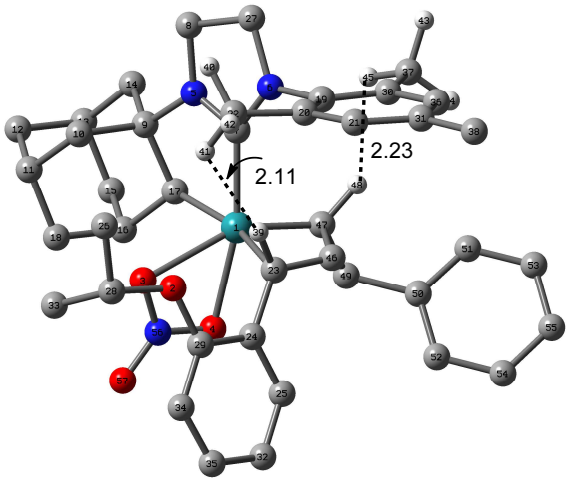


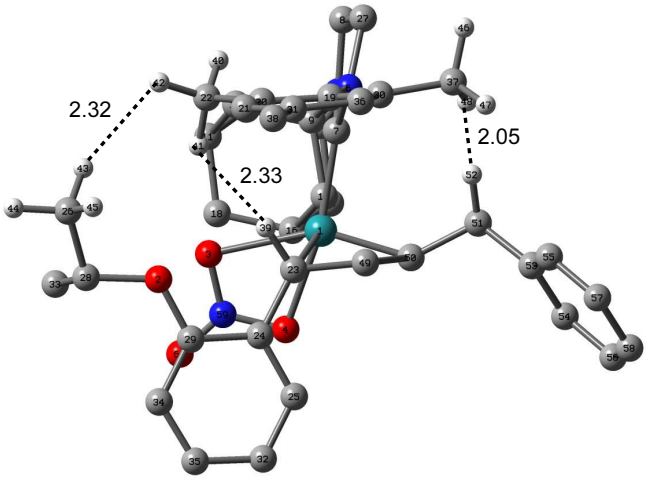
Scheme S8. Possible Side-Bound Pathways for Phenylpropene Homodimerization with Complex **37**



Scheme S9. Key TSs in the Most Favorable Bottom-Bound Pathways for Homodimerization Leading to (*Z*) and (*E*)-Olefin Products







Rh-C(23) 2.32 Rh-C(47) 1.89

C(23)-C(46) 1.42 C(46)-C(47) 2.14

Rh-O(3) 2.32 Rh-O(4) 2.20

TS5, $\Delta G^{\ddagger}$= 24.0 kcal/mol

Rh-C(23) 2.30 Rh-C(50) 1.89

C(23)-C(49) 1.44 C(49)-C(50) 2.03

Rh-O(3) 2.31 Rh-O(4) 2.21

TS14, $\Delta G^{\ddagger}$= 24.0 kcal/mol

Figure S1. Optimized structures of **TS5** and **TS14** with key bond distances listed and H···H interactions marked by dashed lines. H atoms are omitted for clarity except those in question. All distances are in Å. **TS5** and **TS14** are both six-coordinate due to the smaller size of NO_3. The steric repulsions as indicated by the most significant H···H interactions are comparable in **TS5** and **TS14**. There seems to be a combination of similar electronic and steric effects, which leads **TS5** and **TS13** to be isoenergetic coincidently.

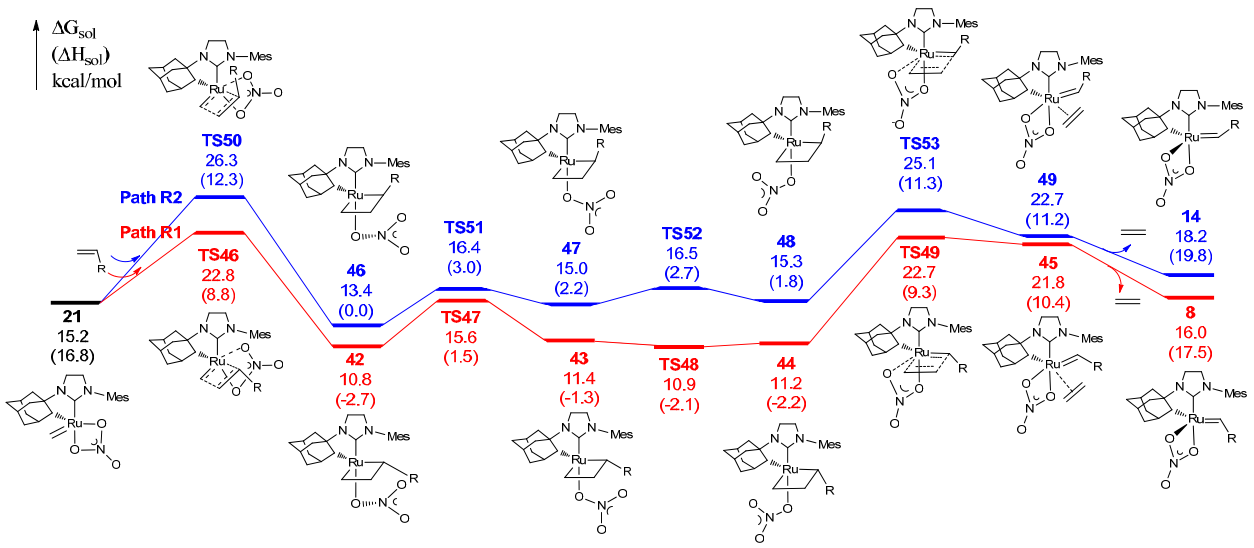


Figure S2. Free energy profiles for the most favorable pathways of regeneration leading to **8** (in red) and **14** (in blue). Note that **TS48** is higher than both **43** and **44** in the gas phase but becomes slightly lower after solvent correction. This computational anomaly could mean a facile isomerization between **43** and **44**.

Cartesian Coordinates (Å), SCF Energies, Enthalpies, and Free Energies at 298.15 K and 1 atm for the Optimized Structures

3cat
B3LYP SCF energy: -1804.087425 a.u.
B3LYP enthalpy: -1803.361772 a.u.
B3LYP free energy: -1803.471121 a.u.
M06 SCF energy in solution: -1803.342247 a.u.
M06 enthalpy in solution: -1802.616594 a.u.
M06 free energy in solution: -1802.725943 a.u.

Cartesian coordinates

C	2.35786700	4.60770900	2.11008700
H	2.78541300	5.59457600	2.26464700
C	2.08328900	4.18714900	0.80405700
H	2.29647500	4.85850500	-0.01793200
C	1.53593200	2.92134100	0.59015000
H	0.01158400	4.74500600	-1.08078500
C	2.08593900	3.78198300	3.20135200
C	1.52611400	2.52650000	2.97996700
H	2.30042100	4.11760400	4.21169300
C	1.23513400	2.06897800	1.68142600
H	1.29592200	1.87394000	3.81910600
Ru	0.18709700	0.24223800	-0.29177600
C	0.62140100	0.76962300	1.42930800
O	1.25465600	2.37961500	-0.64614500
O	-0.76217600	0.05424900	-2.45243000
O	-1.68127600	1.27407900	-0.92293300
N	0.28142600	-2.56623000	0.30293500
N	-1.71805800	0.84615800	-2.13647200
C	-0.55222900	-1.49269400	0.28039300
C	1.78642000	-1.03137900	-0.72986100
H	1.41418100	-1.29035900	-1.73934300
H	0.41031600	0.21650100	2.35397700
C	1.36932300	3.22062700	-1.84168100
C	-0.31681500	-3.74049100	0.94017100
C	1.71373800	-2.33476100	0.10282700
O	-2.59412700	1.18090400	-2.91694000
N	-1.77961000	-1.91097900	0.69861000
C	3.26613900	-0.63136000	-0.89362200
H	2.27165200	3.82648100	-1.71110500
C	1.58671500	2.30816400	-3.03983200
C	0.14039000	4.11715100	-1.96774900
H	-0.10093400	-4.65692700	0.38353400
H	0.06073600	-3.86450900	1.96514600
C	-1.80998300	-3.37182900	0.92082200
C	2.44183500	-2.18574500	1.46339200
C	2.39823400	-3.47384400	-0.68815700
C	-3.01889000	-1.18460100	0.63116700
C	3.96649900	-1.75391300	-1.70530100
H	3.33878700	0.31165300	-1.44776500
C	3.98105100	-0.48073400	0.46328700
H	0.74632000	1.62694200	-3.19217000
H	1.70151900	2.92612100	-3.93754100
H	2.49688600	1.71435700	-2.91551300
H	0.25038800	4.77352500	-2.83844700
H	-0.76565800	3.51793700	-2.09400400
H	-2.32588200	-3.60948600	1.85556800
H	-2.34147800	-3.86834200	0.09933900
H	2.37390600	-3.12933000	2.02428200
H	1.94632700	-1.41359500	2.05973200
C	3.91933600	-1.81509200	1.23459400
C	3.87794900	-3.08978500	-0.93457000
H	2.35373400	-4.42390500	-0.13417400
H	1.87531700	-3.62526400	-1.64157600
C	-3.80601100	-1.24727400	-0.53502900
C	-3.45971400	-0.48080500	1.76629900
H	5.02236600	-1.49954800	-1.87812200
H	3.49497900	-1.85217200	-2.69254300
H	5.02909800	-0.19022000	0.30261000
H	3.51063900	0.31488400	1.05230300
H	4.42084300	-1.70753600	2.20588000
C	4.60102900	-2.93146200	0.41875600
H	4.35853100	-3.88550500	-1.51902400
C	-5.02388500	-0.56046500	-0.55012200
C	-3.38590800	-2.03643800	-1.75533100
C	-4.68740600	0.18456000	1.70300400
C	-2.63816800	-0.42228300	3.03208100
H	5.65900200	-2.68703400	0.25159300
H	4.57614800	-3.87796500	0.97748500
H	-5.62652200	-0.58976600	-1.45543800
C	-5.47969500	0.16716400	0.55173200
H	-3.83577200	-1.60996100	-2.65634400
H	-2.30267800	-2.03379200	-1.89837000
H	-3.71558300	-3.08282900	-1.68906600
H	-5.03096800	0.73315900	2.57774300
H	-3.24092000	-0.04974400	3.86629700
H	-2.24033600	-1.40415100	3.31226300
H	-1.78056000	0.24908100	2.91217600
C	-6.78040100	0.93343100	0.49022300
H	-7.21489900	1.06844200	1.48656300
H	-6.62695200	1.93256300	0.06156600
H	-7.51889400	0.42223500	-0.13708100

TS1
B3LYP SCF energy: -1804.055818 a.u.
B3LYP enthalpy: -1803.331761 a.u.
B3LYP free energy: -1803.440687 a.u.
M06 SCF energy in solution: -1803.312321 a.u.
M06 enthalpy in solution: -1802.588264 a.u.
M06 free energy in solution: -1802.69719 a.u.

Cartesian coordinates

C	0.10185700	5.52214600	-0.23535200
H	0.20342600	6.58737500	-0.04501400
C	1.19440300	4.68386200	-0.01115000
H	2.12524600	5.11632600	0.33416400
C	1.09682400	3.30385400	-0.24794600
H	3.58251900	4.36242800	-1.36479300
C	-1.09726800	5.00260600	-0.71741600
C	-1.19972100	3.62970800	-0.93791800
H	-1.94387200	5.65248800	-0.91856200
C	-0.13780200	2.74669100	-0.68160900
H	-2.12606600	3.22090100	-1.32629900
Ru	-0.46917500	0.20690100	0.58368200
C	-0.29831000	1.27501300	-0.90029700
O	2.13298900	2.43119800	-0.11357200
O	-0.23274000	-0.63672100	2.80100200
O	1.45925600	0.02588500	1.62903100
N	-1.72842400	-1.98834600	-0.74719700
N	1.02820900	-0.44341400	2.75552500
C	-0.52126300	-1.43504200	-0.45941600
C	-2.50957000	-0.27452400	0.70903300
H	-2.33964000	-0.90684300	1.59857200
H	-0.25316200	0.95621900	-1.95130000
C	3.44929900	2.89508100	0.25614600
C	-1.63168300	-3.09379700	-1.70123500
C	-2.93976000	-1.23379300	-0.42160300
O	1.78366600	-0.68282600	3.67923600
N	0.44509100	-2.21182900	-1.02525600
C	-3.69077700	0.64946800	1.06527400
H	3.34619200	3.63152700	1.06398300
C	4.19791300	1.68136900	0.79360000
C	4.15050000	3.52436300	-0.94999600
H	-2.27157400	-3.93292900	-1.41424200
H	-1.92301200	-2.76714800	-2.70950900
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C	-3.46210600	-0.45041900	-1.65055400
C	-4.07289000	-2.14637900	0.10464100
C	1.86300700	-2.16509400	-0.79015100
C	-4.82814800	-0.25198600	1.61902100
H	-3.38393900	1.36247800	1.84194500
C	-4.23221300	1.41154100	-0.15806300
H	4.29010100	0.91455100	0.01730600
H	5.20285100	1.98044600	1.11382800
H	3.66560000	1.23852600	1.63767200
H	5.14190900	3.89224300	-0.66173500
H	4.27836200	2.77406200	-1.73820800
H	0.31456500	-3.63936700	-2.59696400
H	0.05386100	-4.29566200	-0.96734800
H	-3.74932200	-1.14992700	-2.44885200

H	-2.65780900	0.18442300	-2.04016200
C	-4.67465900	0.41165900	-1.24440000
C	-5.26784600	-1.26388400	0.53604400
H	-4.40196900	-2.85558400	-0.67002600
H	-3.70105000	-2.73623500	0.95252400
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C	2.69170500	-1.58409100	-1.76668800
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H	-4.48458000	-0.78150500	2.51736000
H	-5.08170000	2.04193500	0.14026700
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C	-5.79367200	-0.49373900	-0.69274200
H	-6.06114800	-1.90929200	0.93550700
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H	-6.66439700	0.11410800	-0.41173000
H	-6.13070000	-1.19759300	-1.46700600
H	4.22358100	-3.26035000	1.38570100
C	4.64971000	-2.21661000	-0.44562600
H	2.06037600	-3.49652100	2.35308600
H	0.58938800	-2.96357600	1.53865600
H	1.32896000	-4.50937000	1.10560400
H	4.72275100	-1.18138200	-2.33023200
H	2.91183700	-0.69354300	-3.71697500
H	1.37763300	-1.55125000	-3.50084900
H	1.62039900	0.01917000	-2.73831900
C	6.14683300	-2.21488600	-0.24068900
H	6.68245200	-2.13507100	-1.19264200
H	6.45777200	-1.36615800	0.38271900
H	6.48407400	-3.12676900	0.26406100

4

B3LYP SCF energy: -1804.068128 a.u.
B3LYP enthalpy: -1803.34286 a.u.
B3LYP free energy: -1803.456248 a.u.
M06 SCF energy in solution: -1803.323702 a.u.
M06 enthalpy in solution: -1802.598434 a.u.
M06 free energy in solution: -1802.711822 a.u.

Cartesian coordinates

Ru	-0.32311200	-0.19655500	-0.93689200
O	2.85621900	2.32132100	1.07093900
O	-1.71191100	-1.26540900	-2.48973500
O	-2.08879600	0.77691300	-1.87234400
N	-0.15877200	-2.11455300	1.17901800
N	-1.95072800	-0.87808500	1.53062900
C	-0.89991800	-1.08372900	0.69108600
C	-0.58236200	-2.52352700	2.51889400
C	1.14691100	-2.36639400	0.56166900
C	2.27878100	-1.64524500	1.33605700
C	3.61418000	-1.80685000	0.58363100
C	3.95459100	-3.30525100	0.46300400
C	2.82616800	-4.02362100	-0.30528300
C	1.49515300	-3.86989500	0.47411300
C	2.70841300	-3.40016100	-1.71516100
C	2.35145900	-1.89337500	-1.59634000
C	0.99647700	-1.80780600	-0.87051600
C	3.47294000	-1.17800400	-0.81788400
C	-3.10603200	-0.06289100	1.26663500
C	-3.17796700	1.21884200	1.83846000
C	-4.32258000	1.98845200	1.60607500
C	-2.05179200	1.77360000	2.67784600
C	0.62074100	1.10618200	-0.01172900
C	1.36037300	2.14260900	-0.74296800
C	0.95585300	2.56150400	-2.02781400
C	3.66415600	2.65783800	3.26875300
C	-1.98311700	-1.88852200	2.60873300
C	3.95314500	2.91402400	1.79316300
C	2.51205300	2.76100300	-0.17510300
C	-4.16784400	-0.57947500	0.49814200
C	-5.38325600	1.51798800	0.82811500
C	1.65605100	3.53278900	-2.74021600
C	5.28303300	2.30765600	1.34297800
C	3.21155000	3.73923600	-0.88973100
C	2.78348500	4.11779500	-2.16550500
C	-5.28838600	0.22996000	0.29225000
C	-4.12786400	-1.97015900	-0.09545300
C	-6.59118600	2.38230000	0.55202500
H	0.31037600	-2.49555700	-1.39984300
H	0.71132200	1.19652200	1.07487200
H	-0.60571400	-3.61234500	2.62151600
H	0.09703400	-2.12057400	3.28332100
H	2.03768200	-0.58304500	1.43916200
H	2.36296400	-2.06828700	2.34797900
H	4.40753600	-1.29179200	1.14289300
H	4.07732000	-3.74773100	1.46204300
H	4.90918500	-3.43636800	-0.06460400
H	3.06237400	-5.09214500	-0.39498000
H	0.68470100	-4.40563900	-0.03712000
H	1.60262200	-4.31339200	1.47579900
H	1.93897300	-3.92177800	-2.29961200
H	3.65957000	-3.52695400	-2.25193100
H	2.26296500	-1.46040800	-2.60208300
H	3.25138400	-0.10907700	-0.72678000
H	4.42167700	-1.26825800	-1.36573100
H	-4.38242300	2.98311800	2.04302300
H	-2.35015100	2.71493800	3.14940200
H	-1.74755400	1.08100700	3.47157800
H	-1.16488900	1.96927700	2.06541400
H	0.03733100	2.15123700	-2.44229200
H	3.62344800	1.58135800	3.46837000
H	4.45147700	3.09547500	3.89202400
H	2.70550200	3.10016400	3.55663000
H	-2.17983600	-1.41666900	3.57558900
H	-2.77567900	-2.62252300	2.41778100
H	3.94857300	3.99709800	1.61322500
H	1.31243700	3.84297500	-3.72240100
H	5.45271600	2.45442800	0.27241000
H	6.11502300	2.76756300	1.88838100
H	5.29169700	1.23066900	1.54391600
H	4.09250000	4.21013200	-0.46989700
H	3.33848300	4.88196800	-2.70319200
H	-6.10696500	-0.15687100	-0.31085500
H	-4.18251800	-2.74678100	0.67901100
H	-4.97809600	-2.12187500	-0.76652800
H	-3.21557900	-2.14559400	-0.67353700
H	-6.50463800	2.87531800	-0.42507100
H	-7.51342400	1.79086600	0.53491800
H	-6.70464100	3.16771000	1.30670300
N	-2.44042200	-0.21926200	-2.62169700
O	-3.38896700	-0.15503400	-3.37754200

TS2

B3LYP SCF energy: -1804.064978 a.u.
B3LYP enthalpy: -1803.340974 a.u.
B3LYP free energy: -1803.451548 a.u.
M06 SCF energy in solution: -1803.31782 a.u.
M06 enthalpy in solution: -1802.593816 a.u.
M06 free energy in solution: -1802.70439 a.u.

Cartesian coordinates

Ru	0.32764100	-0.28679000	0.95075100
O	-2.58860500	2.40703500	-1.11086300
O	0.91032300	-0.83577600	3.19813400
O	2.21233300	0.33234600	1.90643700
N	0.04856000	-2.14340300	-1.20388400
N	1.89089200	-0.98298500	-1.56054100
C	0.84273800	-1.15123200	-0.70653200
C	0.44189700	-2.54869900	-2.55391000
C	-1.27892600	-2.31318800	-0.60315400
C	-2.35468600	-1.51476600	-1.38309600
C	-3.70417500	-1.59386600	-0.64244000
C	-4.14367400	-3.06756500	-0.53601200
C	-3.07259400	-3.86443800	0.23667200
C	-1.72656000	-3.79122800	-0.52864800
C	-2.92843200	-3.26008300	1.65226600
C	-2.47381100	-1.77901300	1.54951500
C	-1.11289400	-1.77356300	0.83298200
C	-3.53615800	-0.98462300	0.76474100
C	3.08594300	-0.22473600	-1.30764300
C	3.26533300	1.00062900	-1.97291300
C	4.45349600	1.70689100	-1.75860700
C	2.20811300	1.56232000	-2.89436800
C	-0.42656300	1.09000600	-0.01990700
C	-1.07677600	2.20179400	0.68788600
C	-0.61762500	2.64826000	1.94304100
C	-3.37723300	2.73237800	-3.31839200
C	1.87576300	-1.99615500	-2.63591100
C	-3.63933000	3.05816200	-1.85128500

C	-2.19310400	2.87373900	0.11075400
C	4.08314200	-0.74657600	-0.46183300
C	5.45441400	1.22815100	-0.90923100
C	-1.23553300	3.69641100	2.62263200
C	-5.01024900	2.57089800	-1.38024100
C	-2.81024200	3.92774000	0.79188500
C	-2.33223900	4.33108500	2.04240900
C	5.25171000	-0.00311100	-0.27825400
C	3.91212000	-2.07131900	0.24349400
C	6.71242500	2.02689900	-0.65983900
H	-0.46976900	-2.50298000	1.36956200
H	-0.49068200	1.16770000	-1.10932800
H	0.40094200	-3.63453200	-2.68007100
H	-0.21330400	-2.08955300	-3.30796300
H	-2.04380900	-0.46996000	-1.48030000
H	-2.45861600	-1.92753600	-2.39745400
H	-4.45726100	-1.02493100	-1.20519400
H	-4.28662400	-3.49393000	-1.53933300
H	-5.10965100	-3.13842200	-0.01763700
H	-3.37869400	-4.91598900	0.31484600
H	-0.95774100	-4.38229600	-0.01390600
H	-1.85122900	-4.21980100	-1.53466700
H	-2.20053300	-3.83438500	2.24072400
H	-3.89077500	-3.32860700	2.17939100
H	-2.36363900	-1.36023200	2.55807500
H	-3.24108500	0.06747800	0.68298400
H	-4.49454700	-1.01388600	1.30207200
H	4.59705200	2.65708400	-2.26885800
H	2.56377800	2.47917700	-3.37432800
H	1.93174900	0.85668200	-3.68718300
H	1.29087000	1.80285700	-2.34578000
H	0.27433800	2.18797100	2.35986300
H	-3.41782200	1.64990700	-3.48234500
H	-4.13290500	3.20651000	-3.95405000
H	-2.38977200	3.09213900	-3.62359100
H	2.10715500	-1.54165500	-3.60319400
H	2.62461900	-2.77379800	-2.43534100
H	-3.55088500	4.14288500	-1.70723300
H	-0.85219700	4.02364400	3.58431000
H	-5.16409500	2.76382200	-0.31463300
H	-5.80640000	3.07625900	-1.93881800
H	-5.10248000	1.49206000	-1.54719000
H	-3.66590000	4.43873600	0.36653800
H	-2.82407900	5.15348100	2.55509600
H	6.02195900	-0.39622300	0.38180300
H	3.75101800	-2.89847200	-0.45891800
H	4.80063700	-2.30914200	0.83544300
H	3.05410000	-2.05000400	0.92322600
H	6.62721400	2.61537000	0.26313700
H	7.58628900	1.37553500	-0.54778600
H	6.91275400	2.72739600	-1.47746100
N	2.01580500	-0.20091600	3.07542700
O	2.83461300	-0.10206400	3.96492300

5

B3LYP SCF energy: -1804.07293 a.u.
B3LYP enthalpy: -1803.347694 a.u.
B3LYP free energy: -1803.460345 a.u.
M06 SCF energy in solution: -1803.321264 a.u.
M06 enthalpy in solution: -1802.596028 a.u.
M06 free energy in solution: -1802.708679 a.u.

Cartesian coordinates

Ru	0.24325000	-0.72122600	0.98003100
O	2.01381500	-0.87831700	2.25129200
O	0.10082000	-0.74334600	3.27291700
N	-0.09942800	-1.88078500	-1.62651000
N	1.80717500	-0.77899400	-1.66754000
C	0.74643000	-1.11194500	-0.88580800
C	0.28782500	-1.94152500	-3.03876300
C	-1.45385100	-2.08659900	-1.09974900
C	-2.42808800	-1.01358200	-1.65153500
C	-3.80874200	-1.16315400	-0.98409200
C	-4.37221500	-2.56587300	-1.28698400
C	-3.40485300	-3.63491400	-0.73810500
C	-2.02578500	-3.48529500	-1.42691300
C	-3.26679200	-3.44767000	0.78927000
C	-2.68859400	-2.04031200	1.09704700
C	-1.30661100	-1.95155600	0.43235200
C	-3.64933600	-0.97169700	0.53783500
C	3.03743700	-0.18810500	-1.21423900
C	3.30847100	1.15345900	-1.54363100
C	4.52467500	1.70691500	-1.13311300
C	2.31866500	1.99858500	-2.31116500
C	1.74729200	-1.45357800	-2.98135000
C	3.97633500	-0.96826500	-0.51324000
C	5.46861100	0.96785100	-0.41344800
C	5.17815600	-0.36764200	-0.12416400
C	3.71516200	-2.41213700	-0.15252300
C	6.75838700	1.60019800	0.05499200
H	-0.71947100	-2.84110700	0.77509000
H	0.19656500	-2.95421600	-3.44228300
H	-0.33939800	-1.27242800	-3.64405900
H	-2.02272800	-0.01511800	-1.45742900
H	-2.52518300	-1.12825700	-2.74095100
H	-4.48674800	-0.39773500	-1.38526200
H	-4.50698500	-2.69509100	-2.37053600
H	-5.36210700	-2.68509900	-0.82594900
H	-3.80029100	-4.63648600	-0.95251800
H	-1.33136800	-4.25862900	-1.07205100
H	-2.13860900	-3.62068700	-2.51315900
H	-2.61223700	-4.22302800	1.21038500
H	-4.25002000	-3.56753500	1.26593100
H	-2.58389700	-1.91574600	2.18180700
H	-3.26424500	0.03119900	0.75391700
H	-4.62754100	-1.05831400	1.03127500
H	4.73828700	2.74432000	-1.38218400
H	2.75882400	2.96845100	-2.56327100
H	2.00419800	1.52336700	-3.24792400
H	1.41095700	2.18386400	-1.72616800
H	2.00248600	-0.76283900	-3.78957700
H	2.46083900	-2.28796100	-3.00882200
H	5.90514100	-0.96418500	0.42297500
H	3.19445700	-2.95774500	-0.94611600
H	4.65642600	-2.93233000	0.05114600
H	3.09953500	-2.47536700	0.75179500
H	6.64791300	2.01527900	1.06550100
H	7.57342100	0.86936000	0.09271000
H	7.06648500	2.42043200	-0.60228600
C	-0.37331900	0.94689200	0.44779900
H	-0.19511900	1.26227800	-0.58150600
C	-1.10182400	1.98057900	1.19338100
C	-1.71335600	3.05337700	0.47178600
C	-1.22827700	1.99203300	2.59732400
C	-2.40190700	4.06448600	1.15140600
C	-1.91138300	3.00090300	3.27039500
H	-0.76364100	1.19197400	3.16062300
C	-2.49634900	4.03724000	2.54428200
H	-2.87285700	4.87564800	0.60914100
H	-1.98059700	2.97904900	4.35403300
H	-3.03311800	4.83295600	3.05438100
O	-1.57972400	3.01340300	-0.89004300
C	-2.17056300	4.02282900	-1.72815700
H	-2.02705100	5.00418200	-1.25773400
C	-3.66098100	3.74666800	-1.93344700
H	-4.11129300	4.52613500	-2.55871600
H	-3.79769000	2.78124300	-2.43333400
H	-4.19928200	3.71696200	-0.98187500
C	-1.38591700	3.98867400	-3.03572300
H	-1.76939100	4.74526300	-3.72886300
H	-0.32514300	4.18741200	-2.85476500
H	-1.47818600	3.00596600	-3.51151200
N	1.37201500	-0.86232900	3.38794400
O	1.94448000	-0.96271200	4.44948300

TS3

B3LYP SCF energy: -2153.014676 a.u.
B3LYP enthalpy: -2152.115352 a.u.
B3LYP free energy: -2152.244837 a.u.
M06 SCF energy in solution: -2152.102672 a.u.
M06 enthalpy in solution: -2151.203348 a.u.
M06 free energy in solution: -2151.332833 a.u.

Cartesian coordinates

Ru	0.21183400	-0.55163200	-0.68846200
O	2.22095900	3.06785700	1.29697200
O	-0.49793200	-2.21069400	-2.19186800
O	0.36651900	-0.35324700	-2.90111700
N	1.38094200	-1.85290500	1.61257000
N	-0.55915800	-1.13637100	2.33728000
C	0.24544300	-1.21625600	1.22740500
C	1.48118400	-2.05510500	3.05796100

C	2.50883700	-1.92506200	0.67765600
C	3.48104700	-0.73711200	0.88348200
C	4.57603000	-0.76840000	-0.20062700
C	5.37008200	-2.08434700	-0.07737700
C	4.41191900	-3.27876800	-0.26407900
C	3.31770200	-3.23715100	0.83059900
C	3.77160200	-3.19194600	-1.66631300
C	2.95769300	-1.87724800	-1.79182200
C	1.85211700	-1.91322500	-0.71782900
C	3.91030900	-0.68046300	-1.58999100
C	-1.97382700	-0.89626000	2.37382400
C	-2.45285500	0.26562400	3.00614800
C	-3.83652300	0.46826600	3.07136100
C	-1.51416500	1.27941800	3.62014100
C	0.70733900	1.20807100	-0.04364200
C	1.35606300	2.31870300	-0.77897500
C	1.24926100	2.49107700	-2.17109900
C	2.41704000	3.79093400	3.53912600
C	0.02614300	-1.85314000	3.49364100
C	2.99016700	3.95014000	2.13439900
C	2.13838200	3.26470500	-0.05564300
C	-2.86490100	-1.86744300	1.86884500
C	-4.74489300	-0.45361800	2.54587500
C	1.87086300	3.54627600	-2.83403600
C	4.47701500	3.59848600	2.06603900
C	2.77112200	4.31980900	-0.72521500
C	2.63221300	4.45985800	-2.10675600
C	-4.23727800	-1.62071900	1.96393100
C	-2.36874700	-3.13288200	1.20740300
C	-6.23159000	-0.18960700	2.57490100
H	1.32385900	-2.87127400	-0.81672400
H	0.72805000	1.40807900	1.02724200
H	1.86424600	-3.04962700	3.30244500
H	2.15140300	-1.30897300	3.50776600
H	2.92852700	0.20604400	0.83889500
H	3.94066100	-0.80290800	1.88129300
H	5.25152100	0.08586700	-0.05678100
H	5.86219800	-2.14005700	0.90455400
H	6.16374800	-2.12115700	-0.83589200
H	4.97089600	-4.21924500	-0.16871800
H	2.64305400	-4.09808800	0.73358400
H	3.79135600	-3.29893000	1.82244300
H	3.11645300	-4.05562000	-1.84154600
H	4.55988300	-3.22748700	-2.43215000
H	2.51617400	-1.82351300	-2.79214000
H	3.36005200	0.26252400	-1.68645600
H	4.68266500	-0.68441100	-2.37210400
H	-4.21134400	1.37419800	3.54294600
H	-1.10035900	0.92035700	4.57215300
H	-0.66348000	1.50029900	2.96808800
H	-2.04025900	2.21586000	3.82954200
H	0.67138800	1.77314700	-2.74061300
H	2.53227200	2.75742000	3.88406200
H	2.94075100	4.44925500	4.24064200
H	1.35235700	4.04411200	3.55241400
H	-0.07307200	-1.26379600	4.40918600
H	-0.49516800	-2.80792500	3.64481900
H	2.82780500	4.98413300	1.80325200
H	1.76511100	3.64768700	-3.91006300
H	4.85881000	3.65876800	1.04291300
H	5.06028200	4.28430000	2.69110600
H	4.63782000	2.57759600	2.43000800
H	3.37341600	5.03798300	-0.18217200
H	3.12813600	5.28668600	-2.60843300
H	-4.92931500	-2.36003200	1.56595100
H	-1.63797900	-3.66454100	1.82754700
H	-3.20133000	-3.81617600	1.01519700
H	-1.87755900	-2.92141900	0.25015800
H	-6.57716200	0.17461300	1.59855600
H	-6.79723000	-1.10036700	2.80205200
H	-6.49134300	0.56755400	3.32183400
C	-1.26219500	1.22548500	-0.34167100
C	-1.88494700	0.02773500	-0.86031600
H	-1.48688700	1.47406800	0.69053600
H	-1.24442100	2.08109000	-1.01212400
H	-2.44648100	-0.55262200	-0.13608600
C	-2.56808600	0.06364000	-2.22661300
H	-1.99707300	0.68625100	-2.92212400
H	-2.59731900	-0.94917000	-2.64094100
C	-3.99058500	0.58922400	-2.10891500
C	-5.04908200	-0.27935000	-1.80730400
C	-4.27698200	1.95186400	-2.27154500
C	-6.35368500	0.19800100	-1.66694500
H	-4.84810800	-1.34236600	-1.69221100
C	-5.57926700	2.43498600	-2.13230000
H	-3.47191800	2.64034600	-2.52022200
C	-6.62345200	1.55935200	-1.82707700
H	-7.16175200	-0.49536000	-1.44615500
H	-5.77941900	3.49464300	-2.27013800
H	-7.63919700	1.93245500	-1.72528500
N	-0.11137400	-1.51646100	-3.19581900
O	-0.18546400	-1.91136600	-4.34621900

6

B3LYP SCF energy: -2153.022134 a.u.
B3LYP enthalpy: -2152.121124 a.u.
B3LYP free energy: -2152.250184 a.u.
M06 SCF energy in solution: -2152.116909 a.u.
M06 enthalpy in solution: -2151.215899 a.u.
M06 free energy in solution: -2151.344959 a.u.

Cartesian coordinates

Ru	-0.26821400	-0.80459400	-0.32112900
O	-2.08314000	1.96473600	2.46312100
O	0.13119500	-3.12719700	-1.44415100
O	-0.58278900	-2.76050300	0.58155600
N	-1.35650700	1.24873500	-2.03523700
N	0.56425200	2.09354000	-1.41102700
C	-0.23022200	0.97627200	-1.32948700
C	-1.47855400	2.64947000	-2.43889500
C	-2.46499600	0.29525600	-1.97707400
C	-3.43924600	0.63591100	-0.81865500
C	-4.52398400	-0.45261500	-0.71009300
C	-5.31179600	-0.51658000	-2.03446800
C	-4.34672800	-0.84864600	-3.19206400
C	-3.26879700	0.25445400	-3.29713700
C	-3.67865800	-2.21101600	-2.91479100
C	-2.87848100	-2.15071600	-1.58577400
C	-1.78976800	-1.07375000	-1.75280800
C	-3.84394900	-1.80818700	-0.43225800
C	1.98456800	2.17720100	-1.20832900
C	2.48716100	2.97499200	-0.16441900
C	3.87592300	3.08160800	-0.01552600
C	1.57706200	3.74121400	0.76818400
C	-0.22998300	0.22827000	1.41439300
C	-1.06357200	-0.17260400	2.58585000
C	-0.96207300	-1.42003300	3.22168700
C	-2.29426600	4.32273200	2.45898400
C	-0.03241900	3.13130000	-2.28473200
C	-2.90719800	3.02500000	2.97724600
C	-2.00714600	0.75367500	3.10993200
C	2.85736700	1.55694300	-2.12944500
C	4.76610800	2.44477000	-0.88226300
C	-1.74092000	-1.75343600	4.32958500
C	-4.36034800	2.85221800	2.53052600
C	-2.78794100	0.42171400	4.22255800
C	-2.65214500	-0.82851600	4.83070200
C	4.23401200	1.70219200	-1.94255100
C	2.33660000	0.72670900	-3.28104800
C	6.25893500	2.52800700	-0.67142900
H	-1.18823500	-1.30898200	-2.64185900
H	-0.24662800	1.30799000	1.30326100
H	-1.85353500	2.74590800	-3.46151700
H	-2.16360500	3.18756900	-1.76853300
H	-2.87948300	0.71787200	0.11966900
H	-3.90572100	1.61492100	-1.00551500
H	-5.20516300	-0.20128500	0.11371000
H	-5.81639100	0.44218500	-2.22254900
H	-6.09592200	-1.28301000	-1.97068100
H	-4.90364900	-0.89258400	-4.13735400
H	-2.58988900	0.05166000	-4.13608800
H	-3.75108300	1.22465800	-3.48936600
H	-3.00938700	-2.48493600	-3.74122000
H	-4.44653300	-2.99489900	-2.85196100
H	-2.42708900	-3.12967000	-1.41233300
H	-3.29873600	-1.77489200	0.51875300
H	-4.60389500	-2.59603100	-0.33798100
H	4.26822100	3.68289100	0.80191800
H	1.19142400	4.65144700	0.28850200
H	0.71019800	3.15362900	1.08121300
H	2.12071800	4.05610400	1.66425600
H	-0.27532400	-2.15600300	2.82182200

H	-2.30653400	4.33997100	1.36320000
H	-2.86312100	5.18537500	2.82286700
H	-1.25761400	4.42241200	2.79532200
H	0.04703900	4.11941600	-1.82387200
H	0.49696100	3.15934500	-3.24620700
H	-2.84503400	3.01953000	4.07333300
H	-1.63567100	-2.73163400	4.78943100
H	-4.76976900	1.89121000	2.85388700
H	-4.98538800	3.65008600	2.94799900
H	-4.42573900	2.89869600	1.43781400
H	-3.50750300	1.12496600	4.62421600
H	-3.26771500	-1.06962700	5.69331000
H	4.91042100	1.21695800	-2.64306300
H	1.61081700	1.27503400	-3.89287100
H	3.15805000	0.42185100	-3.93628100
H	1.83112700	-0.17972600	-2.92833200
H	6.62566700	1.62801100	-0.16065700
H	6.79564900	2.60393700	-1.62381900
H	6.53174900	3.39186300	-0.05674200
C	1.27977300	-0.30281800	1.35939100
C	1.74412400	-0.93991500	0.00570800
H	1.89950400	0.58402700	1.51546300
H	1.43269900	-1.01812700	2.16756000
H	2.33572600	-0.24050600	-0.57793500
C	2.48619500	-2.27524100	0.11888600
H	1.95640700	-2.95285000	0.79439900
H	2.49876900	-2.74783300	-0.86831400
C	3.91315500	-2.08385800	0.60857700
C	4.93465200	-1.73248300	-0.28612700
C	4.24471100	-2.24047800	1.96186700
C	6.24436600	-1.53857600	0.15579400
H	4.70098200	-1.62316300	-1.34293500
C	5.55242400	-2.04414500	2.41057900
H	3.47273200	-2.53430900	2.66982900
C	6.55781500	-1.69040900	1.50889500
H	7.02349100	-1.28330400	-0.55859400
H	5.78687800	-2.17721700	3.46373000
H	7.57802500	-1.54613700	1.85480300
N	-0.27698600	-3.61517400	-0.35450900
O	-0.39318400	-4.81524400	-0.14907800

TS4

B3LYP SCF energy: -2153.007192 a.u.
B3LYP enthalpy: -2152.107205 a.u.
B3LYP free energy: -2152.236372 a.u.
M06 SCF energy in solution: -2152.107186 a.u.
M06 enthalpy in solution: -2151.207199 a.u.
M06 free energy in solution: -2151.336366 a.u.

Cartesian coordinates

Ru	0.25546700	0.38989300	-0.64617500
O	1.78874200	-0.44242000	3.02068600
O	-0.27285900	4.58124900	-1.13989800
O	0.13150700	2.56258200	-0.47211600
N	1.50883100	-2.12947200	-1.28753500
N	-0.35116800	-2.71192200	-0.28494000
C	0.37328500	-1.63183500	-0.73127300
C	1.71787700	-3.55449200	-1.03223800
C	2.56708200	-1.19275400	-1.66177000
C	3.56882600	-1.00070600	-0.49247100
C	4.61268900	0.07076600	-0.86239700
C	5.37220500	-0.38005700	-2.12710300
C	4.37570700	-0.56757400	-3.29029400
C	3.34453600	-1.65644400	-2.91371300
C	3.65032800	0.76756700	-3.55706500
C	2.88260600	1.22051200	-2.28677500
C	1.84574500	0.13564700	-1.95478200
C	3.88486600	1.40165000	-1.13017600
C	-1.75656300	-2.77638500	0.01434900
C	-2.18331000	-2.91636800	1.34609600
C	-3.55897600	-3.01794300	1.60206100
C	-1.21803000	-3.00086600	2.50596900
C	-0.20700300	0.39133300	1.33673700
C	0.40349500	1.34784600	2.30410900
C	0.01533000	2.69123600	2.43713800
C	2.47902500	-2.54582900	3.87574800
C	0.31470700	-3.99635100	-0.60029300
C	2.74253800	-1.04383000	3.91665900
C	1.41603900	0.87166300	3.18214300
C	-2.69004300	-2.82146600	-1.04894800
C	-4.50644100	-3.01297800	0.57963300
C	0.57584600	3.53410700	3.39418500
C	4.17585700	-0.69906300	3.50562900
C	1.97956700	1.71758300	4.14488300
C	1.55738200	3.04349400	4.25086000
C	-4.04682500	-2.92979400	-0.74187700
C	-2.25280100	-2.76423400	-2.49634200
C	-5.98529500	-3.08039500	0.87880700
H	1.18397700	-0.00859600	-2.83584700
H	-0.17586800	-0.61498000	1.74278100
H	2.07430700	-4.07797600	-1.92385900
H	2.45644700	-3.70003600	-0.23171100
H	3.01612500	-0.70555000	0.40842300
H	4.06976400	-1.95583700	-0.27482200
H	5.31932100	0.18833700	-0.02974900
H	5.91083900	-1.31927400	-1.93426200
H	6.12603800	0.37025700	-2.40004000
H	4.91534400	-0.88641900	-4.19183400
H	2.64192500	-1.82701100	-3.74073600
H	3.86265100	-2.60783200	-2.72104700
H	2.95624100	0.66056300	-4.40251200
H	4.38071800	1.53794600	-3.84054100
H	2.38404100	2.17217100	-2.47333700
H	3.35758400	1.74774600	-0.23408600
H	4.60922200	2.18466100	-1.39010200
H	-3.89053200	-3.10852400	2.63464100
H	-1.23908800	-4.00525400	2.94931700
H	-0.19256900	-2.78387500	2.20445600
H	-1.49202200	-2.29588600	3.29921700
H	-0.72624800	3.09413700	1.76011700
H	2.62559500	-2.93295600	2.86097800
H	3.16991200	-3.06963500	4.54538100
H	1.45504600	-2.76951500	4.18950200
H	0.31930800	-4.65110700	0.27613500
H	-0.22012200	-4.51309900	-1.40695900
H	2.54415700	-0.68235700	4.93384300
H	0.24979200	4.56771600	3.46026700
H	4.33774200	0.38153200	3.46828900
H	4.88875600	-1.12851500	4.21910200
H	4.39245000	-1.10912200	2.51342700
H	2.75360800	1.35961200	4.81209500
H	2.00849900	3.68688000	5.00157200
H	-4.76747900	-2.95130500	-1.55693200
H	-1.73862100	-3.68459600	-2.80150100
H	-3.11901900	-2.64576300	-3.15396600
H	-1.56555800	-1.93444500	-2.68863800
H	-6.44726800	-2.08825400	0.79223700
H	-6.50670500	-3.74256500	0.17835500
H	-6.17353600	-3.44325100	1.89420200
C	-1.61350900	0.70771900	0.69256600
C	-1.73532400	0.48891200	-0.88204900
H	-2.31258700	-0.00617100	1.13498200
H	-1.90583100	1.73162400	0.91146100
H	-2.24603200	-0.44976900	-1.07708200
C	-2.37179200	1.61346700	-1.71352800
H	-1.73643300	2.49811900	-1.71985400
H	-2.44617200	1.24489100	-2.74657200
C	-3.75405500	2.00353300	-1.21413500
C	-4.85634000	1.14647100	-1.34762900
C	-3.94188700	3.24481700	-0.58891200
C	-6.11255100	1.51601000	-0.86472600
H	-4.73103500	0.18342900	-1.83884900
C	-5.19848200	3.61655500	-0.10501700
H	-3.09508300	3.92183900	-0.49990600
C	-6.28719000	2.75295900	-0.23857300
H	-6.95804700	0.84228000	-0.98391900
H	-5.32667900	4.58528900	0.37142500
H	-7.26590400	3.04315800	0.13487700
N	0.57308400	3.69449400	-0.95250600
O	1.78242400	3.84900900	-1.15927200

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B3LYP SCF energy: -2153.0188 a.u.
B3LYP enthalpy: -2152.118033 a.u.
B3LYP free energy: -2152.246173 a.u.
M06 SCF energy in solution: -2152.114178 a.u.
M06 enthalpy in solution: -2151.213411 a.u.
M06 free energy in solution: -2151.341551 a.u.

Cartesian coordinates

Ru	0.33490200	-0.33895900	-0.61326800
O	1.22175700	3.04048300	1.36182000

O	2.13990800	1.34525100	-1.42988100
O	0.54525500	0.46850600	-2.62126600
N	1.44944000	-2.00628300	1.48386500
N	-0.35297600	-1.17538300	2.40576500
C	0.38481900	-1.19304100	1.24440200
C	1.58869800	-2.40690400	2.88532000
C	2.52243700	-2.12558600	0.49865300
C	3.74606300	-1.26088700	0.89920200
C	4.84453800	-1.36169700	-0.17823200
C	5.27357500	-2.83202400	-0.34968500
C	4.05246400	-3.67308500	-0.77426400
C	2.98311600	-3.59727700	0.33728400
C	3.47861600	-3.12298300	-2.09854000
C	3.03788500	-1.64275000	-1.91206600
C	1.93711600	-1.63768600	-0.83420600
C	4.28275800	-0.82331100	-1.50568900
C	-1.71082000	-0.74181300	2.59710000
C	-1.95394800	0.47262200	3.27341100
C	-3.27857000	0.87252800	3.47143800
C	-0.82692000	1.31755200	3.82071600
C	-0.54953000	1.41940400	0.02603100
C	-0.20888000	2.76401700	-0.51161100
C	-0.74467300	3.29603900	-1.69505700
C	2.52231600	2.99576000	3.34701100
C	0.19325000	-2.09379700	3.42830000
C	2.39848700	3.61979400	1.96129500
C	0.69318100	3.58611100	0.21810400
C	-2.77976100	-1.58823500	2.23937900
C	-4.36184100	0.09555800	3.04569500
C	-0.43350100	4.57838500	-2.14539500
C	3.63338600	3.36511400	1.09688900
C	0.99761200	4.87648500	-0.22487100
C	0.43448900	5.37173900	-1.40236900
C	-4.08883000	-1.13840200	2.45193700
C	-2.57025500	-2.98935100	1.70464000
C	-5.78208800	0.57752300	3.22656800
H	1.15145100	-2.36189300	-1.15961200
H	-0.55519400	1.44118400	1.10891400
H	1.85593600	-3.46303100	2.98058200
H	2.36508100	-1.81070300	3.38412100
H	3.42465400	-0.21893200	1.01901300
H	4.13812500	-1.60226700	1.86799400
H	5.70770300	-0.75840000	0.13296700
H	5.69468500	-3.22380400	0.58765200
H	6.06314000	-2.90449600	-1.10954100
H	4.35212100	-4.72086000	-0.90912500
H	2.11577600	-4.22357300	0.08889000
H	3.40479200	-3.97965900	1.27858700
H	2.62811800	-3.73683400	-2.42615300
H	4.24057000	-3.18500900	-2.88779500
H	2.63317100	-1.26752900	-2.85795400
H	4.02413300	0.23258000	-1.41024000
H	5.04265100	-0.90632400	-2.29528700
H	-3.46823800	1.81515100	3.98037000
H	-0.17565000	0.73549000	4.48412300
H	-0.18996100	1.73361400	3.03542700
H	-1.22904600	2.15315400	4.40220500
H	-1.41435400	2.69032000	-2.29429500
H	2.63606100	1.90879200	3.26917500
H	3.40212100	3.39847100	3.86068900
H	1.63857100	3.21129200	3.95537200
H	0.20920700	-1.61482400	4.41129800
H	-0.43202700	-2.99356300	3.49827200
H	2.24041500	4.69920600	2.08621100
H	-0.86592500	4.94667700	-3.07093300
H	3.49712000	3.73750600	0.07873500
H	4.50900200	3.85783000	1.53594200
H	3.83130200	2.29015900	1.03261800
H	1.68383300	5.50265500	0.33245600
H	0.68820700	6.37501500	-1.73401200
H	-4.91563200	-1.77890100	2.15144800
H	-2.62182800	-3.72309300	2.52092700
H	-3.35662000	-3.25335900	0.99009200
H	-1.60575300	-3.11416900	1.20750400
H	-6.09240600	1.21173000	2.38577700
H	-6.48625400	-0.25926700	3.28023100
H	-5.89029900	1.17348800	4.13927200
C	-1.79564000	0.66271300	-0.54188600
C	-1.55645900	-0.86096800	-0.96542500
H	-2.53955800	0.64069200	0.25730600
H	-2.19459700	1.18626300	-1.40844200
H	-2.06429900	-1.51710900	-0.26271800
C	-1.95444300	-1.22436700	-2.40569600
H	-1.41546200	-0.59369400	-3.11757600
H	-1.63035900	-2.25907800	-2.58713900
C	-3.45036800	-1.12464300	-2.65047200
C	-4.32723700	-2.10576000	-2.16281800
C	-3.99674200	-0.04131400	-3.35272300
C	-5.70471300	-2.00344700	-2.35886000
H	-3.92176200	-2.96792700	-1.63615400
C	-5.37517100	0.06680100	-3.55173100
H	-3.33244400	0.71771800	-3.76032600
C	-6.23499100	-0.91268000	-3.05252700
H	-6.36457300	-2.77928100	-1.97799300
H	-5.77528000	0.91378800	-4.10343800
H	-7.30738700	-0.83252000	-3.20984100
N	1.59285000	1.24188700	-2.56160800
O	1.99177000	1.81490300	-3.56485500

TS5

B3LYP SCF energy: -2153.006149 a.u.
B3LYP enthalpy: -2152.107597 a.u.
B3LYP free energy: -2152.236206 a.u.
M06 SCF energy in solution: -2152.094436 a.u.
M06 enthalpy in solution: -2151.195884 a.u.
M06 free energy in solution: -2151.324493 a.u.

Cartesian coordinates

Ru	0.36676500	-0.41975500	-0.45898100
O	0.40753900	3.66704500	0.63618100
O	1.87594300	1.29316100	-0.85254000
O	0.78116600	0.36594200	-2.47486900
N	1.57005700	-1.86469000	1.74463400
N	-0.33207400	-1.16613200	2.56383800
C	0.45378800	-1.14872800	1.43558900
C	1.68068200	-2.21009000	3.16299900
C	2.69659600	-1.91799100	0.80884000
C	3.74734800	-0.82861500	1.14593700
C	4.89925500	-0.86883700	0.12011700
C	5.56160700	-2.26009800	0.13204700
C	4.50778200	-3.32557000	-0.23143300
C	3.39118900	-3.30162100	0.83700500
C	3.92396400	-3.01796600	-1.62902600
C	3.23904500	-1.62280500	-1.62307700
C	2.08795900	-1.69185300	-0.58818400
C	4.32737300	-0.57868500	-1.28025100
C	-1.62280200	-0.58843700	2.79076900
C	-1.69344300	0.72298600	3.30682700
C	-2.95017300	1.27388400	3.56633900
C	-0.43953100	1.50673200	3.61555600
C	-1.00934300	1.41885000	-0.16328600
C	-0.83089100	2.57585300	-1.06906300
C	-1.39262400	2.61942500	-2.35567200
C	1.46804600	4.53589500	2.57337100
C	0.24369800	-1.99310500	3.64375300
C	1.38980400	4.63778100	1.05432600
C	-0.10613000	3.71630800	-0.63091900
C	-2.79011700	-1.35838300	2.62700400
C	-4.13271900	0.55437100	3.35495200
C	-1.25965000	3.72362100	-3.19124000
C	2.73871300	4.38012800	0.38242300
C	0.02568400	4.83032900	-1.47127700
C	-0.54629500	4.83300900	-2.74225700
C	-4.02807000	-0.76192700	2.90159700
C	-2.75392400	-2.80905500	2.19956000
C	-5.48055900	1.18927100	3.60556700
H	1.53673300	-2.61387700	-0.82819300
H	-0.82466700	1.64464900	0.87786500
H	2.02098500	-3.23983600	3.30073000
H	2.39145300	-1.54443900	3.67299200
H	3.26395600	0.15472800	1.12950200
H	4.14369600	-0.99181800	2.15920700
H	5.64176100	-0.10374700	0.38403300
H	5.99099900	-2.47514200	1.12156600
H	6.38987400	-2.28704300	-0.58899000
H	4.97342000	-4.32042100	-0.23671800
H	2.64702300	-4.08542100	0.63959600
H	3.83245400	-3.50856800	1.82396400
H	3.20165800	-3.79523500	-1.91490300
H	4.73038200	-3.04149700	-2.37614600
H	2.83161900	-1.41726400	-2.61970500
H	3.93280000	0.43739900	-1.31301900

H	5.13104700	-0.63793000	-2.02795800
H	-3.00747400	2.28945000	3.95220300
H	0.17861800	0.99027800	4.36115300
H	0.18567300	1.65796100	2.73094400
H	-0.69198300	2.49146400	4.01858200
H	-1.94399600	1.75819800	-2.71686700
H	1.82831500	3.54694800	2.87576500
H	2.16278400	5.28812500	2.96269900
H	0.48562600	4.70365500	3.02608400
H	0.18235700	-1.47271900	4.60407700
H	-0.30919900	-2.93818600	3.73344100
H	1.02377400	5.64124000	0.79998300
H	-1.70279400	3.71337400	-4.18257900
H	2.65534000	4.37328000	-0.70737000
H	3.45578900	5.15708800	0.67329100
H	3.13001100	3.40468700	0.68635200
H	0.58328400	5.70012500	-1.14724400
H	-0.42521000	5.70573200	-3.37833600
H	-4.93318000	-1.34935000	2.75852000
H	-2.94993000	-3.47049200	3.05414300
H	-3.52668800	-3.01653000	1.45099100
H	-1.78786500	-3.09070000	1.77577300
H	-5.81999800	1.75356400	2.72698000
H	-6.24466800	0.43638600	3.82521400
H	-5.44267400	1.89123600	4.44569000
C	-1.90370100	0.34990700	-0.42723900
C	-1.07032800	-1.55500200	-0.93035200
H	-2.43375300	-0.07370600	0.41503800
H	-2.46352100	0.35127900	-1.35701000
H	-1.69778800	-2.12438400	-0.23528200
C	-1.37286900	-1.93207000	-2.37270200
H	-0.87060900	-1.25093000	-3.06536200
H	-0.88618400	-2.91535400	-2.50125600
C	-2.84637400	-2.06125000	-2.71580100
C	-3.63058400	-3.08722800	-2.16671400
C	-3.46127500	-1.14562700	-3.58042600
C	-4.99033500	-3.18734000	-2.46251900
H	-3.16767900	-3.82212600	-1.51079200
C	-4.82256200	-1.24209300	-3.87954100
H	-2.86335300	-0.35735100	-4.03303700
C	-5.59265800	-2.26166200	-3.31873300
H	-5.57899500	-3.99343900	-2.03163600
H	-5.27826600	-0.52251600	-4.55483100
H	-6.65104900	-2.34045400	-3.55214500
N	1.66381600	1.23524000	-2.11535500
O	2.25865300	1.93310900	-2.91788000

8

B3LYP SCF energy: -1650.221133 a.u.
B3LYP enthalpy: -1649.561104 a.u.
B3LYP free energy: -1649.665648 a.u.
M06 SCF energy in solution: -1649.518465 a.u.
M06 enthalpy in solution: -1648.858436 a.u.
M06 free energy in solution: -1648.96298 a.u.

Cartesian coordinates

Ru	-0.53230500	-0.53573200	0.25620000
O	0.13172800	-0.60134800	2.32282100
O	-0.42206500	-2.50285300	1.43147600
N	-1.91264200	1.77421400	-0.67419400
N	0.14642100	2.44204800	-0.28963500
C	-0.67370500	1.36000900	-0.28593700
C	-2.03534600	3.23333700	-0.67754900
C	-2.99625700	0.79431900	-0.51422100
C	-3.52043000	0.77804700	0.94737700
C	-4.55294500	-0.35183200	1.12666500
C	-5.72931900	-0.11400700	0.15702300
C	-5.20615500	-0.10461100	-1.29447700
C	-4.18325800	1.04464000	-1.46544100
C	-4.54108300	-1.46528100	-1.59998200
C	-3.34983700	-1.70028300	-0.63336500
C	-2.33122200	-0.56686500	-0.86078900
C	-3.88095900	-1.70477800	0.81517600
C	1.55377500	2.44719700	-0.00753400
C	1.98282200	2.54932300	1.32991200
C	3.35748200	2.56285900	1.58486100
C	1.00223600	2.64263300	2.47491700
C	-0.55548800	3.65663300	-0.75598600
C	2.47974800	2.40640000	-1.06707100
C	4.30412200	2.48743700	0.55869800
C	3.84405900	2.42211700	-0.75931300
C	2.04077500	2.37402400	-2.51385500
C	5.78259700	2.45811300	0.86842500
H	-2.09204500	-0.53429800	-1.92874400
H	-2.62110200	3.59043200	-1.52884900
H	-2.51294400	3.59268700	0.24611500
H	-2.67735600	0.63338400	1.64044100
H	-3.97080300	1.74951300	1.19833900
H	-4.91955000	-0.34698000	2.16152900
H	-6.22562200	0.83908700	0.38885100
H	-6.48230000	-0.90422300	0.27820100
H	-6.04247800	0.05987200	-1.98643700
H	-3.82081000	1.08744600	-2.50121100
H	-4.67040700	2.00711900	-1.24676900
H	-4.19099300	-1.49095100	-2.64091500
H	-5.28320100	-2.26926700	-1.49262700
H	-2.88220100	-2.66746600	-0.85676300
H	-3.06021600	-1.89522700	1.51816900
H	-4.60464600	-2.52076400	0.94735400
H	3.69572400	2.63470800	2.61638500
H	0.18086800	3.33377200	2.25386900
H	0.55966600	1.66614800	2.69796700
H	1.50516500	2.99445100	3.38108700
H	-0.31629600	4.51015300	-0.11563700
H	-0.25775200	3.90095300	-1.78383000
H	4.56462700	2.37798700	-1.57351400
H	1.84408100	3.38541500	-2.89579200
H	2.82193000	1.93958200	-3.14539200
H	1.12629700	1.79017100	-2.65509700
H	6.12763600	1.42953500	1.03727500
H	6.37450300	2.86924200	0.04373000
H	6.01448900	3.03080800	1.77291200
C	0.60670800	-1.01208300	-1.07934800
H	1.16434100	-0.27462800	-1.67240300
C	0.96957700	-2.44576800	-1.41828100
H	0.36710300	-3.14764900	-0.83398600
H	0.71570900	-2.60269600	-2.47988700
C	2.44992800	-2.72287500	-1.20914400
C	3.37875100	-2.51543400	-2.23723500
C	2.91553000	-3.16437800	0.03769900
C	4.74062900	-2.74188900	-2.02739600
H	3.03116300	-2.18447000	-3.21414200
C	4.27562200	-3.39336000	0.24965200
H	2.20302300	-3.33743300	0.84038700
C	5.19345400	-3.18119900	-0.78187900
H	5.44608900	-2.58245500	-2.83920600
H	4.61750800	-3.74118400	1.22109000
H	6.25246400	-3.36265600	-0.61786800
N	0.00422800	-1.89714100	2.47225100
O	0.27069100	-2.44785100	3.51620300

TS6

B3LYP SCF energy: -2152.993887 a.u.
B3LYP enthalpy: -2152.09549 a.u.
B3LYP free energy: -2152.225522 a.u.
M06 SCF energy in solution: -2152.090124 a.u.
M06 enthalpy in solution: -2151.191727 a.u.
M06 free energy in solution: -2151.321759 a.u.

Cartesian coordinates

Ru	-0.07861900	-0.60069500	-0.40111400
O	-1.93345500	1.67749600	2.57872700
O	-0.13520900	-3.93280700	-1.33043800
O	-0.24119400	-2.59909000	0.42689500
N	-1.38629100	1.59908200	-1.71564000
N	0.44622500	2.49848100	-0.91008500
C	-0.24843500	1.31696700	-1.04045400
C	-1.63826400	3.03082800	-1.87481500
C	-2.36650400	0.52648200	-1.91856100
C	-3.39019800	0.49199800	-0.75406900
C	-4.34607700	-0.70326700	-0.92504900
C	-5.10044400	-0.55761100	-2.26265100
C	-4.08459600	-0.52149600	-3.42389000
C	-3.14206900	0.69162900	-3.24392100
C	-3.26861100	-1.83078400	-3.41918300
C	-2.50012100	-1.97605100	-2.08035300
C	-1.53177200	-0.78151800	-1.95136800
C	-3.52030100	-2.00481200	-0.92304200
C	1.86084900	2.64625700	-0.69169800
C	2.33402000	3.16964500	0.52439200
C	3.71673300	3.33551500	0.69293400
C	1.41213000	3.59124900	1.64482200

C	0.21034000	0.14635200	1.73546500
C	-0.82803200	-0.42905700	2.62883400
C	-0.75847100	-1.73812300	3.13658500
C	-2.18913300	4.01169600	2.95270800
C	-0.24817400	3.61727800	-1.58942300
C	-2.84102000	2.64589100	3.14203400
C	-1.90124700	0.39392600	3.06822400
C	2.76017700	2.36632100	-1.74944500
C	4.63022100	3.02077200	-0.31173200
C	-1.70333500	-2.23383800	4.02930300
C	-4.21339400	2.56637000	2.47086800
C	-2.85153000	-0.10682000	3.96778700
C	-2.75143900	-1.41444700	4.44334500
C	4.12693900	2.55005800	-1.53161600
C	2.28162400	1.89623000	-3.10610500
C	6.11773200	3.17041100	-0.09518400
H	-0.92041200	-0.74727100	-2.86660100
H	0.15049700	1.22363400	1.65839800
H	-2.00374900	3.26932500	-2.87725900
H	-2.38557800	3.37558100	-1.14618300
H	-2.85557700	0.42046700	0.20180100
H	-3.96067900	1.43292100	-0.73311200
H	-5.06492100	-0.71214000	-0.09449300
H	-5.70796000	0.35932500	-2.25857000
H	-5.79286200	-1.39922600	-2.39836200
H	-4.61859700	-0.41557400	-4.37774800
H	-2.43288200	0.75424600	-4.08049800
H	-3.73512800	1.61935500	-3.24356100
H	-2.56094900	-1.83949100	-4.25974400
H	-3.94420500	-2.68617000	-3.56338700
H	-1.92721600	-2.90463000	-2.09013200
H	-2.99977800	-2.12476500	0.03544500
H	-4.18829300	-2.87052200	-1.03267700
H	4.08144400	3.72976600	1.63959700
H	1.55876400	4.65243600	1.88228800
H	0.36273300	3.43838500	1.39123700
H	1.61930800	3.02637700	2.56158900
H	0.03696200	-2.38886700	2.80065600
H	-2.04953600	4.22707600	1.88723400
H	-2.82427500	4.79576200	3.37931600
H	-1.21314000	4.04846500	3.44555000
H	-0.27682700	4.50037400	-0.94422200
H	0.27949300	3.88821100	-2.51250400
H	-2.93427500	2.44895000	4.21744700
H	-1.62146500	-3.25455100	4.38949800
H	-4.64938700	1.56704700	2.55396500
H	-4.90340100	3.28209400	2.93257500
H	-4.12707000	2.80903700	1.40626500
H	-3.67727500	0.50957000	4.30031400
H	-3.50100500	-1.78516200	5.13754800
H	4.81947800	2.32522000	-2.34045600
H	1.81332500	2.71147500	-3.67299300
H	3.12351100	1.53343100	-3.70346300
H	1.54582000	1.09008400	-3.03278600
H	6.57639800	2.20674700	0.16268600
H	6.61980600	3.53636300	-0.99766900
H	6.33660500	3.86568300	0.72154900
C	1.45378100	-0.43424100	1.43983500
C	1.70102400	-0.79169100	-0.92027700
H	2.29798200	0.21885000	1.25048500
H	1.69871600	-1.44220200	1.75222700
C	2.39957300	-2.07393700	-1.32060500
H	1.70139000	-2.90778100	-1.39694400
H	2.79011200	-1.88779500	-2.33554700
C	3.56568800	-2.41106100	-0.40140400
C	4.78474700	-1.72505800	-0.49874900
C	3.43275100	-3.40906700	0.57551800
C	5.84537600	-2.02381800	0.35826300
H	4.90762200	-0.95629200	-1.25926700
C	4.49416300	-3.71011900	1.43190700
H	2.49869800	-3.95858900	0.66251300
C	5.70269000	-3.01815600	1.32847000
H	6.78577400	-1.48642300	0.26220800
H	4.37559400	-4.49211200	2.17746000
H	6.52876100	-3.25653700	1.99329200
H	2.36101000	0.07495800	-1.01157100
N	-0.23097900	-3.79839900	-0.09654200
O	-0.28778500	-4.74986100	0.68797900

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B3LYP SCF energy: -2152.995591 a.u.

B3LYP enthalpy: -2152.096344 a.u.

B3LYP free energy: -2152.231319 a.u.

M06 SCF energy in solution: -2152.092925 a.u.

M06 enthalpy in solution: -2151.193678 a.u.

M06 free energy in solution: -2151.328653 a.u.

Cartesian coordinates

Ru	-0.05103300	-0.70436200	0.05857800
O	2.14221100	2.65340100	-1.91796200
O	-0.04881000	-4.35075100	-0.16232900
O	0.12158200	-2.44685300	-1.26404600
N	1.21347500	0.99571400	1.97331200
N	-0.50401100	2.18956200	1.29502600
C	0.13293400	0.97713100	1.16477000
C	1.49376100	2.30405200	2.56284700
C	2.05530300	-0.20676300	2.04936600
C	3.21803600	-0.14378300	1.02655900
C	4.02154300	-1.45900400	1.06181900
C	4.59885900	-1.66294800	2.47663600
C	3.44401700	-1.72521400	3.49744100
C	2.65807000	-0.39411800	3.45988100
C	2.51187500	-2.90086200	3.13675000
C	1.91894000	-2.69408400	1.71883500
C	1.09434100	-1.39193600	1.73099600
C	3.07963000	-2.62613800	0.70326200
C	-1.90118400	2.43899500	1.05199500
C	-2.29712900	3.26859700	-0.01025600
C	-3.66594400	3.50993300	-0.20242400
C	-1.30655200	3.94118300	-0.93073200
C	0.13602100	0.74474200	-1.95235900
C	1.47149500	0.44949400	-2.51691500
C	1.78362600	-0.77989800	-3.12723900
C	2.18492800	5.03420800	-1.93252100
C	0.18351200	3.06132000	2.27670900
C	3.04441300	3.77605400	-1.99454000
C	2.47844200	1.45579700	-2.49657200
C	-2.86337100	1.92555900	1.95683800
C	-4.63888500	2.97487300	0.63898200
C	3.03292400	-1.02601500	-3.68894200
C	4.07365400	3.71826200	-0.86463100
C	3.73483700	1.20298400	-3.06202800
C	4.00709700	-0.03071300	-3.65512300
C	-4.21195400	2.19678000	1.72350300
C	-2.46940300	1.11692000	3.17382300
C	-6.10988100	3.21773000	0.39622300
H	0.39064900	-1.45077600	2.57270600
H	0.04293500	1.73880200	-1.53860300
H	1.71244900	2.22637800	3.63154500
H	2.35609300	2.77554100	2.07222300
H	2.81872300	0.02597100	0.01831700
H	3.87070000	0.71075600	1.26030300
H	4.83964500	-1.39975100	0.33189900
H	5.28670100	-0.84304800	2.73038500
H	5.18179600	-2.59288000	2.51476000
H	3.85109800	-1.86627800	4.50769600
H	1.85369900	-0.40266500	4.20799900
H	3.33541900	0.43635900	3.71233300
H	1.70133600	-2.98284300	3.87432800
H	3.07554600	-3.84378800	3.17732900
H	1.26779400	-3.53549200	1.47253400
H	2.69452000	-2.49550900	-0.31422300
H	3.63702900	-3.57253200	0.70998200
H	-3.97081200	4.14172300	-1.03453900
H	-1.41790000	5.03187600	-0.88204000
H	-0.27662600	3.69099900	-0.67554500
H	-1.47269100	3.65050100	-1.97490300
H	1.04913400	-1.57428100	-3.11428400
H	1.66047700	5.10212400	-0.97347000
H	2.81448100	5.92416700	-2.04134100
H	1.44123000	5.03430000	-2.73495900
H	0.35080900	4.05678800	1.85353000
H	-0.42984400	3.17794900	3.17820800
H	3.54946300	3.75001200	-2.96774700
H	3.23978100	-1.99344900	-4.13528800
H	4.64074000	2.78331700	-0.88115900
H	4.78059700	4.55174800	-0.94775300
H	3.56975500	3.79321400	0.10593900
H	4.51240300	1.95594800	-3.04201700
H	4.99029700	-0.20596000	-4.08399000
H	-4.95268800	1.79249500	2.41053800
H	-1.95940100	1.73521700	3.92387600

H	-3.35698600	0.69552700	3.65532800
H	-1.79584700	0.29167400	2.92467100
H	-6.59694100	2.31728700	0.00037300
H	-6.63063100	3.48503900	1.32308000
H	-6.26926400	4.02386800	-0.32679000
C	-1.01387100	0.01050500	-2.11370400
C	-1.79157200	-1.01618400	0.53730100
H	-1.96959500	0.44910000	-1.84916900
H	-1.04347800	-0.92015300	-2.66699400
C	-2.45487400	-2.36862100	0.65340200
H	-1.74859100	-3.17951200	0.46280000
H	-2.79307000	-2.45910100	1.70023600
C	-3.66237200	-2.45664900	-0.26752200
C	-4.93734300	-2.06038900	0.15840200
C	-3.50759200	-2.91692400	-1.58386500
C	-6.03313300	-2.12423000	-0.70488700
H	-5.07545300	-1.71193200	1.18014600
C	-4.60173400	-2.98393600	-2.44770000
H	-2.52293300	-3.22747800	-1.92187000
C	-5.86823500	-2.58645200	-2.01198700
H	-7.01666800	-1.82195700	-0.35328500
H	-4.46530000	-3.35242100	-3.46129400
H	-6.72071700	-2.64271300	-2.68392600
H	-2.49438100	-0.19066500	0.70854800
N	0.41636500	-3.71858500	-1.12515900
O	1.12124100	-4.22828900	-1.99947200

TS7

B3LYP SCF energy: -2153.009228 a.u.
B3LYP enthalpy: -2152.10931 a.u.
B3LYP free energy: -2152.237417 a.u.
M06 SCF energy in solution: -2152.108297 a.u.
M06 enthalpy in solution: -2151.208379 a.u.
M06 free energy in solution: -2151.336486 a.u.

Cartesian coordinates

Ru	0.27065300	0.45093000	-0.60182900
O	1.79668700	-0.66766800	3.02002500
O	-0.32032100	4.16687700	-1.06944200
O	0.86226200	2.51049900	-0.23289100
N	1.41114500	-2.07501600	-1.39873000
N	-0.45183500	-2.65082800	-0.39854900
C	0.29855300	-1.57286300	-0.80184200
C	1.57854100	-3.51807100	-1.22512100
C	2.49068500	-1.15491100	-1.75600800
C	3.52482800	-1.04323100	-0.60377700
C	4.59113100	0.01407800	-0.95158000
C	5.30647400	-0.39894300	-2.25425400
C	4.27606300	-0.50203700	-3.39838400
C	3.22538000	-1.58111300	-3.04654300
C	3.58295400	0.86431100	-3.58372600
C	2.86128000	1.27911600	-2.27327400
C	1.80327300	0.20408800	-1.97106300
C	3.89951100	1.37786600	-1.13827500
C	-1.85617500	-2.68823200	-0.08830800
C	-2.27797000	-2.88061700	1.23784100
C	-3.65491000	-2.95250300	1.49924200
C	-1.30867300	-3.04085900	2.38633600
C	-0.15693400	0.35785600	1.39177700
C	0.50712400	1.22589300	2.40390900
C	0.19626800	2.58090500	2.60045500
C	2.40209700	-2.84303200	3.74536500
C	0.17237900	-3.93861400	-0.77982300
C	2.73524100	-1.35926100	3.86453600
C	1.49508600	0.65394800	3.25080800
C	-2.79760300	-2.64994000	-1.14522200
C	-4.60802400	-2.86515000	0.48637200
C	0.80241200	3.34488700	3.59484300
C	4.17603700	-1.05628500	3.44687300
C	2.10562100	1.41963800	4.25136500
C	1.75598900	2.75966400	4.42352300
C	-4.15454900	-2.73098500	-0.83339100
C	-2.36666100	-2.51584100	-2.58914800
C	-6.08653500	-2.89778500	0.79263000
H	1.11564600	0.12118200	-2.83974500
H	-0.17163100	-0.67136900	1.73676100
H	1.89500200	-4.00305700	-2.15293300
H	2.33223400	-3.73025200	-0.45437700
H	3.00181800	-0.77282900	0.32223400
H	4.00198500	-2.02114100	-0.44072600
H	5.32034400	0.07181600	-0.13231800
H	5.82050800	-1.36177000	-2.11925300
H	6.07634900	0.34080800	-2.51083900
H	4.78310300	-0.79135700	-4.32831300
H	2.49956000	-1.69544600	-3.86306900
H	3.72354100	-2.55264000	-2.91042300
H	2.86456700	0.81531600	-4.41417400
H	4.32758700	1.62641900	-3.85181800
H	2.38940800	2.25431300	-2.40958500
H	3.40506800	1.69877300	-0.21590100
H	4.64209400	2.14750600	-1.38642300
H	-3.98261300	-3.08557700	2.52849000
H	-1.46981200	-4.00164000	2.89139100
H	-0.27023400	-2.99569000	2.05569400
H	-1.45064800	-2.25624200	3.13911200
H	-0.52483400	3.05676500	1.94770800
H	2.51021300	-3.17647800	2.70694000
H	3.08097800	-3.43540400	4.36849700
H	1.37512000	-3.03780900	4.06850500
H	0.17674900	-4.62792300	0.06982500
H	-0.39426600	-4.40847700	-1.59293300
H	2.56980500	-1.04663200	4.90367900
H	0.53522200	4.39086500	3.71160700
H	4.38558600	0.01662100	3.46524100
H	4.88013900	-1.55537700	4.12275900
H	4.35801000	-1.42044300	2.42997300
H	2.86030900	0.98779500	4.89668900
H	2.24182700	3.34021700	5.20322600
H	-4.88094100	-2.68627600	-1.64230300
H	-1.82021400	-3.40100400	-2.93811200
H	-3.23824000	-2.39679000	-3.23956500
H	-1.70971700	-1.65329500	-2.74223500
H	-6.51879900	-1.89041100	0.73321900
H	-6.63088200	-3.52643800	0.07869900
H	-6.28016000	-3.28078100	1.79954300
C	-1.55359300	0.78541100	0.79782200
C	-1.71983100	0.60113700	-0.77304400
H	-2.28625500	0.10717500	1.24426400
H	-1.78415400	1.81700300	1.05414900
H	-2.26997100	-0.31275100	-0.97764700
C	-2.32840100	1.77145300	-1.54997400
H	-1.69314900	2.65610700	-1.47063200
H	-2.36253200	1.47813900	-2.60898100
C	-3.73448200	2.11112300	-1.07945300
C	-4.82428000	1.27775900	-1.37295000
C	-3.96571300	3.26861300	-0.32256700
C	-6.10724200	1.58706500	-0.91926600
H	-4.66669000	0.38156600	-1.96987300
C	-5.24850500	3.58068300	0.13416600
H	-3.13270100	3.93411900	-0.10909600
C	-6.32350300	2.74019900	-0.16038300
H	-6.94084100	0.93332400	-1.16565400
H	-5.40800200	4.48617600	0.71431500
H	-7.32270400	2.98476200	0.19072400
N	0.79622600	3.67049200	-0.83831400
O	1.85633100	4.24061000	-1.10639100

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B3LYP SCF energy: -2153.01347 a.u.
B3LYP enthalpy: -2152.112533 a.u.
B3LYP free energy: -2152.242855 a.u.
M06 SCF energy in solution: -2152.112201 a.u.
M06 enthalpy in solution: -2151.211264 a.u.
M06 free energy in solution: -2151.341586 a.u.

Cartesian coordinates

Ru	0.27660900	0.45368700	-0.68281800
O	1.98283700	-0.42863400	2.89233000
O	-0.81853700	3.86863400	-0.29573100
O	0.79913000	2.53294000	-0.99852100
N	1.43520900	-2.14123300	-1.21203100
N	-0.39236100	-2.61587600	-0.09746300
C	0.33277000	-1.58302200	-0.64440200
C	1.63032700	-3.54930400	-0.86650700
C	2.49436600	-1.25735200	-1.70018900
C	3.54928300	-0.99926700	-0.59195000
C	4.58857100	0.02826700	-1.07828900
C	5.28993400	-0.51977700	-2.33811500
C	4.24152500	-0.77532500	-3.44126300
C	3.21476000	-1.82114800	-2.94625800
C	3.52478700	0.55055800	-3.77319000
C	2.81535400	1.10364000	-2.50910600

C	1.78075100	0.05532100	-2.06314800
C	3.86633400	1.34895600	-1.40867500
C	-1.79462100	-2.63662800	0.22734800
C	-2.20691600	-2.67648300	1.56947700
C	-3.58208200	-2.72209300	1.84708900
C	-1.23121300	-2.70210200	2.72321300
C	-0.06365700	0.51804300	1.32064700
C	0.66537100	1.43988900	2.23845400
C	0.36553800	2.80341400	2.38488000
C	2.58415800	-2.56245100	3.74349200
C	0.24073200	-3.93200900	-0.34386100
C	2.93999100	-1.07912300	3.75037900
C	1.70091100	0.90794400	3.05804400
C	-2.74357500	-2.73160900	-0.81989400
C	-4.54210200	-2.75871600	0.83809500
C	1.04067100	3.61864700	3.29236500
C	4.37247000	-0.83024500	3.27215100
C	2.37405400	1.72488700	3.97322900
C	2.04312600	3.07636300	4.08976500
C	-4.09747400	-2.78394400	-0.49111800
C	-2.32382000	-2.76001700	-2.27299500
C	-6.01881900	-2.75246000	1.15343100
H	1.08736300	-0.14182500	-2.90655300
H	-0.07976800	-0.47981300	1.74770000
H	1.93767700	-4.14024000	-1.73398000
H	2.40153600	-3.65368600	-0.09072000
H	3.04242000	-0.63740600	0.31063900
H	4.04823300	-1.94487800	-0.33160100
H	5.33014800	0.19436900	-0.28531700
H	5.82659800	-1.44998700	-2.10138100
H	6.03886800	0.19934100	-2.69573400
H	4.73786400	-1.16524000	-4.33970400
H	2.47748000	-2.03950900	-3.73069900
H	3.73116900	-2.76322000	-2.70845400
H	2.79554800	0.39654100	-4.58071200
H	4.25592300	1.28447300	-4.14012500
H	2.31051000	2.04264200	-2.74375500
H	3.37836700	1.75846300	-0.51687200
H	4.59230100	2.09970500	-1.74909400
H	-3.90250200	-2.73050400	2.88714300
H	-1.33639600	-3.63521000	3.29175200
H	-0.19698400	-2.61972200	2.38756600
H	-1.42199000	-1.87905100	3.42194700
H	-0.40052300	3.24711000	1.76192900
H	2.64275800	-2.96575000	2.72601100
H	3.28320600	-3.12203600	4.37461200
H	1.57070900	-2.72188100	4.12320800
H	0.27354900	-4.51937900	0.57855700
H	-0.33677100	-4.49814700	-1.08498800
H	2.81148600	-0.69514900	4.77058300
H	0.78020800	4.67009700	3.36733500
H	4.59616600	0.23736200	3.19881600
H	5.08734500	-1.28326600	3.96892900
H	4.52543900	-1.27756500	2.28425300
H	3.16343600	1.32409600	4.59648900
H	2.57982400	3.69561800	4.80360500
H	-4.82941200	-2.83746500	-1.29435800
H	-1.79340100	-3.68596900	-2.52873000
H	-3.19962600	-2.69831100	-2.92564100
H	-1.65565000	-1.92932800	-2.52269600
H	-6.46150800	-1.77813200	0.90916200
H	-6.55755200	-3.50877900	0.57064900
H	-6.20427800	-2.94557600	2.21460200
C	-1.48342000	0.91519800	0.74545500
C	-1.72014600	0.55271300	-0.79006500
H	-2.19857000	0.29166500	1.28945500
H	-1.68530100	1.97171400	0.89067900
H	-2.24263900	-0.39649100	-0.86716900
C	-2.41603700	1.59241600	-1.67404800
H	-1.86970500	2.53490100	-1.66113400
H	-2.40728800	1.20319800	-2.70165900
C	-3.85629800	1.83041200	-1.24389500
C	-4.87318500	0.92694800	-1.58556000
C	-4.19285200	2.95339900	-0.47396600
C	-6.18847700	1.13186600	-1.16507100
H	-4.63346100	0.05913300	-2.19676300
C	-5.50781500	3.16096600	-0.05149100
H	-3.41801000	3.67158500	-0.21984600
C	-6.50992500	2.25031400	-0.39208100
H	-6.96443000	0.42534700	-1.45095200
H	-5.74985300	4.04088800	0.53939600
H	-7.53399600	2.41503400	-0.06693500
N	0.33114100	3.73256200	-0.76995600
O	1.05715300	4.68297900	-1.04977200

TS8

B3LYP SCF energy: -2152.995864 a.u.
B3LYP enthalpy: -2152.097671 a.u.
B3LYP free energy: -2152.22723 a.u.
M06 SCF energy in solution: -2152.092759 a.u.
M06 enthalpy in solution: -2151.194566 a.u.
M06 free energy in solution: -2151.324125 a.u.

Cartesian coordinates

Ru	-0.15639000	-0.61498600	-0.38087400
O	-2.25805900	1.39195000	2.40539500
O	0.86361900	-3.65295700	1.15097100
O	-0.71502100	-2.69682200	-0.06686000
N	-1.26072700	1.65706300	-1.76089400
N	0.47037100	2.49202800	-0.69808400
C	-0.21954200	1.32837900	-0.95720400
C	-1.46822800	3.09868200	-1.89492000
C	-2.24219900	0.62198000	-2.10759500
C	-3.39925300	0.60231200	-1.07793800
C	-4.36193700	-0.56067100	-1.38630700
C	-4.93788500	-0.37483700	-2.80485700
C	-3.78497000	-0.35898600	-3.83006200
C	-2.83937200	0.82638600	-3.51739100
C	-3.01478800	-1.69522100	-3.74482900
C	-2.42516300	-1.87613900	-2.32241300
C	-1.45269800	-0.70750200	-2.06266400
C	-3.58277400	-1.88811800	-1.30336900
C	1.85097000	2.59817200	-0.30579900
C	2.18458000	3.05331500	0.98134100
C	3.54022600	3.14984600	1.33024100
C	1.14364000	3.47709900	1.99138400
C	0.06879500	0.01013700	1.76532000
C	-0.98888500	-0.61340400	2.60425900
C	-0.85095500	-1.89418000	3.16575500
C	-2.65688500	3.71191800	2.75312500
C	-0.11839700	3.64839800	-1.41220200
C	-3.23949500	2.31288600	2.92565000
C	-2.15545900	0.12762900	2.93659300
C	2.86648800	2.33989600	-1.25913600
C	4.56111100	2.83585300	0.43503500
C	-1.82187900	-2.44842300	3.99432600
C	-4.57990700	2.15797200	2.20443900
C	-3.12967500	-0.42893300	3.77538800
C	-2.96458500	-1.71209900	4.29725500
C	4.19954100	2.45101200	-0.86275500
C	2.54851900	1.98257700	-2.69553400
C	6.01454700	2.90015900	0.84068800
H	-0.73836700	-0.67821900	-2.90202700
H	0.01371200	1.09088000	1.75504200
H	-1.69810300	3.38010000	-2.92618100
H	-2.29838000	3.43207200	-1.25622300
H	-2.98462400	0.50206100	-0.06669300
H	-3.94091600	1.55993900	-1.11113200
H	-5.17905400	-0.55794500	-0.65216500
H	-5.51274400	0.56099600	-2.86472100
H	-5.63308400	-1.19231400	-3.03835600
H	-4.19263600	-0.22788500	-4.84132600
H	-2.02897700	0.87817900	-4.25722600
H	-3.40403500	1.76945900	-3.57984800
H	-2.21073300	-1.71679300	-4.49386400
H	-3.69507100	-2.52548500	-3.98322400
H	-1.88308000	-2.82408000	-2.26077900
H	-3.18651600	-2.04370000	-0.29450400
H	-4.25662300	-2.72976300	-1.51501500
H	3.79625200	3.48223100	2.33444900
H	1.25489900	4.54301100	2.22904300
H	0.12925800	3.31359800	1.62639600
H	1.25656000	2.92626800	2.93248300
H	0.03611900	-2.47404300	2.94155200
H	-2.47136100	3.92179200	1.69343400
H	-3.35816600	4.46319100	3.13268500
H	-1.71367700	3.81104000	3.29812600
H	-0.21792400	4.50571000	-0.73969900
H	0.52491600	3.94748800	-2.24924800
H	-3.36316300	2.11416700	3.99761800
H	-1.68199200	-3.44743600	4.39496800
H	-4.95698000	1.13322400	2.26171800

H	-5.32765700	2.82447300	2.64980700
H	-4.47363300	2.41879700	1.14642600
H	-4.02686100	0.12466300	4.02220900
H	-3.73549900	-2.12711500	4.94095100
H	4.98053400	2.22848400	-1.58675700
H	2.25121800	2.86999700	-3.26994900
H	3.43033900	1.56388100	-3.19010900
H	1.73572600	1.25599300	-2.77860900
H	6.45071600	1.89430100	0.88890100
H	6.60740300	3.47486600	0.11913900
H	6.13655200	3.36391300	1.82443100
C	1.33116300	-0.55905700	1.48353000
C	1.64632200	-0.84561500	-0.80110600
H	2.17645800	0.11219400	1.37867300
H	1.55846900	-1.58279500	1.75302700
H	2.32845600	0.00340200	-0.88987000
C	2.31289700	-2.14646600	-1.19902500
H	1.73835300	-3.00497100	-0.85365400
H	2.28916800	-2.15405800	-2.30268500
C	3.75613600	-2.23459100	-0.72942400
C	4.77878100	-1.55569800	-1.40718000
C	4.08622100	-2.98174600	0.41030500
C	6.09878500	-1.61357800	-0.95684200
H	4.54164200	-0.98833900	-2.30546600
C	5.40662500	-3.04181000	0.86127100
H	3.30203500	-3.52267600	0.93177200
C	6.41651300	-2.35638500	0.18260700
H	6.88025100	-1.08952200	-1.50198400
H	5.64659500	-3.63135200	1.74255500
H	7.44432900	-2.40807800	0.53253700
N	-0.29279700	-3.69034400	0.66888200
O	-1.05784300	-4.63498600	0.84458900

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B3LYP SCF energy: -2152.999554 a.u.
B3LYP enthalpy: -2152.100756 a.u.
B3LYP free energy: -2152.233857 a.u.
M06 SCF energy in solution: -2152.09433 a.u.
M06 enthalpy in solution: -2151.195532 a.u.
M06 free energy in solution: -2151.328633 a.u.

Cartesian coordinates

Ru	0.02302000	-0.57235400	0.08829800
O	-3.05225600	2.05079900	1.21895000
O	1.20805200	-2.00755900	2.92577700
O	-0.40157900	-2.20322900	1.42081800
N	-0.93322800	0.39727800	-2.43443800
N	0.37052700	2.02397500	-1.75060200
C	-0.10690100	0.77832400	-1.43213700
C	-1.22810500	1.47052000	-3.38555500
C	-1.63350800	-0.89109300	-2.32798400
C	-2.99852000	-0.71667400	-1.61511300
C	-3.67332300	-2.08894000	-1.42484100
C	-3.89052500	-2.74317900	-2.80460200
C	-2.52933900	-2.92173100	-3.50826700
C	-1.87821300	-1.53291400	-3.71117500
C	-1.62192200	-3.81792300	-2.63693000
C	-1.39202400	-3.15183200	-1.25563000
C	-0.68690300	-1.79971000	-1.49409600
C	-2.75711100	-2.97475200	-0.55860700
C	1.53196600	2.65697600	-1.18997300
C	1.37551100	3.78414600	-0.36100500
C	2.52045300	4.38557600	0.17587900
C	0.02301200	4.39292500	-0.07007000
C	-0.46395900	1.23671500	1.77555000
C	-1.60169900	0.76297500	2.58979100
C	-1.42765500	-0.07912300	3.70188000
C	-3.88226300	4.09940600	0.34555400
C	-0.08385300	2.45236300	-3.09221000
C	-4.27471000	2.79019600	1.02323900
C	-2.91714500	1.21105700	2.29691100
C	2.82137800	2.20223700	-1.54671600
C	3.80538400	3.91513700	-0.10196300
C	-2.49724100	-0.48933800	4.48960700
C	-5.27096000	1.98276300	0.19008700
C	-3.99473500	0.80088700	3.09289000
C	-3.78283300	-0.04709600	4.18018100
C	3.93234500	2.83211900	-0.97843800
C	3.04268100	1.11143200	-2.57299300
C	5.02281200	4.54764300	0.53064100
H	0.18716600	-1.99406400	-2.13461200
H	-0.71141800	2.04131500	1.09513100
H	-1.22396100	1.11034900	-4.41735900
H	-2.21303300	1.91406800	-3.18034800
H	-2.84738700	-0.22934700	-0.64154200
H	-3.64473900	-0.05133900	-2.20794200
H	-4.64161400	-1.94892800	-0.92555700
H	-4.55848500	-2.12394000	-3.42118400
H	-4.38027100	-3.71868900	-2.68409500
H	-2.68015900	-3.38782700	-4.49107700
H	-0.92367900	-1.63018300	-4.24617800
H	-2.54069300	-0.90736900	-4.32914800
H	-0.66004600	-3.98535700	-3.14144800
H	-2.09214400	-4.80390500	-2.51243300
H	-0.75529900	-3.79237100	-0.63660600
H	-2.61193400	-2.53245100	0.43177200
H	-3.22574300	-3.95681200	-0.40499000
H	2.39902800	5.24650800	0.83049900
H	-0.11335300	5.31921000	-0.64482300
H	-0.79567300	3.71860900	-0.32586200
H	-0.07032900	4.65698300	0.98893700
H	-0.42901000	-0.42103500	3.94937400
H	-3.41886100	3.90461700	-0.62821900
H	-4.76825400	4.72336700	0.18456000
H	-3.17124400	4.65706900	0.96254800
H	-0.40407400	3.49801400	-3.07887000
H	0.73535800	2.35286200	-3.81696600
H	-4.70238900	3.01818000	2.00758200
H	-2.32605700	-1.15355300	5.33055100
H	-5.49766400	1.01802500	0.65264200
H	-6.20917100	2.53797000	0.07562600
H	-4.86011900	1.79079900	-0.80694400
H	-5.00307700	1.12634400	2.86862300
H	-4.63199400	-0.35999700	4.78183800
H	4.92567100	2.46938200	-1.23489000
H	3.15175500	1.54431000	-3.57721200
H	3.96359000	0.55990700	-2.35911800
H	2.22105700	0.39322400	-2.61047500
H	5.31547100	4.01125800	1.44283200
H	5.88347000	4.52696300	-0.14663500
H	4.83407100	5.58928000	0.81050500
C	0.85825500	0.92756700	1.94924200
C	1.81911900	-0.87341300	-0.09874400
H	1.61183300	1.51288600	1.43519500
H	1.20715200	0.21626400	2.68734900
H	2.53862900	-0.04777400	-0.17723100
C	2.45476500	-2.24326500	-0.17060500
H	1.86410400	-2.95534800	0.41338700
H	2.36124300	-2.56867700	-1.22183400
C	3.91514800	-2.26071500	0.23828200
C	4.93192400	-2.18515600	-0.72337300
C	4.27140200	-2.32045000	1.59389200
C	6.27637600	-2.16619000	-0.34525600
H	4.66885000	-2.15606100	-1.77948400
C	5.61491600	-2.30242800	1.97225600
H	3.48743800	-2.38623100	2.34352400
C	6.62129900	-2.22316600	1.00619100
H	7.05191500	-2.11556200	-1.10568100
H	5.87627500	-2.35513600	3.02618100
H	7.66658100	-2.21284500	1.30432400
N	0.14380500	-2.55217600	2.56155700
O	-0.42811000	-3.41928300	3.21824400

TS9

B3LYP SCF energy: -2152.996154 a.u.
B3LYP enthalpy: -2152.099306 a.u.
B3LYP free energy: -2152.235497 a.u.
M06 SCF energy in solution: -2152.084345 a.u.
M06 enthalpy in solution: -2151.187497 a.u.
M06 free energy in solution: -2151.323688 a.u.

Cartesian coordinates

Ru	0.24404600	-0.50266300	-0.00450200
O	-4.11669600	1.90053600	0.96404100
O	0.98267900	-1.08980600	3.10607200
O	-0.39138900	-1.82732800	1.53595300
N	-0.32636600	0.09361600	-2.73968100
N	0.88397200	1.81089900	-2.11257800
C	0.35242400	0.62507500	-1.69468400
C	-0.46600000	1.01905000	-3.86640400
C	-1.04780500	-1.17044200	-2.53319700
C	-2.49069000	-0.90877100	-2.02774100

C	-3.19396700	-2.24643600	-1.72381300
C	-3.23815200	-3.10148300	-3.00636200
C	-1.79961800	-3.36729100	-3.49663900
C	-1.11930100	-2.01655800	-3.82206500
C	-1.01581700	-4.11118600	-2.39261400
C	-0.96035400	-3.24380000	-1.10755900
C	-0.21986900	-1.93793600	-1.45999400
C	-2.40265700	-2.98172900	-0.62519400
C	1.87251400	2.58605600	-1.41951700
C	1.47602400	3.77793100	-0.78109500
C	2.44443100	4.53226100	-0.11241800
C	0.04555400	4.26194400	-0.83805700
C	-1.48196200	1.68596100	1.68306800
C	-2.52917100	1.08351700	2.51366400
C	-2.24293500	0.38539700	3.69921900
C	-5.34711300	3.39976100	-0.38893300
C	0.64413900	2.03690900	-3.55416800
C	-5.45451600	2.17089900	0.50855100
C	-3.89050200	1.21961400	2.13057700
C	3.22541300	2.19432000	-1.44304900
C	3.78781200	4.14338300	-0.07312100
C	-3.24907700	-0.16304200	4.48733900
C	-6.03104600	0.95900300	-0.22512200
C	-4.90452500	0.67697600	2.92892800
C	-4.58016400	-0.00990200	4.10016200
C	4.15656900	2.97988100	-0.75332700
C	3.70541800	0.99738200	-2.23387600
C	4.80667000	4.94983700	0.69762600
H	0.73074800	-2.21021000	-1.94162200
H	-1.85220900	2.30241800	0.86877200
H	-0.32042800	0.51562700	-4.82538200
H	-1.46131200	1.48674400	-3.86935000
H	-2.45926400	-0.28706300	-1.12093700
H	-3.05209700	-0.34051600	-2.78479800
H	-4.21669300	-2.04517100	-1.37786700
H	-3.81735900	-2.58941800	-3.78858300
H	-3.74665000	-4.05346700	-2.80374000
H	-1.82701300	-3.97830000	-4.40860600
H	-0.10511400	-2.17950800	-4.21129400
H	-1.69317500	-1.49713100	-4.60460800
H	0.00126100	-4.34016800	-2.73987800
H	-1.50448400	-5.07274200	-2.18068600
H	-0.41035400	-3.77611800	-0.32437300
H	-2.38670700	-2.39672100	0.29957300
H	-2.89234700	-3.93689100	-0.38938500
H	2.13954000	5.44632400	0.39288300
H	-0.17616900	4.73111000	-1.80668600
H	-0.66718300	3.44366100	-0.70789000
H	-0.14351500	5.01124000	-0.06369600
H	-1.20872300	0.27148600	4.00694200
H	-4.69442300	3.19232800	-1.24446500
H	-6.33502400	3.68147500	-0.76918900
H	-4.93197200	4.24714100	0.16526400
H	0.34530100	3.07146600	-3.74392300
H	1.55909900	1.83181700	-4.12662300
H	-6.07837000	2.42115800	1.37649900
H	-2.99323000	-0.70964400	5.38922900
H	-6.04835600	0.07152900	0.41387400
H	-7.05586700	1.16465500	-0.55513400
H	-5.42344100	0.73040300	-1.10804200
H	-5.94541700	0.77142100	2.64435800
H	-5.37910000	-0.43116700	4.70459100
H	5.20022600	2.67201500	-0.75349400
H	3.98633000	1.29381400	-3.25420700
H	4.59319800	0.55561600	-1.77050100
H	2.94442400	0.21782600	-2.31272800
H	4.84440900	4.63426800	1.74854100
H	5.81285100	4.82502100	0.28407600
H	4.56394200	6.01791800	0.68780300
C	-0.14271300	1.56402700	1.83189000
C	2.02111300	-0.84158700	0.16025400
H	0.52634500	2.13817600	1.19816800
H	0.31755700	0.97776400	2.61986500
H	2.71904400	0.01049700	0.20961400
C	2.66972500	-2.19640600	0.33139900
H	1.98960100	-2.84693900	0.89482700
H	2.73718900	-2.64861000	-0.67304000
C	4.04555600	-2.15107700	0.96638700
C	5.20203400	-2.30636000	0.19065000
C	4.18348400	-1.92197000	2.34407300
C	6.47047700	-2.23642500	0.77188400
H	5.10848500	-2.49549200	-0.87735700
C	5.45027500	-1.85241100	2.92539900
H	3.29190200	-1.79795400	2.95361500
C	6.59760300	-2.00842900	2.14294100
H	7.35628200	-2.36640600	0.15484700
H	5.54097900	-1.67891200	3.99475200
H	7.58271100	-1.95690700	2.59960500
N	0.04798000	-1.85055100	2.77566200
O	-0.49187200	-2.63536500	3.55071900

TS10

B3LYP SCF energy: -2152.996818 a.u.
B3LYP enthalpy: -2152.097921 a.u.
B3LYP free energy: -2152.228146 a.u.
M06 SCF energy in solution: -2152.090067 a.u.
M06 enthalpy in solution: -2151.19117 a.u.
M06 free energy in solution: -2151.321395 a.u.

Cartesian coordinates

Ru	-0.18632400	-0.82007700	0.02231100
O	-2.55599200	2.58879900	1.50208000
O	0.61860700	-2.66483500	3.04944300
O	-0.55302500	-2.64936400	1.17456400
N	-0.99074900	0.24705700	-2.54725500
N	0.63331300	1.57892700	-1.91907100
C	-0.08388100	0.46422400	-1.55561000
C	-1.05878000	1.32949200	-3.53087000
C	-2.08159900	-0.70475400	-2.31397400
C	-3.31469000	0.02242300	-1.71442400
C	-4.40919500	-1.00322400	-1.36280700
C	-4.82839300	-1.75436600	-2.64340500
C	-3.60320000	-2.47735200	-3.24157000
C	-2.51862500	-1.43397600	-3.60523400
C	-3.05315700	-3.47684300	-2.20223100
C	-2.62064100	-2.72438700	-0.91733500
C	-1.52183000	-1.71864100	-1.30501100
C	-3.84628600	-1.99670900	-0.32759600
C	1.87198600	2.08237400	-1.38798300
C	1.86214600	3.19779900	-0.53067700
C	3.08759700	3.69863000	-0.06780600
C	0.58832600	3.89376600	-0.10885000
C	-0.69703300	0.62054500	1.15447900
C	-1.54042600	0.61997700	2.36060600
C	-1.46218300	-0.35224400	3.37284600
C	-3.07399900	4.69251400	0.54074200
C	0.25729300	2.06448900	-3.26557000
C	-3.56954300	3.61381000	1.49755300
C	-2.49321400	1.67119800	2.51813800
C	3.09692400	1.53162900	-1.83349900
C	4.30828300	3.14110000	-0.44623100
C	-2.26936000	-0.29692100	4.50584500
C	-4.92069500	3.03713900	1.07171800
C	-3.30953600	1.71607900	3.65377400
C	-3.19257300	0.73747500	4.64291800
C	4.28890500	2.06475900	-1.34145500
C	3.15808000	0.39051100	-2.82611300
C	5.61725800	3.67288800	0.08812200
H	-0.70996900	-2.28635000	-1.81708800
H	-0.55156700	1.63168300	0.77846400
H	-1.13440600	0.94391800	-4.55118800
H	-1.93132300	1.96969600	-3.34070500
H	-3.00147000	0.57277700	-0.81926800
H	-3.70578200	0.75368300	-2.43753900
H	-5.27711300	-0.47555000	-0.94412600
H	-5.25106600	-1.05089100	-3.37553900
H	-5.61519500	-2.48450500	-2.41076300
H	-3.89960800	-3.01188500	-4.15391400
H	-1.64906900	-1.92588600	-4.06184300
H	-2.92235600	-0.72578400	-4.34472400
H	-2.19932300	-4.02811700	-2.61973700
H	-3.82576600	-4.22127900	-1.96267300
H	-2.22394300	-3.43169500	-0.18691700
H	-3.56205900	-1.46873500	0.59118700
H	-4.61860600	-2.72916500	-0.05451800
H	3.07935000	4.55434900	0.60461900
H	0.68769800	4.97837800	-0.23541100
H	-0.27537900	3.55666000	-0.68418800
H	0.36006500	3.71466200	0.94885700
H	-0.73370100	-1.14772300	3.27388100
H	-2.95307500	4.28324700	-0.46841500
H	-3.79545900	5.51535900	0.49406200

H	-2.11115200	5.09364400	0.87080000
H	0.15660100	3.15363300	-3.26564500
H	1.03315600	1.79311600	-3.99282100
H	-3.64050800	4.04583500	2.50407000
H	-2.17309400	-1.05915100	5.27307800
H	-5.24164000	2.22730400	1.73272500
H	-5.68913900	3.81843500	1.08899400
H	-4.85465100	2.63992500	0.05266600
H	-4.04213500	2.50403500	3.77852200
H	-3.83341300	0.79235900	5.51915400
H	5.22956100	1.61945400	-1.65861500
H	3.22024700	0.76524500	-3.85700100
H	4.04782200	-0.22117600	-2.64872900
H	2.28377200	-0.26306100	-2.76605200
H	6.10431100	2.93491800	0.73775200
H	6.31882300	3.89885600	-0.72379300
H	5.47085000	4.58686800	0.67209900
C	1.40765300	0.05128700	1.52436700
C	1.94055700	-0.72741500	0.45356800
H	1.59781200	1.12058200	1.52191200
H	1.27726400	-0.41612600	2.49413700
H	2.42669100	-0.15958800	-0.32923700
C	2.59859100	-2.09458900	0.66554000
H	2.27410200	-2.51968900	1.61667300
H	2.29439400	-2.78736900	-0.12898200
C	4.11325400	-1.96130500	0.64197400
C	4.85749000	-2.36490500	-0.47458700
C	4.79961000	-1.41085300	1.73438700
C	6.24717500	-2.22018500	-0.50498700
H	4.34330100	-2.81090800	-1.32374700
C	6.18663400	-1.26429200	1.70936600
H	4.23946000	-1.10327800	2.61450300
C	6.91651900	-1.66644500	0.58730200
H	6.80571200	-2.54893900	-1.37802500
H	6.70014400	-0.84360700	2.57042500
H	7.99780200	-1.55739300	0.56949000
N	-0.04334900	-3.29361800	2.19086700
O	-0.25157200	-4.50237100	2.25980500

TS11

B3LYP SCF energy: -2153.006833 a.u.
B3LYP enthalpy: -2152.107628 a.u.
B3LYP free energy: -2152.236566 a.u.
M06 SCF energy in solution: -2152.096918 a.u.
M06 enthalpy in solution: -2151.197713 a.u.
M06 free energy in solution: -2151.326651 a.u.

Cartesian coordinates

Ru	-0.19869100	-0.87913600	-0.16710000
O	-2.33371100	2.34704700	2.23290200
O	0.54363500	-2.97840100	-1.02531800
O	-0.51915700	-2.82909000	0.86147200
N	-1.29314800	0.78512500	-2.26024000
N	0.58225100	1.80072100	-1.76247400
C	-0.17385300	0.68300800	-1.49604000
C	-1.43887300	2.07644700	-2.93333300
C	-2.40691600	-0.14533700	-2.04552500
C	-3.43730200	0.44115400	-1.04826300
C	-4.52524400	-0.60823900	-0.74729400
C	-5.25542600	-0.96473500	-2.05782500
C	-4.24087800	-1.53536400	-3.07012000
C	-3.15209600	-0.47527700	-3.36323800
C	-3.59840700	-2.80569200	-2.47433500
C	-2.85083800	-2.45055100	-1.16243300
C	-1.74723000	-1.43213700	-1.51264400
C	-3.86083800	-1.86769200	-0.15337300
C	1.98730300	2.00883500	-1.55087300
C	2.40307200	2.98699500	-0.62853500
C	3.77341200	3.24962100	-0.50528700
C	1.41074700	3.76750900	0.20306400
C	-0.70350600	0.40089500	1.18955400
C	-1.44631700	0.16109300	2.44858100
C	-1.36979400	-1.04262300	3.17149000
C	-2.57682800	4.68320500	1.96105500
C	-0.02120100	2.63950800	-2.82499000
C	-3.16427700	3.44984400	2.63949500
C	-2.28378300	1.19024500	2.96572400
C	2.92195400	1.34915200	-2.37677400
C	4.72711100	2.59330600	-1.28813900
C	-2.07293500	-1.23572500	4.35851300
C	-4.62134700	3.20446000	2.24391600
C	-2.99825300	0.99122000	4.15321700
C	-2.88767800	-0.21568900	4.84620600
C	4.27740600	1.65704800	-2.22573300
C	2.49249900	0.30460200	-3.38117700
C	6.20306400	2.86521000	-1.11553000
H	-1.15714700	-1.84714300	-2.34277900
H	-0.65023100	1.46906600	0.97852600
H	-1.77110500	1.95837300	-3.96838800
H	-2.17226000	2.70377200	-2.40822400
H	-2.92949000	0.74229600	-0.12734800
H	-3.89900200	1.34261900	-1.47883000
H	-5.24134800	-0.18912000	-0.02740900
H	-5.74764100	-0.07299100	-2.47276500
H	-6.04479400	-1.70364500	-1.86405800
H	-4.75471300	-1.78293100	-4.00866800
H	-2.43639100	-0.85280300	-4.10543300
H	-3.62409400	0.42416100	-3.78706700
H	-2.89971800	-3.25332900	-3.19378000
H	-4.37848800	-3.55469200	-2.27610900
H	-2.41304100	-3.36303200	-0.74769700
H	-3.35606400	-1.62443400	0.78846200
H	-4.62985600	-2.61821100	0.07817200
H	4.09942000	3.99783500	0.21410300
H	0.75310600	4.38287200	-0.42351800
H	0.76007400	3.11420800	0.79259500
H	1.93141700	4.43951900	0.89207200
H	-0.74911600	-1.84167300	2.78396200
H	-2.61166500	4.57281900	0.87146100
H	-3.14791200	5.57664100	2.23570500
H	-1.53472900	4.82994900	2.26159900
H	0.00595200	3.69646200	-2.54571400
H	0.54168900	2.52249000	-3.75987600
H	-3.08142900	3.57382100	3.72719700
H	-1.98725900	-2.17776100	4.89176500
H	-5.01063500	2.28366300	2.68760100
H	-5.25160200	4.03780800	2.57501600
H	-4.70552100	3.11951800	1.15482900
H	-3.64257100	1.76741100	4.54798800
H	-3.44778900	-0.35076600	5.76774800
H	5.00262600	1.14227000	-2.85232600
H	1.74421900	0.68656200	-4.08509300
H	3.35028500	-0.04191800	-3.96498900
H	2.04749200	-0.56533000	-2.88530000
H	6.67576500	2.08129300	-0.50931300
H	6.72263700	2.88469900	-2.07995100
H	6.37984800	3.82222400	-0.61411800
C	1.26712400	0.03433600	1.43177800
C	1.74981700	-1.14925100	0.76621500
H	1.70831500	0.98179600	1.13724600
H	1.07649400	-0.05836600	2.49750800
H	1.63395300	-2.06529400	1.34616400
C	3.01980300	-1.16632400	-0.06709700
H	3.15373700	-0.20831500	-0.56674000
H	2.92119900	-1.94152100	-0.83474300
C	4.23785200	-1.46603100	0.79481900
C	4.64710400	-2.78712400	1.02191000
C	4.96087100	-0.42954300	1.40264400
C	5.74738100	-3.06666900	1.83492700
H	4.10013800	-3.60296500	0.55381100
C	6.06241200	-0.70471800	2.21478600
H	4.65841800	0.60155400	1.23184600
C	6.45913300	-2.02590000	2.43458100
H	6.04980700	-4.09819000	1.99672400
H	6.61227300	0.11265400	2.67528100
H	7.31698100	-2.24197400	3.06601500
N	0.04927400	-3.58932900	-0.01863400
O	0.09899400	-4.80005300	0.11784500

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B3LYP SCF energy: -2153.014895 a.u.
B3LYP enthalpy: -2152.113555 a.u.
B3LYP free energy: -2152.242805 a.u.
M06 SCF energy in solution: -2152.111598 a.u.
M06 enthalpy in solution: -2151.210258 a.u.
M06 free energy in solution: -2151.339508 a.u.

Cartesian coordinates

Ru	-0.26530400	-0.72948300	-0.43089700
O	0.14133100	-2.97695300	-1.81754600
O	-0.77258500	-2.76391300	0.15720300
N	-1.25056200	1.54035000	-1.88581400

N	0.63755700	2.31080200	-1.09295600
C	-0.13692900	1.18196200	-1.19114500
C	-1.37959400	2.98294200	-2.10071100
C	-2.38200700	0.61017800	-1.95787600
C	-3.36101900	0.83649600	-0.77554400
C	-4.48428400	-0.21736800	-0.81409900
C	-5.25726100	-0.08380500	-2.14214000
C	-4.29067700	-0.30248600	-3.32459500
C	-3.17111800	0.76200600	-3.28098900
C	-3.67385900	-1.71115400	-3.21949300
C	-2.89034600	-1.84823900	-1.88731700
C	-1.76082000	-0.80133000	-1.89759400
C	-3.85663400	-1.62108000	-0.70693100
C	2.03526100	2.43432600	-0.78491100
C	2.43296800	2.98708300	0.44479500
C	3.80178300	3.19541900	0.67256700
C	1.44458100	3.36747900	1.52346800
C	0.04403100	3.46302100	-1.81115500
C	2.98850000	2.14478300	-1.78864500
C	4.76853900	2.89334100	-0.28655600
C	4.33749000	2.37508300	-1.51514600
C	2.57739000	1.57840400	-3.12903500
C	6.23929600	3.10936600	-0.01629000
H	-1.14043300	-0.94321200	-2.79522400
H	-1.70748100	3.21187000	-3.11826600
H	-2.10855400	3.41394900	-1.40073500
H	-2.81483700	0.78068000	0.17275800
H	-3.79343900	1.84609000	-0.84306600
H	-5.16624000	-0.04717900	0.02965800
H	-5.72491000	0.90907100	-2.21190200
H	-6.06852900	-0.82293600	-2.18315500
H	-4.83658100	-0.20337700	-4.27215400
H	-2.48852100	0.63977200	-4.13250900
H	-3.61529900	1.76596700	-3.35499000
H	-3.00423300	-1.90034500	-4.06922300
H	-4.46824600	-2.46937200	-3.26338200
H	-3.31835200	-1.73087400	0.24154400
H	-4.64520000	-2.38597200	-0.72075400
H	4.11253500	3.61860700	1.62573400
H	1.75948200	4.28868700	2.02558600
H	0.43711900	3.51354300	1.12816600
H	1.37491600	2.58777300	2.29230100
H	0.08134000	4.36158900	-1.18820000
H	0.60631300	3.66660900	-2.73072600
H	5.07386100	2.14014400	-2.28085200
H	2.02228900	2.30855700	-3.73152000
H	3.45833900	1.28369900	-3.70653300
H	1.93605100	0.69866100	-3.01508800
H	6.76555600	2.15167800	0.08511700
H	6.72075500	3.65527600	-0.83608700
H	6.39842800	3.67567500	0.90666800
C	-0.22126000	-0.00876900	1.45535600
C	-1.04712000	-0.61402500	2.53928600
C	-2.03919300	0.17642600	3.18053100
C	-0.88807900	-1.93562800	2.98453000
C	-2.81443100	-0.35534400	4.21667400
C	-1.65864400	-2.46837000	4.01751600
H	-0.15976500	-2.56989400	2.49365600
C	-2.62162800	-1.67473000	4.63372500
H	-3.57263600	0.24495000	4.70465000
H	-1.50817700	-3.49792900	4.32828500
H	-3.23358100	-2.07276800	5.43882500
O	-2.16617700	1.46678100	2.72192700
C	-3.03322100	2.40158700	3.38662500
H	-2.97995200	2.22327800	4.46852900
C	-4.47577600	2.25151000	2.89917900
H	-5.13367800	2.94524700	3.43540800
H	-4.53721900	2.47649200	1.82863100
H	-4.84968700	1.23563800	3.05412000
C	-2.46349600	3.78595400	3.09086700
H	-3.06954000	4.56016900	3.57403200
H	-1.43602900	3.86755500	3.45884600
H	-2.46119600	3.97451400	2.01121000
C	1.29670600	-0.51609300	1.30225100
C	1.60213200	-1.37732000	0.04150500
H	1.49231200	-1.14191200	2.17769400
H	1.94648200	0.35954300	1.31013600
H	-0.23864100	1.07466200	1.52499900
H	-2.47920400	-2.85766300	-1.83572600
H	1.51590400	-2.44060900	0.27148000
C	2.89253300	-1.13134900	-0.72396100
H	2.76990900	-1.56420500	-1.72448900
H	3.07949100	-0.06444400	-0.83804600
C	4.08169900	-1.78831600	-0.03826900
C	4.92709700	-1.05248100	0.80367300
C	4.33651100	-3.15676100	-0.21069900
C	5.99850100	-1.66632700	1.45658300
H	4.74658400	0.01122200	0.94350600
C	5.40579400	-3.77320800	0.44042000
H	3.69130000	-3.74061600	-0.86395300
C	6.24111300	-3.02946600	1.27738200
H	6.64495600	-1.07859800	2.10397200
H	5.58822200	-4.83438600	0.29141100
H	7.07518400	-3.50832600	1.78362700
N	-0.40413500	-3.53728300	-0.82822900
O	-0.60393700	-4.74325400	-0.75764700

TS12

B3LYP SCF energy: -2152.995755 a.u.
B3LYP enthalpy: -2152.095999 a.u.
B3LYP free energy: -2152.225034 a.u.
M06 SCF energy in solution: -2152.098686 a.u.
M06 enthalpy in solution: -2151.19893 a.u.
M06 free energy in solution: -2151.327965 a.u.

Cartesian coordinates

Ru	0.31795600	0.57825900	-0.58801900
O	0.91642000	4.81968400	0.23187000
O	0.63845000	2.71370700	-0.15314900
N	1.18746400	-2.02847900	-1.41975400
N	-0.67621200	-2.47663300	-0.35769400
C	0.12022900	-1.44938800	-0.81439100
C	1.26153900	-3.48284600	-1.27453700
C	2.31509200	-1.20151600	-1.85142700
C	3.42375700	-1.16506600	-0.76497300
C	4.55893300	-0.21730700	-1.19895500
C	5.15734300	-0.71853800	-2.52962700
C	4.05664900	-0.74972500	-3.61039200
C	2.93446000	-1.71676100	-3.17246400
C	3.47599500	0.66712200	-3.79108500
C	2.87259700	1.17179400	-2.45371400
C	1.74236500	0.21438600	-2.05257700
C	3.98151900	1.19895400	-1.38346900
C	-2.08382700	-2.47775900	-0.05879300
C	-2.52825500	-2.58496100	1.26982300
C	-3.90876200	-2.67586500	1.51000400
C	-1.58558700	-2.64102000	2.44956100
C	-0.10631800	-3.81100200	-0.66245900
C	-3.00725600	-2.54206300	-1.13147900
C	-4.84369600	-2.70121700	0.47677800
C	-4.36737100	-2.64625000	-0.84066300
C	-2.55426500	-2.49234400	-2.57365800
C	-6.32608900	-2.78374900	0.75639100
H	0.99211800	0.17927900	-2.87147000
H	1.42312400	-3.97198300	-2.24011700
H	2.08950900	-3.76313500	-0.61128700
H	2.98803900	-0.83036400	0.18494900
H	3.81979700	-2.17922700	-0.60558000
H	5.33644500	-0.21080400	-0.42335500
H	5.59143200	-1.72087400	-2.40055100
H	5.97345200	-0.05606300	-2.84719900
H	4.48007600	-1.10576700	-4.55902900
H	2.15517100	-1.77839400	-3.94423800
H	3.34815400	-2.72755500	-3.03936400
H	2.70786100	0.66302200	-4.57751800
H	4.26573500	1.35552700	-4.12224800
H	3.57612500	1.58109600	-0.43986500
H	4.77389500	1.89407400	-1.69045500
H	-4.25239300	-2.74645200	2.54018000
H	-1.84342800	-3.48423600	3.10142300
H	-0.54473500	-2.74756000	2.14123600
H	-1.65439200	-1.73230000	3.05987600
H	-0.03515200	-4.40751300	0.25295400
H	-0.75536200	-4.35016700	-1.36099100
H	-5.07757200	-2.68008500	-1.66422600
H	-2.02833100	-3.40884700	-2.87038200
H	-3.41443700	-2.38287700	-3.24046700
H	-1.87394400	-1.65581800	-2.75953900
H	-6.82947400	-1.84537900	0.49085300
H	-6.80012800	-3.57943200	0.16975100
H	-6.52412100	-2.97977900	1.81470100
C	0.01274700	0.44353300	1.42004800

C	0.81685400	1.17292900	2.44082800
C	1.75037400	0.43431200	3.21990200
C	0.68955000	2.54526100	2.71437600
C	2.48802200	1.06135200	4.23086000
C	1.42807000	3.17068700	3.71646900
H	0.03421000	3.14898000	2.10118300
C	2.32370400	2.42533700	4.47813000
H	3.19946200	0.50307900	4.82665200
H	1.30912400	4.23661400	3.88409800
H	2.90982800	2.89723300	5.26240900
O	1.87072000	-0.90347200	2.91685400
C	2.75763700	-1.74478700	3.67631500
H	2.67700400	-1.47438000	4.73708100
C	4.20387800	-1.58890100	3.20144100
H	4.87471400	-2.19757700	3.81879700
H	4.29701200	-1.92062100	2.16157500
H	4.53672900	-0.54901800	3.25662200
C	2.24650800	-3.17154600	3.50164200
H	2.87979700	-3.87162900	4.05740000
H	1.22038300	-3.26553800	3.86969700
H	2.26554300	-3.45786200	2.44366900
C	-1.38305800	1.01963800	0.93741300
C	-1.53507100	1.33504600	-0.61467000
H	-1.54762300	1.96538000	1.45464600
H	-2.14759100	0.28667800	1.20018900
H	-0.07805200	-0.59948900	1.70244500
H	2.47710200	2.17880200	-2.57730900
H	-1.40095300	2.40570600	-0.78319700
C	-2.79751300	0.85042900	-1.31400800
H	-2.61914700	0.89293700	-2.39688800
H	-3.01768400	-0.18404500	-1.05723600
C	-3.99528100	1.72596400	-0.97438600
C	-4.91846400	1.33329800	0.00448800
C	-4.18353300	2.96088500	-1.61169300
C	-5.99987800	2.15167300	0.33858300
H	-4.79019600	0.37604000	0.50481800
C	-5.26245800	3.78127100	-1.28076100
H	-3.47811300	3.28135700	-2.37572000
C	-6.17524100	3.37896100	-0.30294200
H	-6.70612700	1.82942500	1.09989200
H	-5.39043300	4.73440500	-1.78720400
H	-7.01632000	4.01682000	-0.04459200
N	1.27331900	3.82656900	-0.41297100
O	2.17520800	3.85300300	-1.26068400

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B3LYP SCF energy: -2153.009562 a.u.
B3LYP enthalpy: -2152.109162 a.u.
B3LYP free energy: -2152.238722 a.u.
M06 SCF energy in solution: -2152.107818 a.u.
M06 enthalpy in solution: -2151.207418 a.u.
M06 free energy in solution: -2151.336978 a.u.

Cartesian coordinates

Ru	0.42196100	-0.35866000	-0.60465300
O	2.60966600	1.24658300	-1.29458900
O	1.06923500	0.31555600	-2.53954200
N	1.10894300	-2.00554000	1.67020300
N	-0.78095600	-1.13309900	2.32415600
C	0.10580100	-1.17787100	1.27435000
C	0.91668500	-2.62183700	2.98532200
C	2.26776000	-2.27863100	0.82150800
C	3.52103500	-1.53567100	1.35423000
C	4.72737400	-1.79847100	0.43029000
C	5.00554400	-3.31231200	0.34793500
C	3.76050400	-4.03054000	-0.21102200
C	2.57649900	-3.79766400	0.75185100
C	3.42227400	-3.47072300	-1.60993000
C	3.13160800	-1.94623700	-1.51543000
C	1.91718600	-1.77743900	-0.58611300
C	4.39905100	-1.25089900	-0.97038700
C	-2.03355300	-0.44574000	2.45080600
C	-2.07109600	0.89429100	2.88656500
C	-3.31518900	1.52347900	3.01080000
C	-0.82790700	1.64376100	3.30577700
C	-0.28425400	-1.83890200	3.52403200
C	-3.23162200	-1.17558700	2.28662300
C	-4.51576400	0.85175000	2.76702300
C	-4.45062300	-0.50444700	2.43126800
C	-3.24099900	-2.66929100	2.04364900
C	-5.84277700	1.56644300	2.86955900
H	1.09399300	-2.42209900	-0.98694800
H	0.70320100	-3.69365800	2.88393800
H	1.80729100	-2.51284600	3.61203800
H	3.30470800	-0.46105700	1.39772600
H	3.74331400	-1.87307100	2.37717300
H	5.60756700	-1.28189100	0.83518700
H	5.25903300	-3.71384700	1.33983100
H	5.87038000	-3.49762600	-0.30289700
H	3.95432500	-5.10910100	-0.28130300
H	1.68312900	-4.33553800	0.40565700
H	2.83005100	-4.18993000	1.74762200
H	2.55606600	-4.00007000	-2.03092500
H	4.26465800	-3.64433800	-2.29368300
H	4.24883200	-0.17027200	-0.93338900
H	5.23756200	-1.44432600	-1.65366800
H	-3.34199400	2.56514400	3.32493400
H	-0.77856400	1.70287400	4.40196500
H	0.08753300	1.16748800	2.95307800
H	-0.82968300	2.66926200	2.92590200
H	-0.00005900	-1.10908600	4.29384300
H	-1.06126900	-2.48490600	3.94257100
H	-5.37443500	-1.06249800	2.29078200
H	-3.37968000	-3.20835600	2.99116700
H	-4.06917200	-2.95767900	1.38833400
H	-2.31059100	-3.02410700	1.59543600
H	-6.10789600	2.04361200	1.91687000
H	-6.65268200	0.87470400	3.12413700
H	-5.81602500	2.35448700	3.62963800
C	-0.36283000	1.52473100	-0.24810300
C	0.10803200	2.77056500	-0.90942200
C	0.93248300	3.67369900	-0.18604400
C	-0.23664600	3.12689500	-2.22344100
C	1.34192300	4.87976000	-0.76381600
C	0.18093500	4.32195100	-2.80604000
H	-0.82861400	2.44106400	-2.81936900
C	0.96574400	5.20332900	-2.06815000
H	1.96614900	5.57084200	-0.21012000
H	-0.10096600	4.55367700	-3.82874600
H	1.29968100	6.14206700	-2.50209500
O	1.27443400	3.29863500	1.08922500
C	2.40275800	3.91438000	1.74236000
H	2.29201100	5.00592400	1.69280000
C	3.71615100	3.48867900	1.08640500
H	4.55877300	4.00295100	1.56378300
H	3.85650400	2.40807400	1.19311600
H	3.72639200	3.71689500	0.01805700
C	2.32513600	3.49786900	3.20710800
H	3.14679600	3.95422000	3.76987500
H	1.37949300	3.81677600	3.65628300
H	2.40692000	2.40935600	3.30159900
C	-1.61418300	0.78697100	-0.84758500
C	-1.32169100	-0.62215800	-1.52064100
H	-2.03828400	1.41900400	-1.63018800
H	-2.34579400	0.64373400	-0.05247300
H	-0.46171900	1.67217800	0.82020300
H	2.89147000	-1.56310200	-2.51191100
H	-1.12863100	-0.50482400	-2.59413600
C	-2.36701800	-1.70673800	-1.28408700
H	-1.91882200	-2.67461000	-1.54865800
H	-2.62219300	-1.74650500	-0.22520400
C	-3.62404200	-1.50121400	-2.11479100
C	-4.76256600	-0.89154100	-1.56945900
C	-3.65925200	-1.89200300	-3.46152100
C	-5.90310600	-0.67747200	-2.34682000
H	-4.75610700	-0.58512600	-0.52588300
C	-4.79588800	-1.67848600	-4.24191700
H	-2.78703800	-2.37228300	-3.90068600
C	-5.92360600	-1.06948200	-3.68626100
H	-6.77714100	-0.20602100	-1.90405400
H	-4.80243600	-1.99112400	-5.28298300
H	-6.81093700	-0.90483600	-4.29176200
N	2.16658500	1.02090600	-2.44681300
O	2.70384100	1.41827400	-3.47377300

TS13

B3LYP SCF energy: -2153.000183 a.u.
B3LYP enthalpy: -2152.102342 a.u.
B3LYP free energy: -2152.231278 a.u.
M06 SCF energy in solution: -2152.093378 a.u.
M06 enthalpy in solution: -2151.195537 a.u.
M06 free energy in solution: -2151.324473 a.u.

Cartesian coordinates

Ru	-0.58091500	0.29472600	-0.48018900
O	1.52227000	-3.53337200	-0.40751100
O	-1.35771900	-1.86047300	-0.77532400
O	-1.02291100	-0.54882800	-2.46936400
N	-1.88098700	1.22988600	1.93618200
N	0.23156300	1.01653700	2.50856900
C	-0.65929800	0.85621400	1.46389200
C	-1.90951000	1.49706800	3.37527300
C	-3.08363000	0.88837400	1.16550700
C	-3.62627900	-0.50054000	1.59680500
C	-4.84763200	-0.88170800	0.73606700
C	-5.94906400	0.18449900	0.89449900
C	-5.40071600	1.55320500	0.44186900
C	-4.20682700	1.93682400	1.34689700
C	-4.95149500	1.46002000	-1.03412100
C	-3.82764200	0.39702300	-1.18060200
C	-2.64242600	0.87122600	-0.30729800
C	-4.40909100	-0.96458100	-0.73818400
C	1.49314100	0.36089700	2.69162000
C	1.52888000	-1.04339800	2.84043100
C	2.76295900	-1.65990300	3.06949100
C	0.27263100	-1.88229800	2.79580800
C	1.45236900	-0.76395200	-0.67537100
C	1.67897500	-1.64620400	-1.83865600
C	1.89965500	-1.13752000	-3.13093100
C	1.54965600	-5.21050800	1.27561500
C	-0.41595400	1.59943700	3.70644600
C	1.25562100	-4.93562700	-0.19468800
C	1.70107600	-3.05739600	-1.67817800
C	2.66308500	1.12591300	2.87203600
C	3.95063200	-0.93061500	3.18246000
C	2.13829100	-1.95845300	-4.22667100
C	-0.18262800	-5.27531200	-0.58447400
C	1.93475900	-3.88627400	-2.78509200
C	2.15300800	-3.34090300	-4.04830500
C	3.87363000	0.46144500	3.09888600
C	2.64007600	2.63669600	2.88205700
C	5.27378400	-1.62957500	3.38978200
H	-2.48325600	1.92503500	-0.58119500
H	1.54509300	-1.24991400	0.28673000
H	-2.45114700	2.42078300	3.59704800
H	-2.40050500	0.67685600	3.91715100
H	-2.83397900	-1.24797900	1.47562500
H	-3.91206700	-0.48248100	2.65883000
H	-5.22818900	-1.85761600	1.06635800
H	-6.28542900	0.23807200	1.94032800
H	-6.82503000	-0.08899300	0.29071500
H	-6.18318800	2.31740400	0.54276000
H	-3.82400000	2.93188400	1.08216500
H	-4.54463900	1.98351600	2.39349700
H	-4.59444500	2.43911900	-1.38272600
H	-5.81258400	1.19190800	-1.66303500
H	-3.51560000	0.34383600	-2.22950900
H	-3.67961500	-1.76727000	-0.86105600
H	-5.27419300	-1.21318900	-1.36925500
H	2.79200100	-2.74193100	3.17571800
H	-0.56537200	-1.38682700	3.29691400
H	-0.04448700	-2.09162500	1.76813900
H	0.44232600	-2.84040800	3.29556200
H	1.86323900	-0.06421400	-3.28747200
H	0.85606800	-4.66126600	1.91917300
H	1.43741800	-6.28004200	1.48510000
H	2.57293400	-4.91285100	1.52690800
H	-0.13609600	1.03726600	4.60194600
H	-0.09771400	2.64042300	3.84364300
H	1.96212400	-5.52479300	-0.79268600
H	2.29608000	-1.52394600	-5.20922200
H	-0.39717700	-4.99537700	-1.61937100
H	-0.36202800	-6.35083200	-0.46848000
H	-0.88416800	-4.72894500	0.05358300
H	1.94015100	-4.96318800	-2.67474900
H	2.32716300	-4.00437700	-4.89114400
H	4.77878800	1.05308700	3.22179400
H	2.46598700	3.02244600	3.89605700
H	3.59863200	3.04619000	2.54683900
H	1.85006500	3.04043200	2.24516400
H	5.70614400	-1.94772200	2.43193400
H	6.00351700	-0.97341300	3.87567100
H	5.15975200	-2.52751700	4.00697800
C	1.74406500	0.63757300	-0.70150300
C	0.20303500	1.89057900	-1.12786200
H	2.09004400	1.08198800	0.22316400
H	2.23996900	1.02853400	-1.58695800
C	0.53282700	3.25907900	-0.57011100
H	-0.42624900	3.80375400	-0.61249800
H	0.79380600	3.19102100	0.48916400
C	1.57815500	4.03538500	-1.35057900
C	1.24273400	4.65266000	-2.56502200
C	2.90327300	4.12474200	-0.90370000
C	2.20329800	5.33355000	-3.31356600
H	0.21660100	4.60345400	-2.92420000
C	3.86770300	4.80698900	-1.64869900
H	3.18332500	3.65997700	0.03834400
C	3.52124500	5.41266600	-2.85742800
H	1.92122700	5.80669200	-4.25052900
H	4.88946200	4.86624800	-1.28239300
H	4.27019700	5.94473300	-3.43771900
H	0.22632600	1.90323000	-2.23051800
N	-1.40159500	-1.70566200	-2.05054700
O	-1.79015000	-2.58085600	-2.80477900

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B3LYP SCF energy: -1650.215805 a.u.
B3LYP enthalpy: -1649.555944 a.u.
B3LYP free energy: -1649.660753 a.u.
M06 SCF energy in solution: -1649.514625 a.u.
M06 enthalpy in solution: -1648.854764 a.u.
M06 free energy in solution: -1648.959573 a.u.

Cartesian coordinates

Ru	0.65400900	0.42120200	0.69772200
O	0.10595500	-0.29999200	2.68143900
O	0.95592400	1.69514800	2.53893700
N	1.65285000	-1.39629500	-1.26040500
N	-0.39850200	-2.08406000	-0.88576500
C	0.50090800	-1.10200500	-0.58749800
C	1.65940400	-2.74855000	-1.82010400
C	2.84073100	-0.60273700	-0.92140100
C	3.57263300	-1.17874700	0.32156000
C	4.73078900	-0.24670400	0.73008600
C	5.72218800	-0.12733300	-0.44585700
C	4.99345800	0.44941100	-1.67759500
C	3.84713800	-0.50575100	-2.08679600
C	4.42946300	1.84370500	-1.32379900
C	3.42512300	1.72341600	-0.14804600
C	2.27572800	0.80439300	-0.60446900
C	4.16053900	1.14343300	1.07814400
C	-1.75900200	-2.19372200	-0.44358900
C	-2.02901700	-2.73377100	0.83206500
C	-3.36182500	-2.84378600	1.23769600
C	-0.92820800	-3.22097100	1.74417700
C	0.15770600	-3.08296800	-1.82398700
C	-2.80887700	-1.85842800	-1.32069200
C	-4.42565000	-2.46060000	0.41378500
C	-4.12726400	-1.98814700	-0.86590700
C	-2.57141300	-1.41913700	-2.74958900
C	-5.85363300	-2.56002700	0.89759100
H	1.88468200	1.19788700	-1.55106500
H	2.09884400	-2.77026700	-2.82122900
H	2.22957600	-3.43759000	-1.17993800
H	2.86035400	-1.28299100	1.15502900
H	3.95410800	-2.18719400	0.10543800
H	5.24306600	-0.66948500	1.60427500
H	6.15032900	-1.11159500	-0.68367400
H	6.55973700	0.52533600	-0.16532200
H	5.69799400	0.53743500	-2.51498600
H	3.33423800	-0.13076100	-2.98234500
H	4.26262200	-1.49423100	-2.33503500
H	3.93153500	2.28360600	-2.19874600
H	5.25513700	2.51731400	-1.05358700
H	3.47443700	1.07379800	1.93154900
H	4.97508500	1.81570300	1.38119300
H	-3.57366200	-3.25314700	2.22329600
H	-1.32531200	-3.94300700	2.46489900
H	-0.12443300	-3.70941100	1.18266200
H	-0.48139300	-2.39825100	2.31009900
H	-0.05816500	-4.09662000	-1.47396900
H	-0.28449700	-2.96391500	-2.82083300
H	-4.93985900	-1.71783900	-1.53750700
H	-2.66777600	-2.26891400	-3.43936800

H	-3.31223500	-0.67322700	-3.05576800
H	-1.57836700	-0.98808900	-2.89692800
H	-6.10623500	-1.72010400	1.55797200
H	-6.56241900	-2.54678700	0.06328500
H	-6.01940900	-3.47965500	1.47001100
C	-0.43672600	1.65895300	-0.05615900
H	3.02809500	2.71643000	0.09754800
H	-0.39362300	2.62039800	0.48726300
C	-1.35662900	1.68297500	-1.24806400
H	-0.76344400	2.06738500	-2.09705600
H	-1.65261200	0.66703800	-1.51105800
C	-2.57693500	2.56278300	-1.04532000
C	-3.73089800	2.04577900	-0.43917300
C	-2.56374600	3.91269900	-1.42026800
C	-4.84342900	2.85883800	-0.21646400
H	-3.75579000	0.99925000	-0.14441700
C	-3.67451200	4.72860700	-1.19716200
H	-1.67682800	4.32756900	-1.89520400
C	-4.81883600	4.20329000	-0.59410200
H	-5.73065000	2.44160500	0.25317500
H	-3.64638200	5.77303000	-1.49717700
H	-5.68501800	4.83629400	-0.42058400
N	0.48780100	0.78639700	3.30815800
O	0.40457000	0.89214800	4.50963100

TS14

B3LYP SCF energy: -2152.986593 a.u.
B3LYP enthalpy: -2152.088973 a.u.
B3LYP free energy: -2152.221645 a.u.
M06 SCF energy in solution: -2152.085151 a.u.
M06 enthalpy in solution: -2151.187531 a.u.
M06 free energy in solution: -2151.320203 a.u.

Cartesian coordinates

Ru	0.24463500	0.59900000	-0.23411000
O	0.55320100	3.99705900	-0.16463600
O	1.13222600	2.17296700	0.94198900
N	0.90576300	-1.35540000	-2.23050000
N	-0.86885500	-2.24455100	-1.30603800
C	-0.07844100	-1.11373300	-1.31980300
C	0.95625400	-2.73986900	-2.70188500
C	2.03283700	-0.41942800	-2.33405200
C	3.17031300	-0.81056000	-1.35414500
C	4.30391600	0.23387800	-1.41598000
C	4.85572700	0.29774900	-2.85478800
C	3.72288000	0.69680400	-3.82297700
C	2.60730300	-0.37160400	-3.76726800
C	3.15516700	2.07070200	-3.40852400
C	2.59387400	2.00007900	-1.96439300
C	1.45536600	0.95813200	-1.93996300
C	3.74261900	1.61072000	-1.00952300
C	-2.18414000	-2.42411900	-0.75973000
C	-2.34931900	-3.10482400	0.46355900
C	-3.64671700	-3.30793500	0.95010500
C	-1.18680700	-3.68137500	1.23965400
C	-0.42871300	-3.25075600	-2.29727200
C	-3.31277400	-2.05415900	-1.52659000
C	-4.77860100	-2.89048900	0.24671100
C	-4.58770200	-2.28080500	-0.99788600
C	-3.18812000	-1.48200000	-2.92259500
C	-6.16537200	-3.09324400	0.81148300
H	0.73156200	1.23447200	-2.72147600
H	1.13040900	-2.79430200	-3.77977400
H	1.76186500	-3.29229000	-2.19738400
H	2.76728500	-0.87170100	-0.33222800
H	3.56097900	-1.80844100	-1.60581900
H	5.10544600	-0.06334500	-0.72603600
H	5.28029200	-0.67401000	-3.14728200
H	5.67061900	1.03185100	-2.90937200
H	4.11437400	0.74749900	-4.84785500
H	1.80364900	-0.12729700	-4.47510200
H	3.02182400	-1.34774300	-4.06264500
H	2.36402000	2.37854200	-4.10636500
H	3.94688100	2.83097700	-3.46840500
H	3.38547700	1.59240100	0.02507300
H	4.53934000	2.36543800	-1.05793000
H	-3.77116200	-3.82330400	1.90077800
H	-1.27344500	-4.77432300	1.29272400
H	-0.22640200	-3.44011300	0.78182800
H	-1.17238400	-3.31148100	2.27089400
H	-0.40909900	-4.24813700	-1.84752900
H	-1.12042600	-3.27637200	-3.14883800
H	-5.45584100	-1.98256200	-1.58227700
H	-3.20564300	-2.28431500	-3.67271000
H	-4.02889700	-0.81838600	-3.14763000
H	-2.26342800	-0.91780100	-3.06292900
H	-6.44143900	-2.27251000	1.48662600
H	-6.91965900	-3.13096200	0.01875500
H	-6.23105200	-4.02182400	1.38869800
C	-0.12145700	-0.33100600	1.88081300
C	0.81171500	0.11665000	2.93588700
C	1.97589800	-0.64525600	3.20696500
C	0.56507800	1.24236400	3.73547800
C	2.83232100	-0.27974000	4.25279100
C	1.41624800	1.61211600	4.77104600
H	-0.31534100	1.84411800	3.53853300
C	2.55081700	0.84478700	5.02896700
H	3.72630700	-0.85351300	4.46269800
H	1.19911700	2.49442400	5.36511800
H	3.22972400	1.11885000	5.83192900
O	2.18747700	-1.73375900	2.39525000
C	3.23461000	-2.67619800	2.69791100
H	3.29852600	-2.78564300	3.78820100
C	4.57685700	-2.20376700	2.13599900
H	5.37183500	-2.90621300	2.41222500
H	4.53064700	-2.14832900	1.04328300
H	4.84743700	-1.21375900	2.51301200
C	2.79313000	-4.00747600	2.09754400
H	3.54269200	-4.78126000	2.29642700
H	1.83918900	-4.32951400	2.52650100
H	2.67389200	-3.91620700	1.01193900
C	-1.34605900	0.25976500	1.56899900
C	-1.30214000	1.59440900	-0.44751800
H	-1.66494300	1.17671400	2.05449500
H	-2.13423000	-0.34246600	1.13663600
H	0.00387000	-1.36807000	1.59493500
H	2.19715100	2.98139600	-1.69145900
H	-1.14092500	2.61667000	-0.08437100
C	-2.64844200	1.38809400	-1.08395300
H	-2.51554400	1.69202000	-2.13724100
H	-2.92159400	0.33294600	-1.09764900
C	-3.75564400	2.21959600	-0.45579000
C	-4.80841100	1.60308400	0.23261300
C	-3.73659400	3.61992500	-0.53926400
C	-5.81994300	2.36492500	0.82292400
H	-4.83987100	0.51779000	0.29982000
C	-4.74420000	4.38249300	0.05124700
H	-2.92556100	4.11630400	-1.06745400
C	-5.79034400	3.75717600	0.73471900
H	-6.63063900	1.86903200	1.35101700
H	-4.71250000	5.46624100	-0.02341600
H	-6.57581400	4.35158400	1.19378700
N	1.31231800	3.44239600	0.65363100
O	2.22771700	4.02413400	1.23331100

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B3LYP SCF energy: -2152.987499 a.u.
B3LYP enthalpy: -2152.088794 a.u.
B3LYP free energy: -2152.224639 a.u.
M06 SCF energy in solution: -2152.084746 a.u.
M06 enthalpy in solution: -2151.186041 a.u.
M06 free energy in solution: -2151.321886 a.u.

Cartesian coordinates

Ru	0.16199800	0.63859800	-0.24397000
O	0.46591500	4.04549300	0.09711700
O	0.99843700	2.12869300	1.05769200
N	0.89321500	-1.21680200	-2.29537700
N	-0.85557700	-2.19665700	-1.41196900
C	-0.10009100	-1.04271100	-1.37882700
C	0.99090700	-2.58211100	-2.81238700
C	1.98204600	-0.23282800	-2.36243900
C	3.12535000	-0.60553300	-1.38309000
C	4.21835500	0.48221300	-1.40662300
C	4.77954300	0.60795500	-2.83748100
C	3.63995000	0.98952000	-3.80453100
C	2.56722800	-0.12349300	-3.78772200
C	3.01633700	2.32920700	-3.35789000
C	2.44274300	2.19619600	-1.92259300
C	1.34175200	1.11399600	-1.94822200
C	3.59770100	1.82306900	-0.96762600
C	-2.17305400	-2.42288200	-0.88823900

C	-2.33925000	-3.18401100	0.28579400
C	-3.63751200	-3.42252600	0.75453700
C	-1.17684700	-3.80817000	1.02418100
C	-0.38873500	-3.13882200	-2.45269600
C	-3.30086400	-2.00790900	-1.63292800
C	-4.76837900	-2.95991900	0.07898600
C	-4.57607800	-2.26974500	-1.12292800
C	-3.17165400	-1.34864100	-2.98912500
C	-6.15621000	-3.19840100	0.62694300
H	0.63338600	1.37926200	-2.74439600
H	1.18830400	-2.59481600	-3.88745400
H	1.79943200	-3.13233000	-2.30917100
H	2.72017600	-0.71163000	-0.36560200
H	3.55380500	-1.58121800	-1.65891200
H	5.02446600	0.19809900	-0.71670300
H	5.24415800	-0.33785200	-3.15308500
H	5.56507900	1.37482300	-2.86375800
H	4.03713500	1.08371100	-4.82412400
H	1.76073200	0.10633900	-4.49708000
H	3.02278000	-1.07476300	-4.10325100
H	2.22194300	2.62787000	-4.05604100
H	3.78001100	3.11942300	-3.38704000
H	3.23574000	1.75728000	0.06311300
H	4.36347000	2.61048700	-0.98657300
H	-3.76274500	-3.99969800	1.66890500
H	-1.25652900	-4.90265300	0.99764500
H	-0.21593000	-3.52901200	0.58927100
H	-1.17007400	-3.51383100	2.07948200
H	-0.35656200	-4.15964500	-2.06034700
H	-1.07108100	-3.12572700	-3.31246500
H	-5.44354100	-1.93437400	-1.68787400
H	-3.16126500	-2.10392500	-3.78678800
H	-4.02441300	-0.69122000	-3.18457800
H	-2.25828400	-0.75685300	-3.08169000
H	-6.45412800	-2.39463500	1.31316900
H	-6.90257900	-3.23517100	-0.17345900
H	-6.21006700	-4.13823500	1.18667000
C	-0.09462100	-0.54983700	1.99066800
C	0.91882600	-0.13044600	2.97320400
C	2.10500000	-0.89309200	3.12532500
C	0.73117200	0.97142900	3.82242400
C	3.04227700	-0.55013100	4.10799800
C	1.66215400	1.31737000	4.79425700
H	-0.16677600	1.56890100	3.71274000
C	2.81827500	0.55034200	4.93512300
H	3.95347700	-1.12262100	4.22828200
H	1.49185100	2.18145900	5.42865300
H	3.55936200	0.80737200	5.68717700
O	2.25606000	-1.95544300	2.26926600
C	3.31329900	-2.91363800	2.47287500
H	3.45686400	-3.04690100	3.55280100
C	4.61417900	-2.43998000	1.82199500
H	5.41966900	-3.15698400	2.01900100
H	4.48543400	-2.35616600	0.73767700
H	4.92513700	-1.46260000	2.20122800
C	2.81431400	-4.22686600	1.87828800
H	3.56630800	-5.01284800	2.00791900
H	1.88872700	-4.54673400	2.36667200
H	2.62023500	-4.11126400	0.80585200
C	-1.29395500	0.06023600	1.73021900
C	-1.32282700	1.65226000	-0.60564000
H	-1.58286700	0.99334200	2.20255500
H	-2.07590300	-0.47583900	1.20785800
H	0.06354000	-1.53966500	1.58105500
H	2.00726500	3.15338000	-1.62169400
H	-1.08670900	2.71273100	-0.43336200
C	-2.73953700	1.40549300	-1.03843300
H	-2.77895600	1.68187800	-2.10729500
H	-3.00025500	0.34852900	-0.97579800
C	-3.74908100	2.24308400	-0.26631000
C	-4.66126300	1.62885700	0.60150900
C	-3.77899900	3.63964200	-0.39226000
C	-5.58299700	2.38868700	1.32590500
H	-4.65450700	0.54579300	0.70268600
C	-4.69693100	4.40072000	0.33133500
H	-3.07709300	4.13522400	-1.05895400
C	-5.60279000	3.77764000	1.19365400
H	-6.28475100	1.89393600	1.99278300
H	-4.70424200	5.48190800	0.22157700
H	-6.31802200	4.37116900	1.75682000
N	1.18518400	3.41920100	0.89913300
O	2.06492900	3.94631400	1.57775800

TS15

B3LYP SCF energy: -2153.00546 a.u.
B3LYP enthalpy: -2152.105612 a.u.
B3LYP free energy: -2152.234133 a.u.
M06 SCF energy in solution: -2152.105161 a.u.
M06 enthalpy in solution: -2151.205313 a.u.
M06 free energy in solution: -2151.333834 a.u.

Cartesian coordinates

Ru	0.32518600	0.53366300	-0.52032500
O	-0.19908600	4.11373900	-0.69844500
O	1.19190000	2.50338900	-0.11369800
N	1.21638400	-1.98592100	-1.54577600
N	-0.65024300	-2.54087300	-0.54256800
C	0.13665000	-1.47207000	-0.89738200
C	1.30762500	-3.44652900	-1.50421100
C	2.34256600	-1.11665700	-1.89796400
C	3.44802100	-1.16301700	-0.80769600
C	4.57656900	-0.17222900	-1.15593100
C	5.18089400	-0.54817400	-2.52446500
C	4.08144200	-0.49004500	-3.60550400
C	2.96973600	-1.50572400	-3.25727300
C	3.49153800	0.93519800	-3.66054700
C	2.88402300	1.31292100	-2.28336600
C	1.76168700	0.30639500	-1.98121900
C	3.99288200	1.25207100	-1.21424300
C	-2.04710700	-2.56257400	-0.20362400
C	-2.44761800	-2.78778400	1.12413100
C	-3.81944600	-2.89747000	1.40084000
C	-1.46324100	-2.94652200	2.26011300
C	-0.08550100	-3.83389000	-0.99428200
C	-3.00441600	-2.51331000	-1.24597600
C	-4.78738100	-2.82326000	0.40071200
C	-4.35503600	-2.63786300	-0.92020500
C	-2.59808600	-2.33356100	-2.69203600
C	-6.25993900	-2.94439900	0.71728400
H	1.01658700	0.33476100	-2.80643800
H	1.52996300	-3.86275100	-2.49118800
H	2.10133600	-3.76398500	-0.81524900
H	3.00733500	-0.91270300	0.16607900
H	3.85246800	-2.18359000	-0.73380900
H	5.35310300	-0.22900100	-0.38132900
H	5.62129400	-1.55522700	-2.48566500
H	5.99249800	0.14635300	-2.77856900
H	4.50816900	-0.75448000	-4.58204200
H	2.19150800	-1.50755900	-4.03246300
H	3.39630600	-2.51895600	-3.21556700
H	2.72430200	0.99669800	-4.44526300
H	4.27822600	1.65392300	-3.92819000
H	3.58245400	1.55193800	-0.24526800
H	4.78402400	1.97153400	-1.46445300
H	-4.13036200	-3.06139500	2.43076100
H	-1.66110000	-3.87460200	2.81007800
H	-0.42984700	-2.96617200	1.91046700
H	-1.55122300	-2.12345300	2.97962800
H	-0.05769300	-4.54562300	-0.16323600
H	-0.71087900	-4.26521000	-1.78414800
H	-5.09271200	-2.58599800	-1.71837700
H	-2.15050800	-3.24634000	-3.10648600
H	-3.47049000	-2.09487700	-3.30736200
H	-1.86769400	-1.52853300	-2.81477200
H	-6.79972100	-2.02737400	0.45027000
H	-6.72271800	-3.76391900	0.15399200
H	-6.42661100	-3.13230600	1.78235300
C	0.00931400	0.34764900	1.48264000
C	0.77826800	1.12043600	2.49508800
C	1.75140200	0.44299300	3.27695000
C	0.58368400	2.48812200	2.74367200
C	2.46333100	1.12329000	4.27194300
C	1.29077200	3.16784200	3.73258700
H	-0.12301500	3.03972300	2.13393400
C	2.22912800	2.48056700	4.49875900
H	3.20634800	0.61193600	4.87174900
H	1.11500200	4.22727100	3.89276700
H	2.79267000	2.99452200	5.27294400
O	1.93049000	-0.89005500	2.99064700
C	2.83699900	-1.69053900	3.76979600
H	2.74803800	-1.39836300	4.82420300
C	4.27809500	-1.50520300	3.29072500

H	4.96553900	-2.08867600	3.91413000
H	4.37698200	-1.84819500	2.25483100
H	4.58459700	-0.45640900	3.33098400
C	2.36101600	-3.13277100	3.62430100
H	3.00178900	-3.80496000	4.20537900
H	1.33192400	-3.23900900	3.98099200
H	2.39947800	-3.44450100	2.57423500
C	-1.40039000	0.87822200	1.00504000
C	-1.50020500	1.34576200	-0.50880500
H	-1.63996500	1.76003100	1.60228900
H	-2.13960000	0.09337000	1.17329800
H	-0.03871300	-0.70003700	1.76250400
H	2.48425900	2.32833500	-2.32302500
H	-1.32417200	2.42063900	-0.59154500
C	-2.76018300	0.94810400	-1.26471300
H	-2.57222000	1.09439700	-2.33722200
H	-2.99671600	-0.10471600	-1.11086200
C	-3.94979700	1.80339100	-0.84885900
C	-4.95884100	1.28293700	-0.02780400
C	-4.04349300	3.14252400	-1.25655400
C	-6.03639700	2.07654300	0.37363400
H	-4.90067800	0.24615300	0.29583300
C	-5.11777000	3.93745900	-0.85699500
H	-3.26341100	3.56696400	-1.88441200
C	-6.11962500	3.40662100	-0.04034600
H	-6.81102800	1.65418600	1.00928100
H	-5.17137200	4.97298700	-1.18279800
H	-6.95713500	4.02563800	0.27061000
N	0.97100400	3.68928000	-0.62228100
O	1.95021500	4.35120700	-0.97406000

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B3LYP SCF energy: -2153.006366 a.u.
B3LYP enthalpy: -2152.105529 a.u.
B3LYP free energy: -2152.235973 a.u.
M06 SCF energy in solution: -2152.10564 a.u.
M06 enthalpy in solution: -2151.204803 a.u.
M06 free energy in solution: -2151.335247 a.u.

Cartesian coordinates

Ru	0.33145900	0.57059200	-0.55335500
O	-0.41183800	4.05164500	0.10068600
O	1.16569000	2.58430200	-0.39310600
N	1.25110300	-1.96765100	-1.51889900
N	-0.60109500	-2.52101100	-0.48763400
C	0.16930500	-1.45006300	-0.87630200
C	1.36341100	-3.42501700	-1.44044800
C	2.36481300	-1.09493600	-1.90028200
C	3.47301600	-1.09900700	-0.81230200
C	4.58730700	-0.10248500	-1.18769700
C	5.19491100	-0.50648300	-2.54673500
C	4.09328400	-0.49239900	-3.62695000
C	2.99486400	-1.51292700	-3.24992900
C	3.48508100	0.92312000	-3.71954200
C	2.87289200	1.32979000	-2.35348500
C	1.76493000	0.31619000	-2.02162900
C	3.98232400	1.31126300	-1.28299400
C	-1.99847900	-2.56089300	-0.14963500
C	-2.39900700	-2.74959900	1.18392500
C	-3.76943500	-2.87677700	1.46094400
C	-1.41693900	-2.85510500	2.32773400
C	-0.01595400	-3.81866300	-0.89936400
C	-2.95397900	-2.57248200	-1.19534600
C	-4.73586900	-2.85639400	0.45684600
C	-4.30269100	-2.71341200	-0.86880400
C	-2.54848300	-2.43370300	-2.64606600
C	-6.20735500	-2.98233100	0.77542900
H	1.02160700	0.31329200	-2.84759700
H	1.57652400	-3.86327000	-2.42001700
H	2.17227100	-3.71394600	-0.75666700
H	3.03102000	-0.83126900	0.15596900
H	3.89165300	-2.11176000	-0.71400100
H	5.36533400	-0.12719900	-0.41299600
H	5.64908700	-1.50594800	-2.48103300
H	5.99684900	0.19158800	-2.82124500
H	4.52244400	-0.77787000	-4.59648500
H	2.21595700	-1.54528100	-4.02375000
H	3.43495100	-2.51896100	-3.18200500
H	2.71668600	0.95348200	-4.50495100
H	4.26271400	1.64389300	-4.00816300
H	3.56761400	1.62555500	-0.31951500
H	4.76411500	2.03587800	-1.54849600
H	-4.07973700	-3.01204500	2.49522700
H	-1.62390200	-3.75096000	2.92544900
H	-0.38354400	-2.90197300	1.98122900
H	-1.49722500	-1.99448900	3.00291800
H	0.03512700	-4.49843100	-0.04289200
H	-0.64167300	-4.29145300	-1.66452100
H	-5.03854700	-2.70685100	-1.67024300
H	-2.07071700	-3.34594100	-3.02627500
H	-3.42596700	-2.24518600	-3.27149600
H	-1.84335100	-1.61102000	-2.79667700
H	-6.73926000	-2.04725900	0.55860400
H	-6.68079600	-3.76742200	0.17399600
H	-6.37010900	-3.22080300	1.83103500
C	0.04458700	0.38950400	1.44677000
C	0.84686500	1.14675600	2.44694500
C	1.81271400	0.44602500	3.21932700
C	0.68807900	2.51902100	2.69397200
C	2.55314400	1.11134300	4.20336200
C	1.42711300	3.18276300	3.67124000
H	-0.00734900	3.08787700	2.08645900
C	2.35646500	2.47506000	4.42901300
H	3.29013000	0.58326000	4.79593200
H	1.27908000	4.24685900	3.82918900
H	2.94233800	2.97619500	5.19511600
O	1.95809700	-0.89293300	2.93682500
C	2.86788300	-1.70496300	3.70050700
H	2.80086500	-1.41150100	4.75613100
C	4.30340600	-1.53950000	3.19753000
H	4.99306500	-2.12989900	3.81188300
H	4.38144400	-1.88684900	2.16140500
H	4.62410600	-0.49474000	3.22987700
C	2.37242800	-3.14150300	3.56547800
H	3.01833800	-3.82054100	4.13274300
H	1.35045200	-3.23684500	3.94457800
H	2.38501500	-3.45391300	2.51491300
C	-1.36823200	0.93716100	0.98399700
C	-1.51519800	1.33037200	-0.55102200
H	-1.57110800	1.85278300	1.54030400
H	-2.11099500	0.16926500	1.20625400
H	-0.01726400	-0.65591400	1.73078900
H	2.44975900	2.33444700	-2.41402900
H	-1.40198100	2.41053000	-0.65859600
C	-2.76942200	0.85397200	-1.27142000
H	-2.59836300	0.96081400	-2.35123500
H	-2.96158100	-0.19899000	-1.07078100
C	-3.98893300	1.67655600	-0.87934800
C	-4.91388500	1.19081400	0.05497100
C	-4.19684000	2.95243300	-1.42285100
C	-6.01734700	1.95782100	0.43601500
H	-4.76979000	0.20150100	0.48340000
C	-5.29751000	3.72149000	-1.04460700
H	-3.48725100	3.34829200	-2.14621300
C	-6.21289400	3.22606000	-0.11300300
H	-6.72470500	1.56343300	1.16163400
H	-5.43929300	4.70858700	-1.47680800
H	-7.07084500	3.82433600	0.18224800
N	0.69736800	3.80453100	-0.42102000
O	1.39539800	4.66652400	-0.95509700

TS16

B3LYP SCF energy: -2152.987143 a.u.
B3LYP enthalpy: -2152.090458 a.u.
B3LYP free energy: -2152.217408 a.u.
M06 SCF energy in solution: -2152.085944 a.u.
M06 enthalpy in solution: -2151.189259 a.u.
M06 free energy in solution: -2151.316209 a.u.

Cartesian coordinates

Ru	0.27099900	0.36389800	-0.55730200
O	-0.37584400	3.74896500	-0.43957900
O	1.24840700	2.27787700	-0.72925500
N	0.92333100	-2.37281700	-1.18811500
N	-0.80058400	-2.61995900	0.13700600
C	-0.03086100	-1.67418100	-0.50846900
C	0.97603500	-3.79683200	-0.85335600
C	2.03941900	-1.65446000	-1.81610200
C	3.22266100	-1.50166400	-0.82464800
C	4.34678600	-0.66790800	-1.47052800
C	4.83105400	-1.37223300	-2.75415200
C	3.65173000	-1.50965000	-3.73970600

C	2.54652300	-2.37223600	-3.08704100
C	3.10264200	-0.10555400	-4.07712800
C	2.60767800	0.59376000	-2.78484900
C	1.47645300	-0.26638500	-2.18291300
C	3.79711400	0.72998800	-1.81256100
C	-2.05471600	-2.46676500	0.81774800
C	-2.07962000	-2.33293100	2.22166800
C	-3.31734800	-2.20560400	2.86311900
C	-0.82926600	-2.40354600	3.06884400
C	-0.37658000	-4.00338100	-0.16699800
C	-3.26261900	-2.60659800	0.09703200
C	-4.52562600	-2.25166800	2.16396100
C	-4.47418000	-2.47619300	0.78436900
C	-3.29508500	-2.96963900	-1.37291100
C	-5.84546100	-2.07106300	2.87663200
H	0.73050400	-0.43282900	-2.97627200
H	1.09792500	-4.41596300	-1.74626900
H	1.81663700	-4.00641000	-0.17680100
H	2.86632700	-1.00881500	0.09119600
H	3.60544700	-2.49189100	-0.53443600
H	5.18292800	-0.57905000	-0.76322900
H	5.24357400	-2.36363700	-2.51557800
H	5.64058500	-0.79155400	-3.21615700
H	3.99361200	-2.00646500	-4.65748900
H	1.70886400	-2.51793300	-3.78259600
H	2.95417900	-3.36685100	-2.84945800
H	2.28117800	-0.18687400	-4.80284800
H	3.89206900	0.49195300	-4.55541400
H	3.47750000	1.25596000	-0.90793000
H	4.58818700	1.33770200	-2.27398200
H	-3.33316400	-2.08386900	3.94459100
H	-0.82556800	-3.33310900	3.65380300
H	0.08016300	-2.38376100	2.46709500
H	-0.78351900	-1.57579200	3.78467000
H	-0.31000900	-4.59325600	0.75235800
H	-1.10365500	-4.48949300	-0.82964400
H	-5.40337500	-2.56692700	0.22511800
H	-3.41651700	-4.05459900	-1.49463700
H	-4.14524000	-2.49629200	-1.87447600
H	-2.38453700	-2.67661900	-1.89987000
H	-6.10912100	-1.00813400	2.95570200
H	-6.66119700	-2.57031100	2.34346300
H	-5.80868800	-2.47136400	3.89544900
C	-0.13376100	0.79160800	1.67540700
C	0.75432700	1.78922100	2.31741500
C	1.99343700	1.37254900	2.86820400
C	0.37507000	3.12836900	2.49779200
C	2.80018000	2.28135100	3.56178900
C	1.18354000	4.03751200	3.17516300
H	-0.56874200	3.46776800	2.08912100
C	2.39566200	3.60916600	3.70956300
H	3.75117400	1.97351800	3.97800500
H	0.86491300	5.06965200	3.28209100
H	3.03959100	4.30368300	4.24230300
O	2.32550400	0.05103900	2.68096900
C	3.43476600	-0.52246100	3.40204100
H	3.47010600	-0.06518200	4.39916900
C	4.75481800	-0.28269400	2.66647300
H	5.59200500	-0.67503900	3.25564200
H	4.74755100	-0.79304300	1.69808800
H	4.93174900	0.78071400	2.48510400
C	3.12373300	-2.00819500	3.55564900
H	3.92838700	-2.50891900	4.10528000
H	2.18699300	-2.15467600	4.10197100
H	3.03301000	-2.48352900	2.57246100
C	-1.37020400	1.06479300	1.07919200
C	-1.30357600	1.01016100	-1.29165000
H	-1.70491600	2.08729800	0.94305700
H	-2.13844300	0.30181500	1.08353700
H	0.01821200	-0.21827500	2.03716900
H	2.22197200	1.59000800	-3.02221100
H	-1.24388400	2.09094500	-1.47127200
C	-2.57799600	0.37371600	-1.77551400
H	-2.35721700	0.02402000	-2.79935300
H	-2.80597400	-0.51662000	-1.19079800
C	-3.76875600	1.31642000	-1.80690700
C	-4.79894900	1.19808800	-0.86514000
C	-3.84952200	2.33851600	-2.76356500
C	-5.88302300	2.07888100	-0.87673800
H	-4.75342400	0.40714000	-0.11992800
C	-4.92944300	3.22109900	-2.77632100
H	-3.05857000	2.44530600	-3.50300100
C	-5.95099000	3.09394300	-1.83186100
H	-6.67392900	1.97120800	-0.13862100
H	-4.97326800	4.00838800	-3.52419200
H	-6.79265600	3.78126700	-1.84147400
N	0.84375000	3.51530700	-0.58143400
O	1.70000400	4.39533100	-0.60556600

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B3LYP SCF energy: -2152.991347 a.u.
B3LYP enthalpy: -2152.092878 a.u.
B3LYP free energy: -2152.22618 a.u.
M06 SCF energy in solution: -2152.089133 a.u.
M06 enthalpy in solution: -2151.190664 a.u.
M06 free energy in solution: -2151.323966 a.u.

Cartesian coordinates

Ru	0.02722200	-0.48900400	0.38171900
O	0.39936900	-0.11181100	3.69589600
O	-1.01239700	-0.94078100	2.21188300
N	0.21127200	-1.41977400	-2.35437600
N	1.24725000	0.51107900	-2.39654100
C	0.59016300	-0.36678700	-1.57284600
C	0.39450600	-1.18384400	-3.78762100
C	-0.76850400	-2.35700000	-1.79057300
C	-2.20920500	-1.80609000	-1.96454900
C	-3.21689700	-2.73541000	-1.26153400
C	-3.12454000	-4.14424100	-1.88223400
C	-1.69353400	-4.69222500	-1.70489600
C	-0.69664800	-3.75858100	-2.43384800
C	-1.36550100	-4.75716800	-0.19628100
C	-1.44253500	-3.33801200	0.42398900
C	-0.39864100	-2.45829000	-0.29520600
C	-2.87317500	-2.79322900	0.24026000
C	1.67558700	1.85060500	-2.11164700
C	0.75126800	2.90330200	-2.29672800
C	1.16309400	4.21213500	-2.03887400
C	-0.64652700	2.64489600	-2.81163900
C	1.36443500	0.00575600	-3.78147100
C	3.01195300	2.12550500	-1.77016400
C	2.46990300	4.51068500	-1.63440800
C	3.37845700	3.45713300	-1.52818400
C	4.06931900	1.05145700	-1.66951500
C	2.87979100	5.93140900	-1.32517900
H	0.55191200	-3.00768700	-0.26206200
H	0.80937200	-2.06180700	-4.29039000
H	-0.56110600	-0.93359100	-4.27121800
H	-2.26453100	-0.79497300	-1.53523200
H	-2.45423700	-1.71786000	-3.03354600
H	-4.23340300	-2.34231300	-1.40017500
H	-3.38915400	-4.10800500	-2.94910000
H	-3.84518500	-4.81582000	-1.39663500
H	-1.62595700	-5.69609100	-2.14481200
H	0.32682600	-4.14823800	-2.35150000
H	-0.94726500	-3.71903700	-3.50510900
H	-0.36350900	-5.18153800	-0.04376700
H	-2.07615000	-5.43035900	0.30432400
H	-2.95518700	-1.79975100	0.69634600
H	-3.58958300	-3.44170200	0.76344800
H	0.44796800	5.02201300	-2.16727500
H	-0.63218800	2.33507300	-3.86551500
H	-1.16262200	1.85837700	-2.25416700
H	-1.25235400	3.55349100	-2.74956700
H	1.09819900	0.78409200	-4.50204500
H	2.39806100	-0.30393100	-3.98616400
H	4.41058400	3.67058400	-1.25679500
H	5.02102700	1.41730200	-2.07013700
H	4.25222700	0.75873000	-0.62959300
H	3.79665200	0.14803900	-2.21937600
H	2.59843000	6.20811600	-0.30056800
H	3.96282800	6.06468900	-1.41400900
H	2.39234700	6.64568100	-1.99789700
C	-0.73615100	2.03668000	0.91639200
C	-1.86403800	2.10225700	1.85964900
C	-3.19748500	2.05823200	1.37767900
C	-1.66526000	2.29488900	3.23676200
C	-4.27062300	2.19770900	2.26563300
C	-2.73108000	2.42102300	4.12124100
H	-0.65193300	2.33691300	3.61875200
C	-4.03398700	2.37455000	3.62943500
H	-5.29320500	2.15387600	1.91269700

H	-2.54390900	2.55179800	5.18220100
H	-4.87980600	2.47081200	4.30484000
O	-3.34606100	1.87688100	0.02530100
C	-4.65018400	1.99034400	-0.58039500
H	-5.20254600	2.78651200	-0.06533500
C	-5.41234700	0.66850800	-0.48077000
H	-6.41904500	0.77807800	-0.90077600
H	-4.88819000	-0.11164500	-1.04257200
H	-5.50648300	0.33162100	0.55510000
C	-4.41708100	2.41692900	-2.02595900
H	-5.37548000	2.54386600	-2.54113400
H	-3.87260200	3.36529600	-2.06724900
H	-3.83681700	1.65866800	-2.56327000
C	0.58289300	1.89817300	1.22789800
C	1.67464500	-0.97560400	1.01626100
H	0.91524100	1.71356600	2.24330800
H	1.33964300	2.09612000	0.47998400
H	-0.99274800	2.25787300	-0.11488100
H	-1.20918200	-3.38369600	1.49175800
H	1.73529700	-0.86156200	2.10855900
C	2.85243800	-1.66037000	0.38888600
H	2.57844400	-2.73016200	0.33874500
H	2.96602500	-1.35486400	-0.65811500
C	4.17571900	-1.53406300	1.12786000
C	4.50212600	-0.38519300	1.86269500
C	5.11923600	-2.56931900	1.05990800
C	5.73692200	-0.27287100	2.50651800
H	3.78079700	0.42424100	1.94421600
C	6.35447000	-2.45946700	1.69857100
H	4.88078000	-3.47290400	0.50220800
C	6.66821600	-1.30848900	2.42526600
H	5.96604300	0.62369700	3.07663900
H	7.06920100	-3.27603800	1.63508500
H	7.62761700	-1.22335000	2.92845000
N	-0.68749200	-0.68029500	3.45448200
O	-1.47882400	-1.02162400	4.32947200

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B3LYP SCF energy: -2152.989496 a.u.
B3LYP enthalpy: -2152.090864 a.u.
B3LYP free energy: -2152.223068 a.u.
M06 SCF energy in solution: -2152.084767 a.u.
M06 enthalpy in solution: -2151.186135 a.u.
M06 free energy in solution: -2151.318339 a.u.

Cartesian coordinates

Ru	-0.20949200	-0.81468600	-0.25867500
O	0.57209900	-3.58721600	1.93765000
O	-0.79886300	-2.83170900	0.37647400
N	-1.11901400	1.08187700	-2.24214000
N	0.59092600	2.11992900	-1.34878900
C	-0.10754300	0.93182300	-1.34514800
C	-1.26448300	2.44143300	-2.76589900
C	-2.20150900	0.09415200	-2.30018100
C	-3.39338000	0.54150300	-1.41088200
C	-4.47742100	-0.55321600	-1.39299700
C	-4.98005600	-0.78509700	-2.83278500
C	-3.80057400	-1.22434600	-3.72570000
C	-2.72201100	-0.11537000	-3.74207500
C	-3.20107700	-2.52932900	-3.16162800
C	-2.69032300	-2.29908100	-1.71641900
C	-1.60282700	-1.21110000	-1.75691600
C	-3.87018900	-1.85358000	-0.83024700
C	1.92418800	2.41031600	-0.89327600
C	2.11820300	3.12979400	0.30020600
C	3.42536900	3.48106200	0.66765000
C	0.97424400	3.55414200	1.19177500
C	0.05747200	3.08258200	-2.34104100
C	3.02055300	2.12006200	-1.73979400
C	4.53019300	3.16806000	-0.12428900
C	4.30183200	2.49541900	-1.33090600
C	2.84693800	1.43258000	-3.07691600
C	5.93213600	3.54431400	0.29475400
H	-0.81192500	-1.54434900	-2.47125200
H	-1.41035200	2.44103400	-3.84983100
H	-2.12909400	2.93821000	-2.30645400
H	-3.02890700	0.74067900	-0.39679300
H	-3.81942500	1.47727700	-1.80236100
H	-5.31184000	-0.22173900	-0.75985600
H	-5.43668200	0.13369100	-3.22922800
H	-5.76032000	-1.55802600	-2.84012600
H	-4.15549400	-1.38752200	-4.75210700
H	-1.88735600	-0.39969400	-4.39714800
H	-3.15469900	0.81305600	-4.14432100
H	-2.37785200	-2.87658400	-3.80175600
H	-3.96428100	-3.32045300	-3.16911600
H	-2.26592200	-3.22193300	-1.31888200
H	-3.52231800	-1.70231800	0.19856200
H	-4.63550600	-2.64157700	-0.80205900
H	3.57506600	4.02924500	1.59561000
H	1.16705000	4.54779600	1.61097500
H	0.02305900	3.58218300	0.65618600
H	0.84584500	2.86752400	2.03761100
H	-0.06472200	4.06952100	-1.88429600
H	0.75427800	3.18431000	-3.18103900
H	5.14652300	2.25389500	-1.97292700
H	2.65747000	2.16015200	-3.87774200
H	3.75657400	0.88877500	-3.34931300
H	2.01696800	0.72170300	-3.07343900
H	6.53852100	2.65101400	0.49023100
H	6.44436900	4.11427900	-0.48966600
H	5.92898700	4.15155100	1.20518600
C	-0.67202200	0.21825100	1.26798000
H	-0.55106600	1.29761200	1.18870900
C	-1.43447100	-0.13927500	2.47430000
C	-2.36169400	0.81648800	2.98743800
C	-1.29237500	-1.35505900	3.16621000
C	-3.09747500	0.53507600	4.14357100
C	-2.01711100	-1.62496500	4.32413600
H	-0.58505100	-2.08849200	2.79540100
C	-2.91953300	-0.67991000	4.80851700
H	-3.81325700	1.24867300	4.53315900
H	-1.87557800	-2.57011100	4.83943700
H	-3.49754800	-0.88015400	5.70701800
O	-2.48140300	1.98012700	2.27386400
C	-3.42808700	2.99350900	2.66303500
H	-3.39799500	3.10589000	3.75456100
C	-4.83923400	2.61855800	2.20718900
H	-5.55705700	3.38424700	2.52305600
H	-4.87307800	2.54293100	1.11466300
H	-5.15675600	1.65881700	2.62439600
C	-2.93726200	4.28928700	2.02595300
H	-3.60497400	5.11721100	2.28737600
H	-1.92827300	4.53330600	2.37209000
H	-2.91747900	4.19436100	0.93436300
C	1.46892100	-0.37975000	1.36909400
C	1.81944900	-1.33104100	0.37148600
H	1.88901100	0.62019400	1.32174600
H	1.23998000	-0.75102700	2.36223600
H	1.72169700	-2.36417600	0.69675500
C	2.94554100	-1.12212200	-0.63029000
H	2.69928700	-1.63266400	-1.56993200
H	3.06311400	-0.06202400	-0.84924800
C	4.25992800	-1.67764800	-0.09944400
C	4.66841700	-2.98123800	-0.40805900
C	5.07864600	-0.89953500	0.73158300
C	5.86408000	-3.49596600	0.09726900
H	4.04356000	-3.59993400	-1.04881400
C	6.27467300	-1.40964400	1.23782300
H	4.77507400	0.11500400	0.98058400
C	6.67199700	-2.71094400	0.92141200
H	6.16273900	-4.51060400	-0.15300500
H	6.89749400	-0.79123100	1.87970500
H	7.60309000	-3.10972200	1.31534600
N	-0.23794800	-3.82731300	1.01380100
O	-0.55530400	-4.96698900	0.67806400

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B3LYP SCF energy: -1999.167544 a.u.
B3LYP enthalpy: -1998.333205 a.u.
B3LYP free energy: -1998.459356 a.u.
M06 SCF energy in solution: -1998.299558 a.u.
M06 enthalpy in solution: -1997.465219 a.u.
M06 free energy in solution: -1997.59137 a.u.

Cartesian coordinates

Ru	0.90285800	-0.27177800	-0.42288900
O	1.74531100	-0.46894400	-2.60309800
O	0.81592200	-2.14091000	-1.58695100
N	2.66569600	1.74440200	0.63992400
N	0.70889200	2.73185000	0.60452000
C	1.35630800	1.54910000	0.35091300

C	3.00056400	3.14573300	0.90590800
C	3.64438800	0.68288900	0.36446300
C	4.32645800	0.89805000	-1.01003500
C	5.29906000	-0.26430700	-1.30039200
C	6.37015700	-0.33287900	-0.19464600
C	5.68053700	-0.56352600	1.16536200
C	4.74014700	0.62975500	1.45550200
C	4.87945700	-1.88446300	1.11477300
C	3.78761900	-1.80064800	0.01226100
C	2.83867800	-0.64090600	0.40489000
C	4.50614300	-1.58528600	-1.33797500
C	-0.70685200	2.92811900	0.71594800
C	-1.38858200	3.62105800	-0.30304300
C	-2.77412400	3.78331400	-0.18993400
C	-0.66342000	4.22391100	-1.48538700
C	1.61520000	3.74200800	1.18947600
C	-1.38816300	2.50330000	1.87670000
C	-3.48989000	3.30062200	0.90843400
C	-2.77324700	2.68414800	1.94021200
C	-0.65819200	1.93272200	3.07321000
C	-4.99434500	3.41870500	0.97237100
H	2.60374500	-0.80149600	1.46578100
H	3.68543600	3.24378000	1.75203000
H	3.47337800	3.60461800	0.02642700
H	3.56474900	0.95430800	-1.79444900
H	4.87573800	1.85148400	-1.00632700
H	5.78032400	-0.09413600	-2.27241900
H	6.95730400	0.59661700	-0.16931700
H	7.07369300	-1.15017600	-0.40344000
H	6.43657300	-0.62090100	1.95992400
H	4.26894600	0.52189500	2.44198400
H	5.33106500	1.55814600	1.47318600
H	4.41778000	-2.08406200	2.09175900
H	5.56404400	-2.71981400	0.90912500
H	3.22690700	-2.74318100	-0.01642300
H	3.80397800	-1.56550300	-2.17216300
H	5.19328500	-2.42375600	-1.52021100
H	-3.30762400	4.29374700	-0.98908000
H	0.27452300	3.70715000	-1.70310000
H	-1.28849000	4.19990800	-2.38377800
H	-0.41798600	5.27762400	-1.29289300
H	1.46204700	4.71895800	0.72208700
H	1.42417200	3.84305000	2.26644000
H	-3.30580200	2.33863400	2.82423100
H	-0.32186500	2.73892500	3.73989100
H	-1.31944000	1.28853200	3.66164500
H	0.22198700	1.35127900	2.79109400
H	-5.47143400	2.51944200	0.56072600
H	-5.34482400	3.53235900	2.00402500
H	-5.35526200	4.27499300	0.39309900
C	-0.04015000	-0.89377000	1.03852700
H	-0.81920900	-0.33204300	1.57527100
C	0.12795800	-2.29243400	1.59794700
H	0.70140300	-2.91725300	0.90604800
H	0.76034600	-2.16999700	2.49743200
C	-1.17189300	-2.97278900	1.98513200
C	-1.87250900	-2.59384400	3.13980200
C	-1.71732300	-3.97642700	1.17244000
C	-3.08774500	-3.19510000	3.47070900
H	-1.45560300	-1.82844800	3.79195400
C	-2.93262700	-4.58175700	1.50146000
H	-1.18347600	-4.28281600	0.27586600
C	-3.62340800	-4.19143400	2.65018300
H	-3.61213100	-2.89255800	4.37375300
H	-3.33825600	-5.35895800	0.85909300
H	-4.56768300	-4.66333900	2.90821500
C	-1.72935600	0.07313200	-1.12281500
C	-0.86757200	0.59886300	-2.02735100
H	-2.03293100	0.67585100	-0.27052100
H	-0.52155200	1.62069800	-1.95692100
H	-0.64255200	0.08023200	-2.95409700
C	-2.49731900	-1.21482100	-1.32410500
H	-2.38399400	-1.86771300	-0.45334600
H	-2.08938000	-1.75452900	-2.18596200
C	-3.97629500	-0.91525600	-1.52504700
C	-4.87700500	-1.02036400	-0.45676500
C	-4.46194100	-0.49479400	-2.77100900
C	-6.22849700	-0.70939700	-0.62733300
H	-4.51855400	-1.36134300	0.51211600
C	-5.81153100	-0.18776200	-2.94663600
H	-3.77565400	-0.41072500	-3.61079900
C	-6.69991700	-0.29092200	-1.87321900
H	-6.91408100	-0.80506400	0.21109900
H	-6.17059500	0.12963800	-3.92237800
H	-7.75188200	-0.05382800	-2.00913100
N	1.39605100	-1.70158800	-2.65234400
O	1.59426700	-2.41013400	-3.62379300

TS18

B3LYP SCF energy: -1999.162 a.u.
B3LYP enthalpy: -1998.328241 a.u.
B3LYP free energy: -1998.449019 a.u.
M06 SCF energy in solution: -1998.295636 a.u.
M06 enthalpy in solution: -1997.461877 a.u.
M06 free energy in solution: -1997.582655 a.u.

Cartesian coordinates

Ru	0.81643000	-0.31840000	-0.44493700
O	1.64074000	-0.25059900	-2.67077600
O	0.71908500	-2.02924700	-1.83715600
N	2.53190300	1.38689400	1.15909400
N	0.56747200	2.34640900	1.26305400
C	1.24927400	1.29085400	0.71396700
C	2.81755400	2.63184900	1.87737900
C	3.57113500	0.54632200	0.55538600
C	4.25763500	1.29617200	-0.61602000
C	5.30430300	0.38597800	-1.28937900
C	6.35731400	-0.05102500	-0.25173800
C	5.65962300	-0.81680900	0.89043100
C	4.65085700	0.13003000	1.58259000
C	4.93216300	-2.05030900	0.30936000
C	3.85825900	-1.59681100	-0.71855600
C	2.84833400	-0.71292500	0.04871500
C	4.58421100	-0.84987300	-1.85937200
C	-0.78611700	2.76359500	1.04473800
C	-1.05893100	3.62462200	-0.04182500
C	-2.37329100	4.04856700	-0.24503000
C	0.04305300	4.09636900	-0.96395800
C	1.40626400	3.15226500	2.17396400
C	-1.79851600	2.42052700	1.95904000
C	-3.41617500	3.66570900	0.60818700
C	-3.10264800	2.87185600	1.71227000
C	-1.52722100	1.61819600	3.21266900
C	-4.83983900	4.08502600	0.32749400
H	2.56442500	-1.29143500	0.94620500
H	3.39680900	2.44584700	2.78592100
H	3.38840100	3.32566700	1.24516600
H	3.49501300	1.59537700	-1.34526700
H	4.74285300	2.20987900	-0.24301000
H	5.79285700	0.94025200	-2.10182100
H	6.88993500	0.82380400	0.14891200
H	7.11038600	-0.69239500	-0.72922600
H	6.40534600	-1.14161300	1.62833800
H	4.16975000	-0.36929100	2.43479600
H	5.18701900	1.00739100	1.97549700
H	4.46471800	-2.62942200	1.11777200
H	5.66392800	-2.71269900	-0.17496500
H	3.34825900	-2.48076500	-1.11919200
H	3.87750800	-0.54419500	-2.63363800
H	5.31453100	-1.52416100	-2.32847900
H	-2.59096300	4.69467300	-1.09267400
H	0.57540000	3.26286900	-1.43420700
H	-0.36452800	4.72821900	-1.75860600
H	0.79298800	4.68781100	-0.42328800
H	1.28691600	4.21966000	1.96632000
H	1.10996100	2.97545600	3.21659100
H	-3.89147000	2.59186500	2.40819900
H	-1.64798700	2.24632800	4.10493800
H	-2.23176800	0.78442000	3.31155700
H	-0.51624200	1.20613700	3.22759900
H	-5.33551100	3.35885500	-0.33037300
H	-5.42980800	4.14925400	1.24788000
H	-4.88097400	5.05843700	-0.17282600
C	-0.25683200	-1.06397400	0.92629300
H	-0.67053000	-0.50176200	1.76809100
C	-0.36194500	-2.56859300	1.13027700
H	-0.37006200	-3.09519800	0.17087600
C	-1.60516600	-0.24220900	-0.58127900
C	-0.84901700	0.52254600	-1.52215100
H	-2.08049800	0.32953500	0.21127100
H	-0.86787200	1.60112900	-1.44550200
H	-0.80575800	0.15214100	-2.54432200

C	-2.40120100	-1.45282300	-1.06399900
H	-2.69768100	-2.07506400	-0.21569000
H	-1.76903800	-2.06057000	-1.71857800
C	-3.65219600	-1.00749100	-1.80565200
C	-4.80504900	-0.64090200	-1.09631800
C	-3.67948100	-0.93623000	-3.20490700
C	-5.95101400	-0.20677300	-1.76453500
H	-4.80638300	-0.70575200	-0.00997600
C	-4.82445400	-0.50484100	-3.87754100
H	-2.79954300	-1.23021700	-3.77255300
C	-5.96360300	-0.13576900	-3.15947400
H	-6.83721500	0.06592700	-1.19661400
H	-4.82717100	-0.46295300	-4.96371600
H	-6.85641300	0.19664400	-3.68254500
H	0.60050300	-2.84557200	1.59854600
C	-1.48441000	-3.05632400	2.03225600
C	-1.60893300	-2.57837300	3.34642100
C	-2.40346300	-4.01690500	1.58892000
C	-2.62954200	-3.03109800	4.18314300
H	-0.89010500	-1.85448800	3.72473300
C	-3.42610100	-4.47479100	2.42367500
H	-2.31373900	-4.41476500	0.58081000
C	-3.54587400	-3.97996000	3.72264000
H	-2.70402500	-2.64993700	5.19859500
H	-4.12702200	-5.21996600	2.05657000
H	-4.34010900	-4.33518900	4.37369800
N	1.29140400	-1.46491800	-2.85366100
O	1.47551700	-2.06306500	-3.89987600

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B3LYP SCF energy: -1999.173621 a.u.
B3LYP enthalpy: -1998.337737 a.u.
B3LYP free energy: -1998.456924 a.u.
M06 SCF energy in solution: -1998.312887 a.u.
M06 enthalpy in solution: -1997.477003 a.u.
M06 free energy in solution: -1997.59619 a.u.

Cartesian coordinates

Ru	-0.87691800	-0.36282900	0.40259700
O	-1.70755200	-0.51541600	2.81794800
O	-0.74518000	-2.11758900	1.69824600
N	-2.49726800	1.37820500	-1.25371000
N	-0.50275100	2.27385900	-1.33885200
C	-1.22337700	1.25361600	-0.78253000
C	-2.73245900	2.60828600	-2.01478400
C	-3.56642900	0.60413700	-0.62474400
C	-4.28630800	1.44441600	0.46400100
C	-5.35745300	0.59148100	1.17162700
C	-6.38214200	0.08491100	0.13720300
C	-5.65924900	-0.76645300	-0.92668000
C	-4.61464700	0.11072500	-1.65273100
C	-4.95870800	-1.95843300	-0.24011600
C	-3.91967700	-1.44043900	0.79446300
C	-2.88756200	-0.61110000	0.01620300
C	-4.66442300	-0.60058400	1.85469500
C	0.84840700	2.67523400	-1.07360700
C	1.09670400	3.50369500	0.04381700
C	2.40732000	3.91224300	0.29259300
C	-0.02597500	3.95415100	0.95094000
C	0.69610100	0.36957800	1.42643900
C	-1.30043700	3.09348000	-2.27503400
C	1.88061900	2.34872700	-1.97022200
C	3.46985300	3.54595600	-0.54431800
C	3.18081100	2.78520800	-1.67738200
C	1.63980700	1.57400800	-3.24699300
C	4.88674700	3.94809100	-0.21068700
H	-2.47016200	-1.25728100	-0.79986100
H	0.91622700	1.43208300	1.42100900
H	-3.28332000	2.40884000	-2.93836700
H	-3.30960600	3.33050700	-1.42229100
H	-3.54405300	1.80130100	1.18870800
H	-4.75477300	2.32582400	0.00406600
H	-5.86558100	1.20818500	1.92447800
H	-6.89625800	0.93124800	-0.34056600
H	-7.15346900	-0.51555600	0.63756900
H	-6.38528500	-1.13771500	-1.66176200
H	-4.10867400	-0.46025500	-2.44286400
H	-5.11620000	0.96267300	-2.13475800
H	-4.46598000	-2.59237300	-0.99007700
H	-5.70319800	-2.58640800	0.26825600
H	-3.42919600	-2.29717400	1.26721700
H	-3.96231900	-0.25301400	2.61632200
H	-5.40979300	-1.23116600	2.35850800
H	2.60698800	4.53145100	1.16439100
H	-0.77931300	4.53307000	0.40145000
H	-0.54585300	3.10772400	1.41191300
H	0.36000600	4.59065200	1.75254700
H	-1.16211000	4.15852900	-2.06688800
H	-0.98057600	2.90660500	-3.30824100
H	3.98613500	2.51670600	-2.35861800
H	1.77623100	2.22171100	-4.12300900
H	2.34997300	0.74551100	-3.34636500
H	0.63195300	1.15615900	-3.29238500
H	5.31517600	3.26499800	0.53458300
H	5.53229900	3.92067900	-1.09453900
H	4.92954000	4.95791600	0.21221200
C	1.51091700	-0.44269900	0.35703900
C	0.56015700	-1.03246900	-0.81383500
H	2.12657400	0.29706200	-0.16006300
H	0.74578000	-0.47314000	-1.73092700
C	0.55056100	-2.54288600	-1.11066200
H	0.53010500	-3.12113900	-0.18342600
H	-0.40031300	-2.76027400	-1.62064100
C	1.67669100	-3.03182600	-2.01262200
C	1.82301600	-2.52844900	-3.31513900
C	2.57189400	-4.02245800	-1.58636100
C	2.83866300	-2.98526500	-4.15566900
H	1.12388600	-1.77959400	-3.68145200
C	3.58989400	-4.48496300	-2.42423100
H	2.46653900	-4.44009600	-0.58780600
C	3.73027200	-3.96485800	-3.71122900
H	2.92878100	-2.58315700	-5.16190600
H	4.27084700	-5.25431200	-2.06923900
H	4.52081900	-4.32364900	-4.36493700
C	2.41924900	-1.50527300	1.02612600
H	2.89566100	-2.10195200	0.24146400
H	1.79940100	-2.18212900	1.62212200
C	3.50089500	-0.89193000	1.89348800
C	3.41657400	-0.91166800	3.29218900
C	4.62410000	-0.28983600	1.30558100
C	4.41684300	-0.33825000	4.08118600
H	2.56342700	-1.38954500	3.76829700
C	5.62660000	0.28320300	2.08892700
H	4.71695000	-0.27999300	0.22126900
C	5.52463400	0.26333200	3.48256600
H	4.33103300	-0.36816900	5.16439400
H	6.49465000	0.73294300	1.61241900
H	6.30640900	0.70473900	4.09521700
H	0.76921300	-0.04354100	2.43289300
N	-1.27250200	-1.70255400	2.81696200
O	-1.32569700	-2.44517100	3.78600500

TS19

B3LYP SCF energy: -1999.150542 a.u.
B3LYP enthalpy: -1998.317805 a.u.
B3LYP free energy: -1998.441531 a.u.
M06 SCF energy in solution: -1998.292946 a.u.
M06 enthalpy in solution: -1997.460209 a.u.
M06 free energy in solution: -1997.583935 a.u.

Cartesian coordinates

Ru	-0.86157000	0.25029100	0.28688500
O	-1.51392700	3.60531200	-0.28952300
O	-0.90701300	2.18890500	1.28818100
N	-2.36325100	-2.12856600	-0.37316100
N	-0.32130700	-2.58824800	-1.02443600
C	-1.09463200	-1.63806100	-0.41044800
C	-2.53828500	-3.36421700	-1.14065800
C	-3.46271500	-1.22546700	-0.01528600
C	-4.10088700	-0.60722900	-1.28786700
C	-5.17647300	0.42303300	-0.89049400
C	-6.26781900	-0.28068100	-0.05794100
C	-5.63416500	-0.89347500	1.20818700
C	-4.56915300	-1.93762500	0.79578100
C	-4.98089900	0.23125100	2.03910600
C	-3.87708800	0.93544500	1.20653900
C	-2.81890200	-0.11839000	0.83664100
C	-4.51527200	1.54107000	-0.06042900
C	1.11136600	-2.66414200	-1.08425300
C	1.78132800	-2.31088400	-2.26892900
C	3.17681900	-2.45117300	-2.31622300
C	1.06086300	-1.80105300	-3.49670600

C	-0.50912800	0.91383200	-1.40383400
C	-1.08543000	-3.81578900	-1.33767400
C	1.82472600	-3.20199900	0.01295500
C	3.91090400	-2.94156800	-1.23747400
C	3.21157700	-3.31835800	-0.08283200
C	1.12093800	-3.66768400	1.26876600
C	5.41482100	-3.07033700	-1.30108200
H	-2.46276100	-0.58761600	1.78859500
H	-0.26221600	0.33257700	-2.29667700
H	-3.14065000	-4.09636500	-0.59565600
H	-3.03566100	-3.15655900	-2.09771000
H	-3.31412400	-0.12726700	-1.88234700
H	-4.54963200	-1.40003700	-1.90384800
H	-5.62143000	0.84640900	-1.80080500
H	-6.75752400	-1.06323100	-0.65544600
H	-7.04679100	0.43931500	0.22619000
H	-6.40883800	-1.39434800	1.80387200
H	-4.12735800	-2.41022500	1.68357400
H	-5.04344500	-2.73353200	0.20188300
H	-4.55076000	-0.18007100	2.96302200
H	-5.74585900	0.96010100	2.34066100
H	-3.42336100	1.72703500	1.80891100
H	-3.75342600	2.05984500	-0.65349500
H	-5.26578200	2.29050600	0.22486600
H	3.69682400	-2.17077400	-3.23016500
H	1.32307000	-2.40300500	-4.37503000
H	-0.02380500	-1.82487600	-3.37558300
H	1.35044200	-0.76700800	-3.72110100
H	-0.87094200	-4.15289800	-2.35608600
H	-0.80887100	-4.62259700	-0.64715100
H	3.76361600	-3.71611500	0.76626100
H	0.62802200	-4.63713900	1.11839500
H	1.83795900	-3.79694800	2.08509300
H	0.35071400	-2.96406000	1.59978400
H	5.90045300	-2.39246500	-0.58802900
H	5.73935600	-4.08724300	-1.04952100
H	5.79558300	-2.83300400	-2.29921700
C	1.52665200	0.77516300	-0.13072800
C	1.22723600	0.10408600	1.07300100
H	1.86223500	0.14930500	-0.95232000
H	1.43683000	-0.96057600	1.05945300
C	1.35302100	0.73443700	2.46292100
H	1.06718200	1.78594600	2.43482500
H	0.64032400	0.24325000	3.13889400
C	2.75680300	0.57404400	3.02831300
C	3.21957800	-0.67782400	3.46098800
C	3.61935200	1.67330600	3.13802000
C	4.50679300	-0.83007200	3.97630000
H	2.55708200	-1.53952200	3.40695800
C	4.90971800	1.52595200	3.65289700
H	3.27039400	2.65709400	2.83377800
C	5.35932400	0.27293100	4.07078100
H	4.84225700	-1.80780400	4.31350900
H	5.55938300	2.39362500	3.73395400
H	6.36111900	0.15726100	4.47580600
C	1.95464300	2.23209400	-0.20301700
H	2.87786400	2.30883500	0.39256100
H	1.21265200	2.86259300	0.29177400
C	2.23550900	2.74000900	-1.60308500
C	1.45564500	3.75810500	-2.16791300
C	3.29666600	2.21125100	-2.35350800
C	1.72525500	4.22908500	-3.45532700
H	0.62782000	4.17166600	-1.59713200
C	3.56581700	2.67856300	-3.64075200
H	3.92483800	1.43436800	-1.92098100
C	2.77862600	3.69050600	-4.19621800
H	1.10993800	5.01953500	-3.87713200
H	4.39564400	2.26087800	-4.20569300
H	2.98966700	4.05973300	-5.19648000
H	-0.61891600	1.99180500	-1.54238500
N	-1.52061200	3.28792500	0.91652400
O	-2.05188900	3.96756000	1.79394500

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B3LYP SCF energy: -1999.153217 a.u.
B3LYP enthalpy: -1998.319944 a.u.
B3LYP free energy: -1998.447248 a.u.
M06 SCF energy in solution: -1998.296112 a.u.
M06 enthalpy in solution: -1997.462839 a.u.
M06 free energy in solution: -1997.590143 a.u.

Cartesian coordinates

Ru	-0.82027200	0.16081800	0.29773200
O	-1.87187900	3.30633400	1.38563400
O	-0.86043500	1.46005700	2.03846500
N	-2.15143800	-1.88862700	-1.23847500
N	-0.11062000	-1.84145200	-2.03828700
C	-0.93658700	-1.28905600	-1.09671800
C	-2.24626600	-2.74165300	-2.42556000
C	-3.30346200	-1.32165200	-0.53043800
C	-4.08246600	-0.33678800	-1.44227500
C	-5.21073400	0.34328700	-0.64310800
C	-6.18206400	-0.73605800	-0.12513600
C	-5.41556900	-1.72272400	0.78050400
C	-4.28978100	-2.40538700	-0.03352400
C	-4.81137100	-0.94716400	1.96982900
C	-3.82779300	0.13621100	1.45340100
C	-2.70698500	-0.57737100	0.67992600
C	-4.59486700	1.11493200	0.54135700
C	1.31394700	-1.70683500	-2.14914000
C	1.85455100	-0.78134800	-3.06222800
C	3.24719400	-0.71800900	-3.20340500
C	0.98905200	0.15009600	-3.87800700
C	-1.07200600	1.44527900	-0.97593400
C	-0.76609900	-2.94055100	-2.77932600
C	2.15634200	-2.57551100	-1.42019400
C	4.10640500	-1.54252800	-2.47452100
C	3.53868100	-2.46733900	-1.59107900
C	1.60882100	-3.62543600	-0.47710700
C	5.60655600	-1.43874400	-2.62325800
H	-2.27209100	-1.35055200	1.36159500
H	-1.06557200	1.31099400	-2.06439000
H	-2.76099100	-3.68193500	-2.20893600
H	-2.79254500	-2.22890300	-3.22936200
H	-3.39260100	0.41547700	-1.84023700
H	-4.50556700	-0.88219100	-2.29827600
H	-5.74798500	1.03793400	-1.30253700
H	-6.64168500	-1.27148900	-0.96844200
H	-6.99937500	-0.26879000	0.44040200
H	-6.10237100	-2.49560400	1.15035400
H	-3.75228900	-3.13362500	0.58896000
H	-4.72663400	-2.95639600	-0.87973900
H	-4.28947700	-1.63653400	2.64823800
H	-5.61491500	-0.47651200	2.55303300
H	-3.41107400	0.67298100	2.31015000
H	-3.91978000	1.89963200	0.18278500
H	-5.38655600	1.61310400	1.11682900
H	3.66735400	-0.00326000	-3.90797800
H	1.43987300	0.33614700	-4.85837600
H	-0.01714700	-0.24899700	-4.02797400
H	0.88321900	1.12148800	-3.37916600
H	-0.56165200	-2.85952600	-3.85083100
H	-0.38841500	-3.91108600	-2.43186300
H	4.18958500	-3.12500200	-1.01822700
H	1.46565700	-4.58610200	-0.99032900
H	2.30657400	-3.80316900	0.34756800
H	0.64484000	-3.33634700	-0.04909200
H	6.05945400	-0.96778600	-1.74131400
H	6.06768000	-2.42724700	-2.73160300
H	5.88217900	-0.83921000	-3.49645700
C	1.72265700	0.88622500	0.30604800
C	1.51039400	-0.19365400	1.11521300
H	1.90374600	0.69018500	-0.74718400
H	1.60603300	-1.17218000	0.65434700
C	1.51960400	-0.20077300	2.63632100
H	1.40727300	0.81191300	3.02662500
H	0.65820000	-0.76677800	3.01191100
C	2.79895300	-0.84546700	3.14893500
C	2.85535900	-2.22212000	3.40608900
C	3.95707400	-0.08202300	3.35248500
C	4.03545000	-2.82237600	3.85009400
H	1.96062100	-2.82719300	3.27186000
C	5.13832700	-0.67700300	3.79752500
H	3.92861800	0.99019900	3.17273700
C	5.18231700	-2.05074600	4.04593800
H	4.05546000	-3.89023800	4.05272400
H	6.02286000	-0.06575500	3.95742300
H	6.10036300	-2.51395700	4.39747400
C	1.94464100	2.31316400	0.76420400
H	2.92965700	2.34406500	1.25800100
H	1.20668800	2.57425900	1.52672900
C	1.93199800	3.33501000	-0.35608000

C	0.93164400	4.31386200	-0.42265500
C	2.93143800	3.32585800	-1.34053800
C	0.93018700	5.25838600	-1.45258800
H	0.14400400	4.32314000	0.32680600
C	2.92927500	4.26629600	-2.37180800
H	3.72407300	2.58103000	-1.29375100
C	1.92640100	5.23753600	-2.43015400
H	0.14694500	6.01121200	-1.48768700
H	3.71495800	4.24741400	-3.12319700
H	1.92566600	5.97473600	-3.22890300
H	-1.27401700	2.46121500	-0.62235000
N	-1.63376700	2.48960000	2.29535800
O	-2.06561300	2.60481500	3.44249100

TS20

B3LYP SCF energy: -1999.141925 a.u.
B3LYP enthalpy: -1998.310593 a.u.
B3LYP free energy: -1998.445004 a.u.
M06 SCF energy in solution: -1998.277755 a.u.
M06 enthalpy in solution: -1997.446423 a.u.
M06 free energy in solution: -1997.580834 a.u.

Cartesian coordinates

Ru	-1.10015600	0.21022000	-0.42259400
O	0.03457300	-0.10265500	-3.47835800
O	-0.75252800	1.41955400	-2.08901300
N	-2.76769300	0.00361700	1.93359500
N	-0.80714400	-0.73208700	2.59152400
C	-1.49324200	-0.23344500	1.53578900
C	-3.04776400	-0.51703200	3.27719800
C	-3.78346700	0.26642900	0.90167400
C	-4.46987400	-1.05039000	0.45967400
C	-5.43069100	-0.77184500	-0.71311500
C	-6.50715500	0.23386900	-0.25636100
C	-5.82790900	1.54662800	0.18650700
C	-4.87216300	1.25929900	1.37030600
C	-5.04145700	2.13348900	-1.00698200
C	-3.94990900	1.13010600	-1.46274000
C	-3.00802400	0.89908200	-0.27327100
C	-4.63111400	-0.18442200	-1.89421900
C	0.60948400	-0.95155600	2.66770700
C	1.09877700	-2.26659600	2.57231400
C	2.47667900	-2.47311100	2.70349000
C	0.17179600	-3.43909400	2.35011800
C	-1.19010100	-1.51937800	-0.94737700
C	-1.62839300	-0.75333100	3.82246500
C	1.47189700	0.13380000	2.91666700
C	3.36367700	-1.41702600	2.93043800
C	2.84019900	-0.12401100	3.03890600
C	0.94811500	1.54512000	3.05468400
C	4.85191900	-1.65707100	3.02788400
H	-2.66011000	1.90027600	0.08118800
H	-0.50920600	-2.29946800	-0.57534300
H	-3.61836800	0.19744000	3.87661600
H	-3.62242300	-1.45110700	3.21493000
H	-3.70410200	-1.77617300	0.16334700
H	-5.02703900	-1.48202700	1.30340300
H	-5.90811400	-1.71266700	-1.01750500
H	-7.09475300	-0.18943900	0.57067000
H	-7.20831400	0.43513400	-1.07720000
H	-6.59065800	2.26428400	0.51551300
H	-4.39973300	2.18761700	1.71853600
H	-5.44279400	0.84517000	2.21483900
H	-4.57967700	3.08973500	-0.72660400
H	-5.73185900	2.34350700	-1.83575900
H	-3.38090100	1.55258500	-2.29675300
H	-3.87978800	-0.90365200	-2.24055200
H	-5.30255700	0.00713600	-2.74220500
H	2.86364700	-3.48627000	2.62118000
H	0.74277500	-4.35100500	2.15361200
H	-0.45984000	-3.62953400	3.22816400
H	-0.50098900	-3.27054300	1.50342500
H	-1.52101000	-1.70660100	4.34671000
H	-1.30855600	0.04857500	4.50020500
H	3.51504000	0.71030400	3.21713300
H	0.28822000	1.65335800	3.92493900
H	1.77323300	2.25231900	3.17698300
H	0.37240900	1.85108500	2.17379800
H	5.34574300	-1.44310800	2.07091100
H	5.31445800	-1.01052300	3.78165700
H	5.07515400	-2.69695500	3.28732200
C	2.49486300	-0.40109200	-0.87619600
C	2.36823900	0.90879500	-0.61398200
H	2.20433500	-1.10678700	-0.09944000
H	1.98133400	1.19374000	0.36271700
C	2.74765800	2.06006500	-1.51797000
H	3.36626500	1.69593300	-2.34762100
H	1.84588300	2.48381600	-1.97778100
C	3.48509100	3.15945000	-0.77138200
C	2.95317200	4.45198700	-0.68372300
C	4.71350600	2.90158700	-0.14393000
C	3.62780100	5.46136900	0.00842100
H	2.00517200	4.67020900	-1.17043600
C	5.39170900	3.90619300	0.54630200
H	5.13860600	1.90166300	-0.19970600
C	4.84976700	5.19211800	0.62596400
H	3.19795400	6.45858800	0.06123200
H	6.34564700	3.68730600	1.02025100
H	5.37757900	5.97635200	1.16249500
C	3.03356500	-1.01226500	-2.16067000
H	4.10992000	-0.79653500	-2.24066200
H	2.55428800	-0.53831900	-3.02324100
C	2.82399700	-2.51266200	-2.23424800
C	1.73896800	-3.04999200	-2.94113300
C	3.69832300	-3.39333300	-1.58187100
C	1.53452000	-4.43131200	-2.99161200
H	1.05922100	-2.37647000	-3.45575700
C	3.49564900	-4.77380000	-1.62881100
H	4.55180700	-2.99278300	-1.03784400
C	2.41038600	-5.29825300	-2.33482200
H	0.69270900	-4.82984900	-3.55282400
H	4.19010200	-5.44014600	-1.12254400
H	2.25433800	-6.37315600	-2.37935400
H	-1.85527800	-1.84635100	-1.75798600
N	-0.11294900	1.09599700	-3.20253600
O	0.27428700	2.02444500	-3.90902400

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B3LYP SCF energy: -1379.861776 a.u.
B3LYP enthalpy: -1379.318227 a.u.
B3LYP free energy: -1379.406111 a.u.
M06 SCF energy in solution: -1379.29385 a.u.
M06 enthalpy in solution: -1378.750301 a.u.
M06 free energy in solution: -1378.838185 a.u.

Cartesian coordinates

Ru	0.22099400	1.04077800	0.24723300
O	0.31939200	3.29006100	0.48087200
O	-1.29786300	2.31607400	-0.60090800
N	0.95677800	-1.59252300	-0.65339800
N	-1.21499400	-1.62902300	-0.29237300
C	-0.10829100	-0.84427200	-0.24935400
C	0.61908400	-3.01194900	-0.79955500
C	2.29264900	-1.05634500	-0.36555000
C	2.79501100	-1.55678300	1.01214300
C	4.13205500	-0.87867100	1.36727300
C	5.17698200	-1.22058000	0.28640200
C	4.67921200	-0.71903600	-1.08497300
C	3.34287600	-1.41934300	-1.43905300
C	4.48296000	0.81167000	-1.01523600
C	3.42159400	1.15770400	0.06347100
C	2.10715300	0.47639500	-0.34604800
C	3.91336600	0.64661100	1.43175900
C	-2.57466700	-1.18596100	-0.14743500
C	-3.26396100	-1.50015800	1.03922500
C	-4.59820400	-1.10220400	1.15933700
C	-2.59221900	-2.24247100	2.17071100
C	-0.91801000	-2.95824300	-0.86660000
C	-3.21392900	-0.50955400	-1.20308000
C	-5.25796500	-0.41031600	0.13858500
C	-4.55081400	-0.13356500	-1.03421200
C	-2.49867600	-0.16248800	-2.48805700
C	-6.68994900	0.04200700	0.30542200
H	1.88175800	0.78861100	-1.39516700
H	1.06609300	-3.44574200	-1.69861800
H	0.96650400	-3.58737300	0.06976500
H	2.04034000	-1.32425100	1.77090600
H	2.92241900	-2.64832900	0.98815200
H	4.47510800	-1.24661500	2.34341900
H	5.34983200	-2.30578200	0.25582600
H	6.13986000	-0.75061400	0.52815400
H	5.42026500	-0.96066800	-1.85806700

H	2.98705200	-1.09615200	-2.42652600
H	3.49716100	-2.50766600	-1.48700100
H	4.16679100	1.20121800	-1.99252700
H	5.43997500	1.29510800	-0.77379900
H	3.27638800	2.24418100	0.10082700
H	3.17846100	0.88854000	2.20914700
H	4.85126900	1.15099500	1.70159100
H	-5.13528300	-1.33936700	2.07530500
H	-2.21171200	-3.22222000	1.85646700
H	-1.73945600	-1.67990000	2.56593400
H	-3.29505100	-2.40947200	2.99240200
H	-1.40216200	-3.75252400	-0.29220200
H	-1.28591700	-3.01105200	-1.90006300
H	-5.05003800	0.39220100	-1.84549500
H	-1.78881400	-0.93672400	-2.79605800
H	-3.21775000	-0.02196400	-3.30127300
H	-1.93905000	0.77312800	-2.37543000
H	-6.73522500	1.07599200	0.67191900
H	-7.23372800	0.01167700	-0.64503800
H	-7.22774600	-0.58364500	1.02558300
C	0.23016900	0.68637600	2.02857500
H	-0.07083300	-0.23963500	2.53193300
H	0.49759500	1.51041000	2.70730400
O	-1.26685400	4.51236300	-0.42587900
N	-0.76232800	3.44189800	-0.18291200

TS21

B3LYP SCF energy: -1999.161247 a.u.
B3LYP enthalpy: -1998.326588 a.u.
B3LYP free energy: -1998.446599 a.u.
M06 SCF energy in solution: -1998.30656 a.u.
M06 enthalpy in solution: -1997.471901 a.u.
M06 free energy in solution: -1997.591912 a.u.

Cartesian coordinates

Ru	0.96080100	-0.42952800	-0.15179400
O	-0.10523900	-3.96655900	-0.57773700
O	1.23007200	-2.31775700	-1.19390300
N	2.57267800	1.73850500	0.87231600
N	0.55672100	2.59002300	0.76657800
C	1.28447600	1.46083700	0.51356200
C	2.80101100	3.14890700	1.19760700
C	3.62446500	0.83843600	0.39726400
C	4.12207800	1.27928700	-1.00781800
C	5.13861900	0.26025600	-1.55544500
C	6.33568000	0.17306800	-0.58579600
C	5.84121300	-0.27154600	0.80664300
C	4.83452100	0.76641600	1.35537200
C	5.15880000	-1.65024900	0.68435900
C	3.95115300	-1.56321600	-0.28755200
C	2.96396700	-0.53979200	0.29094300
C	4.45354700	-1.11493300	-1.67426700
C	-0.79734800	2.88604600	0.39632300
C	-1.04995700	3.34718700	-0.91602500
C	-2.36484500	3.64174900	-1.27609700
C	0.07379700	3.57088100	-1.90384700
C	-0.40514500	-0.03669500	-1.53919600
C	1.36671600	3.65661500	1.39311800
C	-1.82751000	2.83074000	1.35053600
C	-3.42619100	3.52669100	-0.36771200
C	-3.13245000	3.14129700	0.94031500
C	-1.57785200	2.49020900	2.80248900
C	-4.84348500	3.81012200	-0.80538600
H	2.65013800	-0.87130500	1.31177200
H	-0.58761900	0.96841500	-1.90955500
H	3.41311300	3.25836900	2.09698300
H	3.31061800	3.66331600	0.37122800
H	3.25803600	1.35620700	-1.68086400
H	4.58303400	2.27521900	-0.94623600
H	5.48571800	0.59338500	-2.54243700
H	6.84145300	1.14686500	-0.51721300
H	7.07486100	-0.54470400	-0.96532000
H	6.69224600	-0.33857900	1.49682700
H	4.49286100	0.48067800	2.35932000
H	5.32243000	1.74857700	1.44214200
H	4.82611500	-1.99913200	1.67172200
H	5.87987300	-2.39072200	0.31164700
H	3.46644200	-2.53753800	-0.37226400
H	3.61264400	-1.07136500	-2.37642600
H	5.16155500	-1.85590800	-2.06855000
H	-2.56881000	3.97418900	-2.29163400
H	0.69714000	4.42476700	-1.60526700
H	0.73623100	2.70478800	-1.98831600
H	-0.32575000	3.79155600	-2.89804100
H	1.17832900	4.61803900	0.90730900
H	1.10418700	3.75415900	2.45445000
H	-3.93705300	3.07710800	1.67017700
H	-1.67066000	3.38770500	3.42849500
H	-2.31171000	1.76436500	3.16832800
H	-0.58139300	2.07276700	2.96412200
H	-5.20611200	3.02162500	-1.47710500
H	-5.52579200	3.86182600	0.04877800
H	-4.91257000	4.75730400	-1.35305700
C	-1.38895100	-0.42589300	-0.34410600
C	-0.62841700	-0.65656000	1.04837400
H	-1.96486000	0.48601700	-0.17438600
H	-0.83088000	0.18530900	1.71015000
C	-0.73225500	-1.97876600	1.82196800
H	-0.63611900	-2.82809500	1.14387400
H	0.13952500	-2.01472200	2.49288300
C	-1.98056900	-2.11029200	2.68565000
C	-2.19168400	-1.25816000	3.78096400
C	-2.93130500	-3.10954100	2.43418900
C	-3.32518600	-1.38325400	4.58525500
H	-1.44882500	-0.49942100	4.01845900
C	-4.06698200	-3.24017200	3.23769200
H	-2.77308900	-3.79616000	1.60650700
C	-4.27167200	-2.37414300	4.31261100
H	-3.46393900	-0.71570300	5.43237900
H	-4.78887700	-4.02425700	3.02392500
H	-5.15394300	-2.47619300	4.93896900
C	-2.33928400	-1.58186600	-0.74851600
H	-2.96730200	-1.81641400	0.11708400
H	-1.75195600	-2.47654700	-0.97042900
C	-3.23578500	-1.22260000	-1.91628700
C	-2.98659000	-1.71260500	-3.20569700
C	-4.34908800	-0.38883900	-1.72794500
C	-3.81355600	-1.36888500	-4.27793500
H	-2.14393400	-2.38067800	-3.36777100
C	-5.17939200	-0.04425200	-2.79524000
H	-4.57151200	-0.01512100	-0.73022300
C	-4.91135900	-0.53073300	-4.07736300
H	-3.60281800	-1.76407400	-5.26841400
H	-6.04480500	0.59214900	-2.62450000
H	-5.55930300	-0.26764200	-4.90944700
H	-0.39388100	-0.77735000	-2.34092900
N	0.84083900	-3.56388900	-1.28198800
O	1.44653200	-4.28453800	-2.07418000

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B3LYP SCF energy: -1999.170851 a.u.
B3LYP enthalpy: -1998.334976 a.u.
B3LYP free energy: -1998.456759 a.u.
M06 SCF energy in solution: -1998.316221 a.u.
M06 enthalpy in solution: -1997.480346 a.u.
M06 free energy in solution: -1997.602129 a.u.

Cartesian coordinates

Ru	-0.97259200	-0.45495800	0.19021900
O	-1.75009700	-3.36249200	-0.59472000
O	-0.90690500	-2.36159200	1.17684600
N	-2.49738600	1.72402100	-0.97542800
N	-0.44837600	2.49173000	-0.94804700
C	-1.21787700	1.41202700	-0.61638600
C	-2.66890700	3.12058600	-1.38597200
C	-3.57153800	0.91670300	-0.39429800
C	-3.96021300	1.46963800	1.00569500
C	-5.00448100	0.55413000	1.67024000
C	-6.25863700	0.48838700	0.77449900
C	-5.87359500	-0.06522200	-0.61365400
C	-4.83744400	0.87133300	-1.27794100
C	-5.27113400	-1.47505300	-0.44362000
C	-4.00426300	-1.40984000	0.45181200
C	-2.98777400	-0.49636600	-0.25246500
C	-4.39614800	-0.85207600	1.83455300
C	0.94304600	2.71983400	-0.68574700
C	1.31455000	3.29071400	0.55217900
C	2.66969200	3.51207300	0.80256100
C	0.28331000	3.72389900	1.57069100
C	0.26996600	0.05567700	1.64448500
C	-1.21798700	3.54640600	-1.64083800
C	1.90211100	2.48639700	-1.68702500

C	3.65707700	3.22092500	-0.14797600
C	3.25039700	2.72785100	-1.38851800
C	1.52382800	2.03533500	-3.07971000
C	5.11681900	3.44609800	0.16939000
H	-2.77098200	-0.90554000	-1.26100100
H	0.43449800	1.08950100	1.93763500
H	-3.29605800	3.20268600	-2.27780000
H	-3.13432500	3.71032500	-0.58412300
H	-3.05662200	1.53053200	1.62709400
H	-4.36224700	2.48803300	0.90817900
H	-5.27239300	0.96517700	2.65264400
H	-6.70584700	1.48792100	0.67582200
H	-7.01782800	-0.15702400	1.23588300
H	-6.76576700	-0.11615100	-1.25138300
H	-4.57472200	0.50700400	-2.27998600
H	-5.26661800	1.87757500	-1.39558500
H	-5.01396700	-1.90425600	-1.42087800
H	-6.01343000	-2.14399900	0.01369000
H	-3.59222400	-2.41403800	0.54866700
H	-3.51624600	-0.81313900	2.49005900
H	-5.12205400	-1.52321700	2.31336800
H	2.96364600	3.92780800	1.76408200
H	-0.16430700	4.68601400	1.28458900
H	-0.53471200	3.00707700	1.67388900
H	0.74375100	3.86174700	2.55366100
H	-0.97769200	4.53160300	-1.23119400
H	-0.97102300	3.55117700	-2.71048200
H	3.99796000	2.52359400	-2.15217800
H	1.50745100	2.89062900	-3.76912000
H	2.25110500	1.31737800	-3.47072800
H	0.53663000	1.56756400	-3.10966900
H	5.45233500	2.77564600	0.97067000
H	5.75039300	3.26616300	-0.70451600
H	5.29782300	4.47178500	0.51283100
C	1.35790600	-0.45940100	0.59602900
C	0.73060200	-0.83695800	-0.82583900
H	1.97441700	0.41833500	0.39084700
H	0.98885200	-0.06765900	-1.55161800
C	0.96786800	-2.22938700	-1.43649100
H	1.05168300	-2.99414500	-0.66255500
H	0.07702500	-2.49639800	-2.01617200
C	2.17928500	-2.29025300	-2.35594800
C	2.16193000	-1.63345400	-3.59679500
C	3.32529100	-3.02174700	-2.01621600
C	3.25928300	-1.68424500	-4.45704700
H	1.26855100	-1.09122300	-3.89936000
C	4.42738500	-3.07711300	-2.87390100
H	3.35025600	-3.57054000	-1.07814000
C	4.40150600	-2.40335700	-4.09511100
H	3.21767100	-1.17507900	-5.41697400
H	5.30258700	-3.65491400	-2.58787000
H	5.25608700	-2.44818500	-4.76500300
C	2.22292300	-1.58241400	1.22180100
H	2.92134100	-1.94109900	0.45872400
H	1.57585200	-2.41814000	1.50263700
C	3.01919600	-1.11453500	2.42360500
C	2.64571100	-1.46782600	3.72743500
C	4.16292400	-0.31948900	2.25278100
C	3.38432700	-1.03044500	4.82957000
H	1.77464600	-2.10129800	3.87784300
C	4.90437700	0.11888200	3.35042900
H	4.47967000	-0.05108400	1.24668200
C	4.51477300	-0.23293400	4.64531700
H	3.07879500	-1.32016000	5.83176900
H	5.79316400	0.72632900	3.19581400
H	5.09340800	0.10368100	5.50159000
H	0.18100500	-0.60841400	2.50813800
N	-1.26062200	-3.46222200	0.54745900
O	-1.08166400	-4.53026300	1.12694600

TS22

B3LYP SCF energy: -1999.160188 a.u.
B3LYP enthalpy: -1998.326794 a.u.
B3LYP free energy: -1998.448272 a.u.
M06 SCF energy in solution: -1998.29677 a.u.
M06 enthalpy in solution: -1997.463376 a.u.
M06 free energy in solution: -1997.584854 a.u.

Cartesian coordinates

Ru	0.89817200	0.24383300	-0.47920600
O	0.93784000	1.99105100	-1.81363600
O	0.96993300	0.08850500	-2.85664900
N	2.47278100	-1.79468300	0.83789200
N	0.40747100	-2.30836300	1.35193100
C	1.17867400	-1.43603600	0.62253200
C	2.64223800	-2.80486200	1.88234800
C	3.54319600	-0.92206100	0.34957600
C	3.99493700	0.07962200	1.44327900
C	5.01962200	1.06734200	0.85374700
C	6.25137600	0.28144000	0.36019700
C	5.81372000	-0.73015100	-0.71944100
C	4.78752000	-1.71767400	-0.11444700
C	5.18551900	0.04335500	-1.89894400
C	3.93558700	0.82357600	-1.41217200
C	2.92894300	-0.21017100	-0.87091100
C	4.36576700	1.82456200	-0.32107600
C	-0.99395600	-2.57831300	1.21073500
C	-1.86389500	-2.23197000	2.26156600
C	-3.21761000	-2.56924600	2.14689000
C	-1.36223400	-1.53434000	3.50504400
C	-1.33433800	0.11329400	-0.83337400
C	1.22063100	-3.36384800	1.99745900
C	-1.46179100	-3.29270300	0.08760200
C	-3.71818600	-3.25418300	1.03662100
C	-2.82072900	-3.61672700	0.02583100
C	-0.53839200	-3.68221000	-1.04399400
C	-5.19013600	-3.56994400	0.91491100
H	2.79553100	-0.98002400	-1.64546300
H	3.37529600	-3.56386900	1.59517600
H	2.97847900	-2.34190100	2.82083500
H	3.12182300	0.62014300	1.82458900
H	4.44228100	-0.46503300	2.28767300
H	5.32441500	1.77916600	1.63283000
H	6.72857200	-0.24069300	1.20209100
H	6.99967000	0.97030300	-0.05463000
H	6.68645300	-1.29693300	-1.07012100
H	4.48716100	-2.46536800	-0.86045800
H	5.25057600	-2.25736100	0.72572500
H	4.90174000	-0.64860000	-2.70294400
H	5.92778400	0.73624900	-2.32049400
H	3.50737800	1.36981600	-2.25846200
H	3.49533000	2.39113100	0.03210400
H	5.07641900	2.55134700	-0.73872000
H	-3.89615500	-2.29342300	2.95141800
H	-0.79207100	-2.21801100	4.14834100
H	-0.69869900	-0.69804200	3.26608100
H	-2.19757400	-1.15137100	4.09895000
H	0.90102800	-3.52445100	3.03068700
H	1.10478300	-4.31158000	1.45458700
H	-3.18701100	-4.17020600	-0.83669800
H	0.35402800	-4.20905700	-0.68802900
H	-1.05304200	-4.33824700	-1.75226100
H	-0.18486200	-2.80180600	-1.59392200
H	-5.70909300	-2.78568100	0.34794800
H	-5.35591800	-4.51680600	0.38952800
H	-5.67021600	-3.63650800	1.89675100
C	0.70339600	1.25057400	1.08846000
C	-1.31459000	0.97320000	0.30249100
H	0.55728500	0.91982300	2.12424700
H	0.79944000	2.34057100	1.01707000
H	-1.53986200	0.49170900	1.25033600
C	-1.76368700	2.43098300	0.19797600
H	-2.77885500	2.41118800	-0.22463700
H	-1.13940500	2.96058600	-0.52814600
C	-1.80630500	3.19023800	1.50912400
C	-2.65379000	2.77465800	2.54731800
C	-1.02870800	4.33886400	1.70650300
C	-2.70829000	3.47472600	3.75300300
H	-3.28694400	1.90098500	2.40482600
C	-1.08184700	5.04470700	2.91073600
H	-0.37825600	4.68585300	0.90650700
C	-1.91932200	4.61244500	3.93998400
H	-3.37365300	3.13743000	4.54381200
H	-0.46980800	5.93328700	3.04170900
H	-1.96351700	5.16074900	4.87718600
H	-1.55616900	-0.92411900	-0.61178500
C	-1.86555300	0.56556900	-2.19302300
H	-1.53905600	1.58293700	-2.42051300
H	-1.43450600	-0.08045700	-2.96423300
C	-3.38562300	0.50128200	-2.28230700
C	-4.14515200	1.66129400	-2.48901600
C	-4.06314700	-0.72469600	-2.19405900

C	-5.53762000	1.60423700	-2.59341900
H	-3.63885600	2.61902700	-2.58627200
C	-5.45271300	-0.78699700	-2.29996300
H	-3.49611100	-1.64056200	-2.04865000
C	-6.19745800	0.37926600	-2.49644500
H	-6.10310100	2.51805400	-2.75690300
H	-5.95534700	-1.74962300	-2.24184100
H	-7.27980400	0.33065900	-2.58154600
N	1.01456600	1.36287600	-2.94274400
O	1.11757400	1.95752700	-4.00181500

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B3LYP SCF energy: -1999.167612 a.u.
B3LYP enthalpy: -1998.333068 a.u.
B3LYP free energy: -1998.458958 a.u.
M06 SCF energy in solution: -1998.299869 a.u.
M06 enthalpy in solution: -1997.465325 a.u.
M06 free energy in solution: -1997.591215 a.u.

Cartesian coordinates

Ru	0.88385300	-0.32186700	-0.33870300
O	1.54031600	-0.79556300	-2.55113000
O	0.83128100	-2.34722300	-1.21766800
N	2.67926600	1.80896000	0.41592100
N	0.72405600	2.79315000	0.42026700
C	1.35520400	1.59049600	0.22198700
C	3.02577100	3.22609300	0.54678300
C	3.65056300	0.73003600	0.19291300
C	4.24652300	0.80473900	-1.23529500
C	5.21316500	-0.37594000	-1.46230100
C	6.34796600	-0.32926500	-0.42097300
C	5.74264600	-0.42112300	0.99440300
C	4.81133700	0.79343400	1.21540300
C	4.95140500	-1.74238600	1.12773000
C	3.79635600	-1.77384400	0.08993500
C	2.86254200	-0.58306700	0.41996200
C	4.43021500	-1.69532000	-1.31657700
C	-0.67785100	3.04267700	0.58499100
C	-1.37113700	3.71243400	-0.44529400
C	-2.73215700	3.97934900	-0.27242700
C	-0.66766600	4.15538800	-1.70831600
C	1.66309000	3.83724800	0.88454700
C	-1.31951700	2.73246600	1.79921800
C	-3.41620200	3.61753400	0.89455600
C	-2.68739800	3.01139700	1.92062000
C	-0.56776500	2.18756500	2.99364200
C	-4.90147100	3.85861200	1.02757600
H	2.68915900	-0.63279300	1.50298000
H	3.76996800	3.38914800	1.32994000
H	3.42858100	3.61459700	-0.39908100
H	3.43789800	0.77390200	-1.97375500
H	4.78172900	1.75720500	-1.36486300
H	5.63475100	-0.30494000	-2.47348100
H	6.92791800	0.59924800	-0.52529800
H	7.04491600	-1.16175200	-0.58734900
H	6.54499000	-0.39352700	1.74379400
H	4.40104100	0.78888000	2.23442100
H	5.39435700	1.71956600	1.09919300
H	4.54997700	-1.84140900	2.14573400
H	5.63017000	-2.59236300	0.96784200
H	3.24503700	-2.71670600	0.19052200
H	3.67905900	-1.76150300	-2.10417800
H	5.11073400	-2.54726200	-1.45497000
H	-3.27258300	4.48283100	-1.07147400
H	-0.02084900	3.37216200	-2.11430200
H	-1.39292200	4.43622700	-2.47786400
H	-0.03268500	5.03242400	-1.52475500
H	1.47560500	4.78580800	0.37427600
H	1.54145900	3.99841800	1.96457500
H	-3.19161600	2.75438600	2.85011400
H	-0.20803600	3.00970200	3.62782300
H	-1.22138400	1.56860300	3.61685200
H	0.29788600	1.58766500	2.70688600
H	-5.47111700	3.04713900	0.55571600
H	-5.20854900	3.90704100	2.07732600
H	-5.20164100	4.79303100	0.54080700
C	0.00734700	-0.79874500	1.20624600
H	-0.80872600	-0.21710200	1.66216900
C	0.22313400	-2.12189100	1.91443400
H	0.98710900	-2.71091100	1.39870900
H	0.62541100	-1.87799700	2.91367100
C	-1.05090800	-2.93518700	2.06913300
C	-1.89572800	-2.76656400	3.17485400
C	-1.41579800	-3.85951900	1.07881100
C	-3.07666700	-3.50247100	3.29278600
H	-1.61935800	-2.06253400	3.95759700
C	-2.59417700	-4.59952500	1.19694800
H	-0.76969500	-3.99449800	0.21487800
C	-3.42941000	-4.42309600	2.30362100
H	-3.71580600	-3.36301000	4.16097300
H	-2.85604800	-5.31972500	0.42586900
H	-4.34384300	-5.00280800	2.39757500
C	-1.70316900	-0.54389700	-1.27409600
C	-1.03534100	0.50032100	-1.82636500
H	-1.27648400	1.51143800	-1.52697000
H	-0.40901800	0.37427400	-2.70170200
H	-1.54665100	-1.54751400	-1.66288600
C	-2.83427200	-0.39460000	-0.27982800
H	-2.77807000	0.59246200	0.19234000
H	-2.74357800	-1.14640500	0.51066400
C	-4.18636200	-0.56306400	-0.96173200
C	-4.88284200	-1.77540100	-0.88226500
C	-4.75438200	0.48977000	-1.69358400
C	-6.11743800	-1.93293600	-1.51679700
H	-4.45707500	-2.59828200	-0.31255000
C	-5.98878300	0.33681400	-2.32541900
H	-4.22191400	1.43563200	-1.76609400
C	-6.67487300	-0.87751000	-2.23983000
H	-6.64442500	-2.88088100	-1.44269400
H	-6.41550200	1.16491200	-2.88601800
H	-7.63613000	-0.99831700	-2.73237400
N	1.27915400	-2.04005800	-2.38887500
O	1.44382900	-2.87506200	-3.25980600

TS23

B3LYP SCF energy: -1999.160128 a.u.
B3LYP enthalpy: -1998.326255 a.u.
B3LYP free energy: -1998.445727 a.u.
M06 SCF energy in solution: -1998.296452 a.u.
M06 enthalpy in solution: -1997.462579 a.u.
M06 free energy in solution: -1997.582051 a.u.

Cartesian coordinates

Ru	0.88275200	-0.39229400	-0.43858400
O	1.76560900	-0.26052700	-2.63193300
O	0.89649300	-2.09146500	-1.85544600
N	2.52265600	1.30241000	1.25255400
N	0.56474900	2.28129300	1.26557900
C	1.26138500	1.22180300	0.73949900
C	2.78355500	2.53290700	2.00252900
C	3.59350900	0.48597300	0.67338000
C	4.31654600	1.27126200	-0.45251700
C	5.39235000	0.38599200	-1.11236900
C	6.41213000	-0.07049700	-0.05054300
C	5.68117900	-0.86891700	1.04771300
C	4.64054600	0.05278600	1.72791900
C	4.98541700	-2.09229600	0.40961000
C	3.94438600	-1.62065500	-0.64364200
C	2.90343700	-0.76452800	0.11269900
C	4.70209700	-0.83871600	-1.73971800
C	-0.70699200	2.81785300	0.88842400
C	-0.81125100	3.55378400	-0.31101300
C	-2.04047800	4.14127500	-0.62755800
C	0.37646500	3.73394700	-1.22791100
C	1.36583400	3.06245000	2.23385100
C	-1.79287700	2.73868000	1.78126700
C	-3.14951100	4.04779500	0.22137100
C	-2.99865200	3.35531300	1.42569700
C	-1.68380800	2.01984400	3.10636700
C	-4.47843700	4.65529900	-0.16224600
H	2.59636100	-1.36689000	0.98562200
H	3.31280800	2.32610900	2.93663200
H	3.39383100	3.22913500	1.41116600
H	3.57960500	1.58691600	-1.20073600
H	4.78350000	2.17683000	-0.03881000
H	5.90461300	0.96502700	-1.89231900
H	6.92515300	0.79724500	0.38912200
H	7.18520400	-0.69543600	-0.51771400
H	6.40315600	-1.20679400	1.80312100
H	4.13428700	-0.47156800	2.54987900
H	5.15478200	0.92387300	2.16161500
H	4.49446200	-2.69599300	1.18540500

H	5.73943600	-2.73599400	-0.06554100
H	3.45647100	-2.49830700	-1.08302400
H	4.01986700	-0.51724700	-2.52950000
H	5.45310000	-1.49493100	-2.20149300
H	-2.12855200	4.70096000	-1.55635000
H	0.74920100	2.77763300	-1.60984700
H	0.11172200	4.36231700	-2.08348900
H	1.21290100	4.21578500	-0.70585600
H	1.26710400	4.13356800	2.03546200
H	1.01759100	2.87074900	3.25646100
H	-3.84420200	3.28205900	2.10682500
H	-1.34038400	2.69617600	3.90095300
H	-2.65707900	1.62743300	3.41734400
H	-0.97629400	1.18746600	3.05698700
H	-5.13463900	3.90111200	-0.61648500
H	-5.00356900	5.05770700	0.71080600
H	-4.35513300	5.46511900	-0.88875600
C	-0.19607000	-1.20578700	0.87821600
H	-0.71648900	-0.67607600	1.68600800
C	-0.21376000	-2.71571900	1.05885700
H	0.12336400	-3.21258000	0.14417700
H	0.57244700	-2.90522600	1.81249800
C	-1.51424100	-3.32829500	1.54774300
C	-1.98650700	-3.08226500	2.84618900
C	-2.27029100	-4.16001500	0.71106700
C	-3.18480800	-3.64093000	3.29205900
H	-1.40370500	-2.45504700	3.51820200
C	-3.46820900	-4.72623000	1.15537800
H	-1.91244900	-4.37206700	-0.29396800
C	-3.93160300	-4.46529800	2.44637000
H	-3.53139500	-3.44047800	4.30269400
H	-4.03498800	-5.37565800	0.49312000
H	-4.86166000	-4.90666700	2.79421600
C	-1.52676300	-0.66192700	-0.77097800
C	-0.86108300	0.30489100	-1.57728100
H	-1.12377800	1.34760700	-1.43624200
H	-0.60066500	0.03941100	-2.59701200
H	-1.56774000	-1.67067500	-1.17705500
C	-2.75018100	-0.27816000	0.06171400
H	-2.60781800	0.72203200	0.47775200
H	-2.88793100	-0.97182400	0.89502000
C	-4.00495500	-0.30303900	-0.80193300
C	-4.86955400	-1.40485900	-0.76386500
C	-4.31934400	0.76434000	-1.65614400
C	-6.01892900	-1.44068300	-1.55703000
H	-4.64125200	-2.23970600	-0.10549400
C	-5.46637200	0.73111700	-2.44975700
H	-3.66006800	1.62768000	-1.69750400
C	-6.32151700	-0.37299700	-2.40278400
H	-6.67813500	-2.30396000	-1.51166700
H	-5.69320400	1.56778200	-3.10598700
H	-7.21542500	-0.39945500	-3.02036900
N	1.48838000	-1.49117900	-2.83943100
O	1.75766800	-2.06986700	-3.87673100

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B3LYP SCF energy: -1999.174922 a.u.
B3LYP enthalpy: -1998.338898 a.u.
B3LYP free energy: -1998.457888 a.u.
M06 SCF energy in solution: -1998.316101 a.u.
M06 enthalpy in solution: -1997.480077 a.u.
M06 free energy in solution: -1997.599067 a.u.

Cartesian coordinates

Ru	0.91655500	-0.47680600	-0.36938100
O	1.72052400	-0.68730700	-2.69771000
O	0.77845600	-2.29884700	-1.58437300
N	2.56504000	1.29095400	1.22626300
N	0.61134600	2.27706000	1.22081800
C	1.29595300	1.19956400	0.72450200
C	2.83599900	2.53195300	1.95448500
C	3.62343300	0.48144800	0.62808700
C	4.36973300	1.28270700	-0.47285700
C	5.42387400	0.39112500	-1.15754600
C	6.43168300	-0.11604900	-0.10705500
C	5.68465200	-0.92714100	0.97134900
C	4.65479700	-0.01325500	1.67342000
C	4.96092700	-2.11744600	0.30721500
C	3.93893200	-1.59847000	-0.74460400
C	2.92569200	-0.72849900	0.01039300
C	4.70679200	-0.79873100	-1.81918100
C	-0.66112500	2.81756900	0.84277400
C	-0.77085100	3.51341100	-0.38083100
C	-1.99069500	4.11930700	-0.69483200
C	0.40033400	3.62993900	-1.32840100
C	1.42348300	3.08916200	2.15476500
C	-1.73069100	2.79565700	1.75698100
C	-3.08656100	4.08076700	0.17615900
C	-2.92920000	3.42668100	1.39984400
C	-1.61718400	2.13409400	3.11144000
C	-4.40700300	4.70539800	-0.20860800
H	2.47448600	-1.34441500	0.83461700
H	3.34863300	2.33574800	2.90059600
H	3.46505600	3.20738200	1.35950000
H	3.64123600	1.64467900	-1.20854800
H	4.85777300	2.16043700	-0.02710500
H	5.94939900	0.98020200	-1.92048200
H	6.96259400	0.72873700	0.35470000
H	7.19151100	-0.74502400	-0.58957800
H	6.39836000	-1.29857500	1.71825500
H	4.13197900	-0.55694700	2.47167700
H	5.17033200	0.83843600	2.14051300
H	4.45061000	-2.72471400	1.06721700
H	5.69241300	-2.77240600	-0.18565800
H	3.43250300	-2.45521100	-1.19929500
H	4.01565600	-0.45119500	-2.59113400
H	5.43895300	-1.45721100	-2.30619500
H	-2.08263000	4.64868200	-1.64082700
H	0.70225000	2.65446700	-1.72469000
H	0.14865100	4.27679400	-2.17403300
H	1.27853000	4.05805100	-0.82887700
H	1.34037800	4.15102300	1.90563500
H	1.06834000	2.95139600	3.18309200
H	-3.76289700	3.39669100	2.09856700
H	-1.32401300	2.85826500	3.88391100
H	-2.57847600	1.70961300	3.41786600
H	-0.87467500	1.33215800	3.11143500
H	-5.05046600	3.97387500	-0.71514100
H	-4.95280600	5.06552300	0.66984000
H	-4.26798000	5.54857600	-0.89351000
C	-0.53778100	-1.06025900	0.89133200
C	-0.47748100	-2.52078100	1.36967600
H	-0.13040900	-3.15977400	0.55068200
H	0.28252600	-2.57932400	2.16250300
C	-1.79022300	-3.06412900	1.90979900
C	-2.26993400	-2.67034200	3.16846500
C	-2.55946400	-3.96520300	1.16027100
C	-3.48484500	-3.15105700	3.65842100
H	-1.68002600	-1.98459400	3.77394700
C	-3.77583600	-4.45133400	1.64742300
H	-2.19664100	-4.29417100	0.18912100
C	-4.24474900	-4.04274000	2.89721400
H	-3.83575200	-2.83534500	4.63788700
H	-4.35219000	-5.15516200	1.05216600
H	-5.18931800	-4.42112500	3.27881500
C	-1.46049900	-0.78966400	-0.38607700
C	-0.73345300	0.15742600	-1.38894800
C	-2.85026300	-0.23165400	0.04815600
H	-2.72564800	0.79105300	0.41322700
H	-3.20563000	-0.83747300	0.88854800
C	-3.87768000	-0.27048200	-1.06468900
C	-4.64470200	-1.42592700	-1.27625500
C	-4.08441300	0.82745300	-1.91247900
C	-5.58493100	-1.48586200	-2.30593900
H	-4.50558500	-2.28260800	-0.62044100
C	-5.02394500	0.77128200	-2.94405100
H	-3.50497900	1.73439400	-1.75947900
C	-5.77761600	-0.38668400	-3.14540200
H	-6.17017700	-2.39064500	-2.45021900
H	-5.16791100	1.63373300	-3.59042700
H	-6.50995400	-0.43134200	-3.94725600
H	-0.81785600	-0.39092000	1.71063600
H	-1.04011500	1.19712600	-1.31047200
H	-0.76484400	-0.19227500	-2.42082500
H	-1.60658000	-1.75388200	-0.87944500
N	1.31317700	-1.88985900	-2.69806200
O	1.40965400	-2.63456400	-3.65893900

TS24

B3LYP SCF energy: -1999.144862 a.u.
B3LYP enthalpy: -1998.312211 a.u.
B3LYP free energy: -1998.436114 a.u.

M06 SCF energy in solution: -1998.288597 a.u.
M06 enthalpy in solution: -1997.455946 a.u.
M06 free energy in solution: -1997.579849 a.u.

Cartesian coordinates

Ru	-0.88814000	-0.41666500	-0.15817300
O	-1.02022100	-3.41956600	1.66948500
O	-1.20241400	-2.57647000	-0.35903300
N	-2.24108500	2.11959300	-0.48631300
N	-0.15768800	2.69595900	-0.14845500
C	-0.99177800	1.61743700	-0.27771300
C	-2.33188000	3.57195800	-0.32393300
C	-3.39566900	1.22178200	-0.39847300
C	-3.96579100	1.20313500	1.04540900
C	-5.09897400	0.16434100	1.15004800
C	-6.22033100	0.53721700	0.15899000
C	-5.65427000	0.55385400	-1.27642400
C	-4.52955600	1.61268800	-1.37349100
C	-5.09662800	-0.84593000	-1.61305800
C	-3.96196700	-1.22005200	-0.62338100
C	-2.85037400	-0.16566600	-0.76235800
C	-4.53353200	-1.22873600	0.80887000
C	1.27521200	2.73824300	-0.13896600
C	1.94270400	3.02606400	1.06555600
C	3.33826900	3.15925900	1.04067000
C	1.19884500	3.22714900	2.36596200
C	-0.85651800	3.98007100	-0.37791600
C	1.98766100	2.63742600	-1.35395600
C	4.07516000	3.02428600	-0.13731500
C	3.37808800	2.76670000	-1.32454700
C	1.27872000	2.43333800	-2.67420200
C	5.58152600	3.14062700	-0.13812100
H	-2.53930500	-0.13674500	-1.83568300
H	-2.92874000	4.02934700	-1.11784900
H	-2.79310500	3.82589000	0.64014600
H	-3.15550000	0.95503300	1.74154300
H	-4.34513900	2.19992200	1.31301700
H	-5.49539100	0.16724700	2.17417800
H	-6.64179400	1.52032800	0.41420100
H	-7.04075200	-0.18948200	0.22824100
H	-6.45061000	0.81791800	-1.98482100
H	-4.13351400	1.66136400	-2.39709300
H	-4.93632900	2.60606000	-1.13132500
H	-4.71797800	-0.86619100	-2.64452300
H	-5.90447900	-1.58876100	-1.55686700
H	-3.56859600	-2.20962100	-0.86819600
H	-3.75124800	-1.50610200	1.52627500
H	-5.32468000	-1.98620400	0.88889700
H	3.85821700	3.37786000	1.97129700
H	0.23792900	2.70816300	2.36934900
H	1.78761700	2.86245400	3.21339100
H	0.99895500	4.29275600	2.54468000
H	-0.58115500	4.71212000	0.38642500
H	-0.57638800	4.38812200	-1.35783100
H	3.93198400	2.67348300	-2.25645900
H	0.81539300	3.36514100	-3.02534900
H	1.98567900	2.11231400	-3.44499700
H	0.48514100	1.68406900	-2.60517800
H	6.05419300	2.15552700	-0.24300600
H	5.93436100	3.75680400	-0.97300900
H	5.94998400	3.58615300	0.79126000
C	1.14347200	-0.76880700	-0.96243700
C	0.99701800	-1.71647300	-2.16094900
H	0.50320800	-2.63835500	-1.84459000
H	0.35725600	-1.25742600	-2.92626000
C	2.35612200	-2.01301600	-2.77644100
C	2.78258200	-1.35510900	-3.93723000
C	3.22298600	-2.94064900	-2.18001200
C	4.03960700	-1.61277500	-4.48925300
H	2.11698600	-0.64271900	-4.42089900
C	4.47915500	-3.20194400	-2.72768600
H	2.90392000	-3.47057800	-1.28513700
C	4.89312400	-2.53667800	-3.88470100
H	4.34805900	-1.09666100	-5.39505400
H	5.13261200	-3.93071600	-2.25499100
H	5.86999900	-2.74246100	-4.31408600
C	1.35549200	-1.24451900	0.35355600
C	-0.46068800	-0.42767900	1.64222700
C	2.45968800	-0.66813800	1.21566400
H	2.52451400	0.41279100	1.06240200
H	3.38881800	-1.07478200	0.77751200
C	2.47537300	-0.98003300	2.70326700
C	1.87683500	-2.12180500	3.25449800
C	3.17606900	-0.11763700	3.56078400
C	1.96893900	-2.38233700	4.62445000
H	1.31217000	-2.80725000	2.62999400
C	3.27302000	-0.37852400	4.92773500
H	3.65703600	0.76615600	3.14624400
C	2.66587400	-1.51510200	5.46631200
H	1.48821800	-3.26847900	5.03023000
H	3.82025400	0.30597200	5.57129300
H	2.73503300	-1.72138400	6.53108200
H	1.66559200	0.15326300	-1.20812900
H	-0.07335400	0.41334100	2.22557700
H	-0.65132000	-1.35151400	2.19697400
H	1.08350300	-2.27810100	0.54687100
N	-1.53425800	-3.47784200	0.53353500
O	-2.32354000	-4.35653900	0.19078400

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B3LYP SCF energy: -1999.151423 a.u.
B3LYP enthalpy: -1998.317666 a.u.
B3LYP free energy: -1998.442646 a.u.
M06 SCF energy in solution: -1998.295049 a.u.
M06 enthalpy in solution: -1997.461292 a.u.
M06 free energy in solution: -1997.461292 a.u.

Cartesian coordinates

Ru	0.78561400	0.05395400	-0.40745800
O	1.85287400	2.39051500	-2.87170500
O	1.19496600	0.31655400	-2.55564500
N	1.91582400	-1.09889600	1.98380600
N	-0.12550900	-0.57214700	2.57988600
C	0.74622200	-0.56489500	1.52575200
C	1.93147600	-1.32377800	3.43180900
C	3.13471800	-0.93859300	1.18135000
C	3.89827400	0.34289400	1.60434300
C	5.10766600	0.56869700	0.67651000
C	6.05340000	-0.64505800	0.77913100
C	5.29754300	-1.92258800	0.35833500
C	4.09283200	-2.14534700	1.30570200
C	4.80710800	-1.75862500	-1.09671200
C	3.84714100	-0.54391000	-1.19952700
C	2.65218500	-0.82119200	-0.27235100
C	4.60355000	0.72833700	-0.77172400
C	-1.52802900	-0.26929800	2.60583900
C	-1.94823600	1.01190100	3.01349100
C	-3.32237800	1.25812500	3.12671000
C	-0.96818900	2.11549400	3.33461100
C	0.44071800	-1.23576900	3.77455400
C	-2.46849400	-1.29431100	2.37059600
C	-4.27973400	0.27714000	2.85304700
C	-3.82968100	-0.99379400	2.48225800
C	-2.04938800	-2.70867400	2.03497400
C	-5.75693600	0.57995200	2.94728400
H	2.23363400	-1.81497200	-0.55984800
H	2.36858500	-2.29402200	3.68390200
H	2.51491700	-0.54384700	3.93949900
H	3.21580400	1.19807700	1.55345200
H	4.23732800	0.24876200	2.64589500
H	5.63719500	1.47769400	0.99177800
H	6.43179100	-0.74700100	1.80657200
H	6.92700200	-0.49856300	0.12999900
H	5.96812300	-2.78923000	0.42931500
H	3.55942800	-3.06846900	1.04056600
H	4.45249100	-2.26013700	2.33917700
H	4.29746900	-2.67309100	-1.43145900
H	5.66978300	-1.61430200	-1.76219500
H	3.48996100	-0.43386700	-2.22653000
H	3.94601900	1.59997200	-0.86120100
H	5.45392800	0.89644100	-1.44673800
H	-3.65055600	2.24410800	3.44965600
H	-0.70878800	2.68519500	2.43459000
H	-1.40327200	2.81877100	4.05207800
H	-0.03478600	1.72971400	3.75376800
H	0.23503600	-0.64883900	4.67436200
H	-0.01096000	-2.22769200	3.90395500
H	-4.55583400	-1.77984000	2.28441400
H	-1.99977500	-3.32924600	2.94017800
H	-2.77137100	-3.17967300	1.36067400
H	-1.06759000	-2.74563100	1.55609500
H	-6.17420300	0.82065100	1.96067700

H	-6.31829800	-0.27722100	3.33475900
H	-5.94952400	1.43660300	3.60119900
C	-1.43259200	-0.74083200	-0.97072300
C	-0.96770800	-1.93706400	-1.79672800
H	-0.44448100	-1.58099500	-2.68984800
H	-0.25712400	-2.55009700	-1.22399500
C	-2.14692700	-2.81869600	-2.18832900
C	-2.32312200	-4.08675900	-1.62121300
C	-3.08594300	-2.36883700	-3.12768600
C	-3.41123900	-4.88764100	-1.97859100
H	-1.59557900	-4.45625100	-0.90143000
C	-4.17214200	-3.16573500	-3.48818100
H	-2.95794500	-1.38996100	-3.58387200
C	-4.34038200	-4.42809100	-2.91228100
H	-3.52729700	-5.87160200	-1.53125000
H	-4.88595400	-2.80318800	-4.22332500
H	-5.18609300	-5.04950600	-3.19436300
C	-1.54122900	0.52662300	-1.47445200
C	1.06562400	1.77957600	0.10809700
C	-2.43981600	1.57728800	-0.86561700
H	-2.69024800	1.29891600	0.16292700
H	-3.38574600	1.50142500	-1.43221200
C	-1.98924200	3.02878200	-0.90944800
C	-1.35280200	3.58601100	-2.02781400
C	-2.27154800	3.86325900	0.18172700
C	-0.99318200	4.93495000	-2.04086100
H	-1.11701100	2.97547600	-2.89448100
C	-1.91874500	5.21429900	0.16738000
H	-2.78258500	3.44884300	1.04791100
C	-1.27321800	5.75481000	-0.94584000
H	-0.48510000	5.33926400	-2.91182900
H	-2.14782300	5.84165800	1.02549500
H	-0.99120900	6.80433600	-0.96036700
H	-1.97095300	-0.97823400	-0.05896300
H	1.00622200	2.18715500	1.12302100
H	1.33053400	2.49727200	-0.67874900
H	-1.15421500	0.72483100	-2.47084800
N	1.12908100	1.44715400	-3.21540700
O	0.33227900	1.50938900	-4.16574800

TS25

B3LYP SCF energy: -1999.143071 a.u.
B3LYP enthalpy: -1998.311206 a.u.
B3LYP free energy: -1998.441139 a.u.
M06 SCF energy in solution: -1998.286707 a.u.
M06 enthalpy in solution: -1997.454842 a.u.
M06 free energy in solution: -1997.584775 a.u.

Cartesian coordinates

Ru	-0.89609300	-0.25210700	0.29758800
O	-1.63849600	-0.30765600	3.62246500
O	-0.31776200	-1.20685200	2.10766900
N	-2.40715300	-0.15659000	-2.15652800
N	-0.59597800	1.02168600	-2.54365000
C	-1.24676800	0.29063700	-1.59724600
C	-2.67725000	0.44038000	-3.46727100
C	-3.41449200	-0.72937100	-1.25855600
C	-4.41044900	0.35775000	-0.77797300
C	-5.36696700	-0.22766000	0.27818800
C	-6.15591600	-1.39495400	-0.34924700
C	-5.16983200	-2.48041200	-0.82857500
C	-4.22077500	-1.88367200	-1.89753500
C	-4.35896000	-2.99097000	0.38340200
C	-3.55715800	-1.82026900	1.01370100
C	-2.60921100	-1.29313000	-0.07016300
C	-4.53979400	-0.72895200	1.47883400
C	0.75212100	1.51111800	-2.47460700
C	0.97365000	2.86839200	-2.18396200
C	2.29029200	3.34777400	-2.20159700
C	-0.15776700	3.80618300	-1.83592000
C	-1.28741600	0.97566000	-3.85007000
C	1.82652400	0.65213300	-2.78792200
C	3.37690300	2.52161500	-2.49504800
C	3.12188600	1.17531300	-2.78430800
C	1.60506300	-0.80199000	-3.13731100
C	4.78966900	3.05807500	-2.51021400
H	-2.01398400	-2.15878800	-0.45139300
H	-3.05739000	-0.29760700	-4.17924200
H	-3.41537200	1.25041100	-3.38372600
H	-3.85192300	1.20110400	-0.35813900
H	-4.98284500	0.73719200	-1.63645300
H	-6.06312000	0.55599100	0.60529700
H	-6.76349900	-1.03390200	-1.19138200
H	-6.85078400	-1.82091600	0.38670000
H	-5.72636900	-3.31333400	-1.27768100
H	-3.53145700	-2.65177400	-2.27343500
H	-4.80795900	-1.52314500	-2.75506900
H	-3.67556500	-3.79394100	0.07363500
H	-5.04033000	-3.42370300	1.12888100
H	-2.97416600	-2.17717100	1.86771700
H	-3.98493400	0.09566200	1.93890500
H	-5.20467500	-1.13765400	2.25143200
H	2.46583300	4.39980400	-1.98629400
H	-0.41059800	3.72780500	-0.77149000
H	0.12720100	4.84501400	-2.03056000
H	-1.06787100	3.58867200	-2.40268200
H	-1.31685500	1.96720600	-4.31037400
H	-0.76136200	0.29628300	-4.53351800
H	3.95390000	0.51456100	-3.02010900
H	1.21498200	-0.92028700	-4.15716000
H	2.54496800	-1.35896600	-3.08208300
H	0.88955000	-1.27891800	-2.46008900
H	5.41872300	2.54359100	-1.77347100
H	5.26073200	2.91377500	-3.49033600
H	4.81411200	4.12792400	-2.28132500
C	2.77871600	-0.67339000	0.61055800
C	2.50658200	-2.15927000	0.52724400
H	2.02636400	-2.48706900	1.45635600
H	1.79229500	-2.36893300	-0.28304400
C	3.76877000	-2.96882700	0.26340400
C	3.89794800	-3.75902400	-0.88505500
C	4.83663500	-2.93633500	1.17247800
C	5.05870700	-4.50013000	-1.12310400
H	3.07642100	-3.80234800	-1.59781800
C	5.99561400	-3.67629500	0.94143900
H	4.75349400	-2.32153100	2.06531700
C	6.11208000	-4.46102200	-0.20960100
H	5.13660800	-5.10890200	-2.02058000
H	6.80991800	-3.64184200	1.66091900
H	7.01572700	-5.03733600	-0.39001500
C	2.58383200	0.07291500	1.70705700
C	-1.54892600	1.32270700	0.93480500
C	2.97662600	1.52591400	1.83061500
H	3.32111400	1.89729100	0.85774600
H	3.84533300	1.58468600	2.50788100
C	1.89458900	2.45067000	2.37195300
C	1.19918800	2.15443400	3.55425000
C	1.59755100	3.64955100	1.70974000
C	0.23139900	3.02869700	4.05197500
H	1.39455600	1.22807800	4.08750200
C	0.63487500	4.53085600	2.20946100
H	2.12946800	3.89468800	0.79325000
C	-0.05406100	4.22186700	3.38351100
H	-0.30227700	2.77026400	4.96240100
H	0.42755400	5.45949300	1.68255900
H	-0.80395200	4.90398700	3.77576500
H	3.21812900	-0.21591600	-0.27689500
H	-1.83617300	2.20955300	0.35640000
H	-1.69165800	1.40546000	2.01946400
H	2.14945400	-0.39621900	2.58851400
N	-0.57258000	-0.87964700	3.35718400
O	0.28199500	-1.17493200	4.19871700

TS26

B3LYP SCF energy: -1999.163447 a.u.
B3LYP enthalpy: -1998.328781 a.u.
B3LYP free energy: -1998.449234 a.u.
M06 SCF energy in solution: -1998.309868 a.u.
M06 enthalpy in solution: -1997.475202 a.u.
M06 free energy in solution: -1997.595655 a.u.

Cartesian coordinates

Ru	1.01459600	-0.47080400	-0.16625100
O	-0.17606800	-3.93145400	-0.43168400
O	1.19306700	-2.38033300	-1.19087900
N	2.68347200	1.68880900	0.79898200
N	0.68774100	2.58036500	0.75110300
C	1.37865200	1.43142800	0.47882300
C	2.95286700	3.09422300	1.10766300
C	3.70807600	0.76471300	0.31819500
C	4.18219100	1.16883600	-1.10590000
C	5.16443100	0.11857500	-1.65676600

C	6.38091200	0.02190700	-0.71235200
C	5.90857700	-0.38573700	0.69904000
C	4.93836200	0.68496600	1.25032300
C	5.19285100	-1.75034000	0.61857100
C	3.96566900	-1.65581100	-0.32884900
C	3.01813000	-0.59760900	0.25431800
C	4.44772700	-1.24324300	-1.73390400
C	-0.68134600	2.92493900	0.50223300
C	-1.02392000	3.44205200	-0.76654800
C	-2.33753300	3.86490100	-0.98072900
C	0.01091000	3.59440500	-1.85818300
C	1.53961000	3.62247600	1.36559300
C	-1.61700300	2.91190500	1.55182100
C	-3.30801800	3.81380600	0.02924900
C	-2.92248100	3.34812100	1.28694700
C	-1.25345900	2.48224600	2.95534700
C	-4.73202200	4.23423500	-0.24744400
H	2.71179600	-0.90171800	1.28626800
H	3.60772000	3.19576600	1.97725800
H	3.43209400	3.59747500	0.25618900
H	3.30426500	1.25128800	-1.76005900
H	4.66394700	2.15626600	-1.07311300
H	5.49650000	0.42607800	-2.65719400
H	6.90986600	0.98499400	-0.67347400
H	7.09490400	-0.71953800	-1.09457200
H	6.77348100	-0.45894700	1.37116300
H	4.61386300	0.42612000	2.26721600
H	5.44984400	1.65722300	1.30666600
H	4.87453000	-2.07310800	1.61946000
H	5.88765900	-2.51463500	0.24436300
H	3.46325200	-2.62288800	-0.38749900
H	3.59310800	-1.19456400	-2.41934300
H	5.13052600	-2.00728600	-2.12849800
H	-2.60879800	4.25840800	-1.95826500
H	0.54632500	2.66127600	-2.05571200
H	-0.45710200	3.92363900	-2.79064300
H	0.76539600	4.34463900	-1.58639900
H	1.34875700	4.59542100	0.90457300
H	1.31880800	3.70322500	2.43787600
H	-3.65502700	3.32042100	2.09103800
H	-1.09398700	3.35611300	3.60153700
H	-2.06200500	1.89527700	3.40358800
H	-0.34266300	1.87945700	2.98038500
H	-5.27886100	3.43780900	-0.76873000
H	-5.27305100	4.45355000	0.67843500
H	-4.77143400	5.12500000	-0.88439900
C	-0.60780300	-0.67009000	1.00775800
C	-0.67187100	-1.89313000	1.93072700
H	-0.24102000	-2.76136300	1.42833900
H	-0.05572800	-1.67005200	2.81295100
C	-2.08339700	-2.23398300	2.38572100
C	-2.71224200	-1.50481400	3.40553400
C	-2.78975700	-3.28604900	1.78320500
C	-4.01497200	-1.80664700	3.80683100
H	-2.16913300	-0.70160400	3.90067700
C	-4.09275700	-3.59102800	2.18453300
H	-2.30559900	-3.87110600	1.00605700
C	-4.71177000	-2.85040600	3.19376500
H	-4.48252300	-1.23306900	4.60355500
H	-4.62133500	-4.41557400	1.71260600
H	-5.72460500	-3.08999600	3.50677900
C	-1.29559300	-0.77227200	-0.41545800
C	-0.39221300	-0.12527700	-1.54558200
C	-2.70028200	-0.09277400	-0.39112000
H	-2.58222100	0.98608800	-0.27001300
H	-3.22976600	-0.46383300	0.49290900
C	-3.51794600	-0.39785300	-1.62983500
C	-4.13958600	-1.64729600	-1.77558600
C	-3.67267100	0.54483300	-2.65536300
C	-4.88471900	-1.94867600	-2.91558600
H	-4.04104200	-2.38550000	-0.98309100
C	-4.41956900	0.24780300	-3.79781200
H	-3.20919600	1.52302400	-2.55250900
C	-5.02646100	-1.00164600	-3.93293700
H	-5.35774500	-2.92291400	-3.00858300
H	-4.52861800	0.99419200	-4.58099100
H	-5.60774200	-1.23511300	-4.82110100
H	-0.93157500	0.23007100	1.53267200
H	-0.68333600	0.89139000	-1.80354200
H	-0.30724200	-0.77329300	-2.41968500
H	-1.40207800	-1.83304700	-0.64556300
N	0.92067900	-3.63843900	-0.94272000
O	1.76723500	-4.47508300	-1.25663400

26

B3LYP SCF energy: -1999.16999 a.u.
B3LYP enthalpy: -1998.334098 a.u.
B3LYP free energy: -1998.454966 a.u.
M06 SCF energy in solution: -1998.317603 a.u.
M06 enthalpy in solution: -1997.481711 a.u.
M06 free energy in solution: -1997.602579 a.u.

Cartesian coordinates

Ru	-1.02103200	-0.53968400	0.14384600
O	-1.75946800	-3.42572500	-0.77611600
O	-0.94797100	-2.48745800	1.04240000
N	-2.63518100	1.64670300	-0.88752700
N	-0.61510600	2.47726300	-0.92190900
C	-1.33609000	1.36840700	-0.56730000
C	-2.86750600	3.03556700	-1.28754200
C	-3.67290900	0.80172200	-0.30236000
C	-4.03491600	1.30805400	1.12199900
C	-5.03715300	0.34953600	1.78936300
C	-6.31373600	0.27305100	0.92697200
C	-5.95395200	-0.23426700	-0.48563000
C	-4.96160200	0.74646100	-1.15280300
C	-5.30996300	-1.63055600	-0.36959500
C	-4.01992700	-1.55398600	0.49187200
C	-3.05076000	-0.59464000	-0.22007100
C	-4.38743000	-1.04306700	1.89965400
C	0.75119100	2.82147800	-0.66137700
C	1.07476800	3.39030200	0.59027600
C	2.38782800	3.81239900	0.81058800
C	0.02143200	3.59981000	1.65435100
C	-1.44338500	3.50058200	-1.59831600
C	1.70548700	2.75900600	-1.69221700
C	3.37639200	3.70988900	-0.17750400
C	3.00978100	3.19453600	-1.42164200
C	1.35703600	2.28184400	-3.08393400
C	4.79835500	4.13135500	0.10803300
H	-2.85000100	-0.97129600	-1.24536900
H	-3.53126000	3.09759500	-2.15397800
H	-3.31970200	3.61032600	-0.46695000
H	-3.11513900	1.37423100	1.71804600
H	-4.46269900	2.31880900	1.06206300
H	-5.28824600	0.72718700	2.78941600
H	-6.78968700	1.26229000	0.86717200
H	-7.04229200	-0.40432000	1.39190300
H	-6.86195100	-0.29286200	-1.09981200
H	-4.71763600	0.41502200	-2.17090200
H	-5.41999300	1.74334400	-1.23199000
H	-5.06961900	-2.02916300	-1.36375600
H	-6.01921900	-2.33103500	0.09268200
H	-3.58917800	-2.55210200	0.55490000
H	-3.49205100	-0.99875600	2.53336000
H	-5.08195400	-1.74684500	2.37788900
H	2.64437300	4.24567900	1.77522900
H	-0.53406000	2.68395900	1.87494700
H	0.47633000	3.95619600	2.58338000
H	-0.71422000	4.35206800	1.33965700
H	-1.21652100	4.49671800	-1.20887900
H	-1.23580400	3.49882000	-2.67615800
H	3.75641000	3.12807600	-2.21027900
H	1.14927500	3.13254200	-3.74728700
H	2.19172000	1.72796600	-3.52557100
H	0.47608300	1.63521400	-3.09004100
H	5.32332400	3.36275800	0.68994100
H	5.36372200	4.28900900	-0.81582800
H	4.83299800	5.05866200	0.69096600
C	0.66873200	-0.76913100	-0.95581300
C	0.83964300	-2.01704800	-1.83079700
H	0.39404200	-2.88702500	-1.34862900
H	0.26371400	-1.85515800	-2.75170700
C	2.28659400	-2.31349900	-2.19284200
C	2.95557100	-1.57649700	-3.18130300
C	2.98953400	-3.33741800	-1.54115800
C	4.28888000	-1.84112200	-3.49869900
H	2.41980900	-0.79617500	-3.71831500
C	4.32356700	-3.60715500	-1.85620600
H	2.48107000	-3.93723400	-0.78968100
C	4.97998500	-2.85630800	-2.83327000
H	4.78596000	-1.26070700	-4.27216500

H	4.84601000	-4.41123800	-1.34410100
H	6.01681800	-3.06667700	-3.08153400
C	1.29439400	-0.80489200	0.49423100
C	0.32291400	-0.15938400	1.56869000
C	2.68423700	-0.09656900	0.51916000
H	2.54839100	0.97526200	0.36316100
H	3.26616900	-0.47682000	-0.32669600
C	3.44555400	-0.34968000	1.80470600
C	4.11653200	-1.56640800	2.00090800
C	3.49880000	0.60907800	2.82577500
C	4.80876200	-1.82163600	3.18485400
H	4.10099400	-2.31476200	1.21175800
C	4.19196700	0.35853500	4.01223100
H	2.99941400	1.56432600	2.68424500
C	4.84728000	-0.85972700	4.19717500
H	5.32202900	-2.77085800	3.31589800
H	4.22172000	1.11702600	4.79072000
H	5.38716600	-1.05696200	5.11955300
H	0.99367800	0.12205500	-1.49442400
H	0.59541300	0.86099800	1.83416000
H	0.20935400	-0.80136500	2.44587400
H	1.41735100	-1.85494900	0.76807300
N	-1.37631800	-3.55581200	0.40444000
O	-1.37203100	-4.62213300	1.01147200

TS27

B3LYP SCF energy: -1999.154531 a.u.
B3LYP enthalpy: -1998.321666 a.u.
B3LYP free energy: -1998.44214 a.u.
M06 SCF energy in solution: -1998.291784 a.u.
M06 enthalpy in solution: -1997.458919 a.u.
M06 free energy in solution: -1997.579393 a.u.

Cartesian coordinates

Ru	-0.86352800	0.04058700	0.64836200
O	-0.79742000	-1.30956900	2.56705700
O	-0.95856000	0.85171100	2.69500100
N	-2.36811000	-1.20698100	-1.47847000
N	-0.28489800	-1.49757900	-2.08775600
C	-1.08485800	-0.97084200	-1.09722300
C	-2.50092400	-1.72226900	-2.83947300
C	-3.46943800	-0.70952100	-0.65037300
C	-3.97357100	0.66776000	-1.14577600
C	-5.02841000	1.21945600	-0.16736600
C	-6.22284300	0.24523900	-0.11482100
C	-5.73355600	-1.13734600	0.36288800
C	-4.67637200	-1.68007200	-0.62926000
C	-5.12251900	-0.99119900	1.77333700
C	-3.90956200	-0.02418800	1.72560000
C	-2.86858600	-0.63992700	0.76840500
C	-4.39513500	1.35438200	1.23400400
C	1.09964600	-1.85644500	-1.99090000
C	2.01918600	-1.26979100	-2.88018600
C	3.36476500	-1.65085400	-2.80374100
C	1.58744700	-0.27338700	-3.93220400
C	-1.07850300	-2.22069400	-3.10821600
C	1.50861600	-2.87004300	-1.09545800
C	3.81020600	-2.61104200	-1.89375800
C	2.86095400	-3.21955700	-1.06350000
C	0.53293000	-3.56593300	-0.17478800
C	5.27273200	-2.97212200	-1.78770200
H	-2.70501500	-1.68012500	1.08610300
H	-3.24821800	-2.51786500	-2.90105900
H	-2.79482500	-0.92148500	-3.53360000
H	-3.12745700	1.35847100	-1.22057300
H	-4.40565400	0.56623800	-2.15237300
H	-5.36938800	2.20268000	-0.51880300
H	-6.68892600	0.16394800	-1.10744900
H	-6.99303100	0.62612700	0.56950200
H	-6.57922800	-1.83714800	0.39599300
H	-4.33901700	-2.67907500	-0.32249500
H	-5.12923800	-1.77611500	-1.62769800
H	-4.80450400	-1.97013500	2.15583500
H	-5.88677200	-0.61034600	2.46585500
H	-3.49359100	0.07551400	2.73336600
H	-3.55805600	2.06251300	1.20637000
H	-5.13477200	1.76097700	1.93768400
H	4.07996600	-1.18285100	-3.47723600
H	0.69880900	0.28433100	-3.62396600
H	2.38951600	0.43926000	-4.15073500
H	1.34342800	-0.77811000	-4.87737100
H	-0.72297900	-1.99026200	-4.11580600
H	-0.98528300	-3.30424300	-2.95171400
H	3.18160400	-3.99509400	-0.37075100
H	-0.37779100	-3.87665900	-0.69880300
H	0.98994100	-4.46043100	0.25952700
H	0.21598600	-2.91618300	0.64891200
H	5.73617700	-2.46035000	-0.93397500
H	5.41066400	-4.04866600	-1.63561200
H	5.82549900	-2.68212000	-2.68704200
C	1.44557900	0.00873200	0.86340500
C	1.95568400	-0.32187200	2.26562600
H	1.54402800	0.38720400	2.99046600
H	1.62862100	-1.32137000	2.56298000
C	3.47622300	-0.25656400	2.30156900
C	4.24763600	-1.41269000	2.12249300
C	4.14333600	0.96162000	2.49570900
C	5.64329100	-1.35572500	2.13338000
H	3.74708700	-2.36791800	1.98285400
C	5.53748700	1.02508700	2.50692000
H	3.56311700	1.86833500	2.65517000
C	6.29367100	-0.13480900	2.32302300
H	6.22202900	-2.26749300	2.00633000
H	6.03352500	1.97895400	2.66781600
H	7.37935500	-0.08840600	2.33676600
C	1.24144500	1.34725700	0.47334100
C	-0.91204500	1.69734700	-0.20547600
C	1.87746200	1.89860600	-0.80139800
H	1.64211200	1.24749600	-1.64644600
H	2.96313100	1.79943400	-0.64194700
C	1.58097100	3.34693500	-1.14268200
C	1.82541300	4.36959700	-0.21369900
C	1.10031100	3.70534400	-2.40899600
C	1.57749900	5.70481700	-0.53327800
H	2.22162400	4.12272700	0.76882900
C	0.85473600	5.04076400	-2.73595700
H	0.91815600	2.92923700	-3.14923500
C	1.08883200	6.04574400	-1.79665800
H	1.77138300	6.47989800	0.20352700
H	0.48064900	5.29402500	-3.72461400
H	0.89716300	7.08557100	-2.04705000
H	1.84555800	-0.64929300	0.09728000
H	-0.78264000	1.94971600	-1.26361200
H	-1.10579300	2.59057200	0.40699200
H	1.13845800	2.06753600	1.28414100
N	-0.93636500	-0.28050100	3.31885800
O	-1.03564500	-0.35216900	4.53049700

TS28

B3LYP SCF energy: -1999.159017 a.u.
B3LYP enthalpy: -1998.32563 a.u.
B3LYP free energy: -1998.448238 a.u.
M06 SCF energy in solution: -1998.294657 a.u.
M06 enthalpy in solution: -1997.46127 a.u.
M06 free energy in solution: -1997.583878 a.u.

Cartesian coordinates

Ru	0.36767800	0.11699100	0.72425000
O	0.54529300	-1.11491000	2.70086500
O	0.33830400	1.04672900	2.72816700
N	1.96059400	-1.34810200	-1.20343300
N	-0.11321000	-1.62286200	-1.88223600
C	0.66757200	-1.03370300	-0.91028500
C	2.11477500	-2.29415200	-2.31105400
C	2.99770400	-1.14392700	-0.18125600
C	3.17484100	-2.42500200	0.67798200
C	4.20870300	-2.17328500	1.79515700
C	5.55890100	-1.76884700	1.17164600
C	5.36980700	-0.48510500	0.33791800
C	4.36506700	-0.77230100	-0.80267800
C	4.84231100	0.64332500	1.25364100
C	3.47299600	0.23390100	1.86461300
C	2.50363900	0.02816400	0.67934700
C	3.69197300	-1.04303000	2.70477100
C	-1.50883400	-1.95557200	-1.80744300
C	-1.90819500	-3.01143100	-0.95274900
C	-3.25444600	-3.37828100	-0.92430000
C	-0.91027000	-3.74242400	-0.08347000
C	0.69289200	-2.35151200	-2.88861900
C	-2.43829500	-1.34885700	-2.66994200
C	-4.21240000	-2.75334000	-1.73343100
C	-3.77880500	-1.75719300	-2.60704000

C	-2.05499400	-0.29131000	-3.68112300
C	-5.66811500	-3.14901900	-1.65604100
H	2.60541900	0.92605100	0.05383300
H	2.84751600	-1.93426700	-3.03983400
H	2.45574500	-3.27169000	-1.94636400
H	2.20907300	-2.70182200	1.11668200
H	3.50768700	-3.26212600	0.04682600
H	4.33304000	-3.09412300	2.38050900
H	5.94876800	-2.57918600	0.53832200
H	6.30041600	-1.59713800	1.96367600
H	6.33013400	-0.18432800	-0.10217100
H	4.24654900	0.11143600	-1.44340700
H	4.75183000	-1.58729700	-1.43388600
H	4.73825400	1.57607200	0.68302100
H	5.57275500	0.83627200	2.05242300
H	3.10608500	1.04381900	2.50612400
H	2.76693800	-1.35584700	3.19313700
H	4.42692500	-0.83885300	3.49631100
H	-3.56328200	-4.18127000	-0.25830800
H	-0.45458600	-3.08105500	0.66187400
H	-1.39665200	-4.56470900	0.44946300
H	-0.09135700	-4.16935500	-0.67587200
H	0.32055000	-3.37395700	-3.00574000
H	0.62120900	-1.85588700	-3.86466200
H	-4.49865000	-1.28159500	-3.27072800
H	-2.48759000	-0.52460700	-4.66083400
H	-2.43569500	0.69609500	-3.39200700
H	-0.97397700	-0.20311200	-3.80034700
H	-6.16546100	-2.65423000	-0.81158700
H	-6.20929200	-2.86785100	-2.56528700
H	-5.78331600	-4.22899200	-1.51143500
C	-0.03531100	1.70620500	-0.20904700
H	-0.01787600	2.57888500	0.46351300
C	-0.19214000	2.13803400	-1.65005100
H	-0.24522600	1.26974300	-2.30848600
H	-1.12105500	2.71619700	-1.77885300
C	0.99033600	3.01694200	-2.02781300
C	0.95017800	4.40311000	-1.82467200
C	2.16168600	2.44971900	-2.54974300
C	2.04942900	5.20400600	-2.13824000
H	0.04714100	4.86009600	-1.42512500
C	3.26146900	3.24843400	-2.86802400
H	2.20831000	1.37463400	-2.70348700
C	3.20928100	4.62849300	-2.66142900
H	1.99784600	6.27776100	-1.97825000
H	4.15937400	2.79242500	-3.27718700
H	4.06466600	5.25128900	-2.90875100
C	-1.94705500	0.85048000	0.44531400
C	-1.73292800	-0.34707500	1.17456100
H	-2.26804600	0.73212800	-0.58720500
H	-2.00257200	-1.28997800	0.71901400
H	-1.85996700	-0.31039800	2.25419400
C	-2.48261100	2.09590700	1.15628600
H	-2.30594100	2.98956000	0.54678400
H	-1.93951100	2.22736400	2.09782400
C	-3.97454400	1.97040600	1.42156300
C	-4.90465100	2.29558100	0.42457900
C	-4.45264100	1.51440400	2.65748100
C	-6.27537400	2.16220000	0.65065100
H	-4.55112000	2.66510500	-0.53639800
C	-5.82272600	1.38090000	2.88859800
H	-3.74621900	1.27108500	3.44763700
C	-6.73892500	1.70230100	1.88499900
H	-6.98076200	2.42387900	-0.13404800
H	-6.17397100	1.03130600	3.85596900
H	-7.80586100	1.60214100	2.06578100
N	0.46796400	-0.04659600	3.40560600
O	0.51448700	-0.05272500	4.62307300

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B3LYP SCF energy: -1999.172789 a.u.
B3LYP enthalpy: -1998.33728 a.u.
B3LYP free energy: -1998.459602 a.u.
M06 SCF energy in solution: -1998.313722 a.u.
M06 enthalpy in solution: -1997.478213 a.u.
M06 free energy in solution: -1997.600535 a.u.

Cartesian coordinates

Ru	-0.46020000	0.73725800	0.08019400
O	-0.64457700	2.91188800	-1.26931700
O	-0.54589400	2.74807900	0.90468500
N	-1.86806200	-1.40296600	-1.24871900
N	0.21682600	-2.08038500	-1.28859800
C	-0.60534500	-1.05534100	-0.88411500
C	-1.98058100	-2.69964300	-1.91767500
C	-2.93740400	-0.40478900	-1.22906000
C	-3.13525900	0.19585600	-2.64733100
C	-4.20887000	1.30161700	-2.61244700
C	-5.53858100	0.71313000	-2.10027000
C	-5.33386500	0.14121100	-0.68237200
C	-4.28355300	-0.99055500	-0.73493100
C	-4.84869800	1.26328800	0.26059800
C	-3.50173800	1.84517900	-0.25775200
C	-2.48951400	0.69334500	-0.26079900
C	-3.73179900	2.42242200	-1.67122600
C	1.64148300	-2.03376400	-1.47374700
C	2.16901900	-1.26749800	-2.53947300
C	3.55250000	-1.24582800	-2.72453100
C	1.27404300	-0.48639500	-3.47588700
C	-0.51014600	-3.13429800	-2.03256100
C	2.48400800	-2.84423500	-0.69192800
C	4.42387400	-1.97444600	-1.90501600
C	3.86664600	-2.78377500	-0.91536600
C	1.96156200	-3.81370100	0.34490200
C	5.92008500	-1.87233000	-2.08099800
H	-2.44444100	0.26217700	0.77271000
H	-2.57474300	-3.39732600	-1.31545600
H	-2.46600300	-2.60375800	-2.89499600
H	-2.17953500	0.60618700	-2.99496700
H	-3.43392000	-0.59656000	-3.34839400
H	-4.34533400	1.69972500	-3.62640700
H	-5.89631700	-0.07500100	-2.77848400
H	-6.31133100	1.49322100	-2.08189900
H	-6.28048500	-0.27046400	-0.30823300
H	-4.14466400	-1.43753900	0.25800800
H	-4.62818200	-1.78713900	-1.41101200
H	-4.72865100	0.87627000	1.28136800
H	-5.60012100	2.06349200	0.30641800
H	-3.16368700	2.63253900	0.42328700
H	-2.80904400	2.87179000	-2.04707500
H	-4.48815800	3.21766700	-1.61921400
H	3.96248700	-0.64131200	-3.53074200
H	0.74582400	0.32191000	-2.95907800
H	1.86323000	-0.04060600	-4.28260800
H	0.51168200	-1.12596500	-3.93773700
H	-0.16023100	-3.16935700	-3.07120300
H	-0.32416800	-4.11668600	-1.58652300
H	4.52137500	-3.39443300	-0.29622400
H	2.21007900	-4.84462600	0.06217300
H	2.41685500	-3.63408200	1.32562400
H	0.87876800	-3.74980900	0.46272400
H	6.31674400	-1.02108400	-1.51195100
H	6.43000600	-2.77338900	-1.72390900
H	6.19275600	-1.71880700	-3.13072400
C	0.32827400	0.12195600	1.80492800
H	0.06114200	0.88380000	2.55042000
C	0.30985700	-1.26418900	2.44072900
H	0.49938400	-2.02153400	1.67822700
H	1.13796500	-1.33111500	3.16746400
C	-0.99297600	-1.56593400	3.15431600
C	-1.29056300	-0.96690100	4.38727800
C	-1.93948300	-2.43570000	2.59603800
C	-2.49808500	-1.22241800	5.03815900
H	-0.56552400	-0.29689000	4.84470200
C	-3.14780700	-2.70046600	3.24606500
H	-1.72378600	-2.91266100	1.64257600
C	-3.43256700	-2.09137400	4.46923300
H	-2.70688400	-0.74786700	5.99348400
H	-3.86341900	-3.38627700	2.79898700
H	-4.37061600	-2.29601400	4.97824400
C	1.70446900	0.51892400	1.09319000
C	1.48539900	1.18165300	-0.30118000
H	2.23649500	-0.42186800	0.92224700
H	2.02027300	0.68287900	-1.10238400
H	1.67456100	2.25595900	-0.30728700
C	2.52649000	1.43201000	2.04612000
H	2.54696500	0.95814900	3.03722100
H	1.99497500	2.38352400	2.15568600
C	3.94674700	1.66834800	1.57536400
C	4.91921200	0.66778300	1.72107400
C	4.32396500	2.87642600	0.97311200
C	6.22609000	0.86280600	1.27252100

H	4.64941600	-0.27257900	2.19817600
C	5.63053900	3.07718400	0.52214800
H	3.58905100	3.67057900	0.86429400
C	6.58627600	2.07040100	0.66827600
H	6.96636200	0.07746600	1.40544600
H	5.90130700	4.02364100	0.06128200
H	7.60481400	2.22758000	0.32306500
N	-0.61931500	3.50783000	-0.15238400
O	-0.66238400	4.72325000	-0.03540200

TS29

B3LYP SCF energy: -1999.139972 a.u.
B3LYP enthalpy: -1998.307537 a.u.
B3LYP free energy: -1998.429592 a.u.
M06 SCF energy in solution: -1998.286163 a.u.
M06 enthalpy in solution: -1997.453728 a.u.
M06 free energy in solution: -1997.575783 a.u.

Cartesian coordinates

Ru	-0.56585700	0.31856200	0.34278500
O	-0.80457500	3.49199700	1.82025700
O	-1.28501300	1.36183000	2.13095000
N	-1.39845300	-0.84113500	-2.17488100
N	0.73086400	-1.35075800	-2.08798500
C	-0.28870300	-0.75264800	-1.38798500
C	-1.14143000	-1.36752300	-3.51836900
C	-2.56806800	-0.00926200	-1.86231900
C	-2.48211600	1.34551800	-2.61710700
C	-3.64999800	2.25873900	-2.19762800
C	-4.98149200	1.56386900	-2.54699300
C	-5.07160800	0.21817600	-1.79661500
C	-3.90221500	-0.69649100	-2.23445000
C	-4.99500000	0.48112700	-0.27786800
C	-3.65286700	1.17409700	0.07548400
C	-2.50840600	0.23846800	-0.34890500
C	-3.56970900	2.51607600	-0.67989000
C	2.07949200	-1.64311000	-1.68911200
C	3.11176800	-0.72683700	-1.97633400
C	4.42252000	-1.05479500	-1.60466600
C	2.88513300	0.56825900	-2.72279900
C	0.28291800	-1.91736700	-3.37889500
C	2.38827800	-2.91422400	-1.15259800
C	4.74355600	-2.27033900	-0.99819200
C	3.71139200	-3.19325400	-0.80002300
C	1.35270800	-4.00838700	-1.00925300
C	6.15934500	-2.58408400	-0.57427500
H	-2.65715400	-0.74153300	0.16569800
H	-1.86829700	-2.13779900	-3.79220700
H	-1.20058100	-0.56518800	-4.26482600
H	-1.52243000	1.82088200	-2.38119200
H	-2.51557000	1.17583500	-3.70295500
H	-3.57547900	3.20895400	-2.74316800
H	-5.05276500	1.40079300	-3.63229700
H	-5.82683700	2.20554100	-2.26462600
H	-6.01953900	-0.27903300	-2.04194400
H	-3.96737100	-1.67070600	-1.73114600
H	-3.96360600	-0.88163400	-3.31747500
H	-5.08691000	-0.46350700	0.27584500
H	-5.83760400	1.11487300	0.03157700
H	-3.60748000	1.35195900	1.15285000
H	-2.63544800	3.03205800	-0.42858600
H	-4.39283500	3.17202900	-0.36626700
H	5.21489900	-0.33927800	-1.81565600
H	1.84293000	0.69920800	-3.01861900
H	3.18149800	1.43155100	-2.11604200
H	3.50077500	0.59033100	-3.63061700
H	0.95043300	-1.59829600	-4.18555600
H	0.30149100	-3.01302700	-3.33934200
H	3.94259500	-4.16621800	-0.37060300
H	1.37871700	-4.67859200	-1.87935500
H	1.55077700	-4.62480800	-0.12675600
H	0.33704200	-3.61735500	-0.92490300
H	6.31917800	-2.33844100	0.48395400
H	6.38804200	-3.64829600	-0.69661000
H	6.88844300	-2.01034200	-1.15565000
C	0.73107700	-0.52221600	1.95019200
H	0.24213700	-0.13166700	2.84392900
C	0.83748700	-2.04445400	1.94241700
H	1.08139100	-2.40165600	0.94258400
H	1.68891700	-2.31712100	2.58600400
C	-0.40242300	-2.73369200	2.48274000
C	-0.56007300	-2.91403000	3.86403800
C	-1.42317800	-3.18538400	1.63537400
C	-1.70395400	-3.51927700	4.38551300
H	0.22453500	-2.57728800	4.53867100
C	-2.56899200	-3.79570600	2.15148300
H	-1.32302100	-3.05827800	0.56062700
C	-2.71406900	-3.96303200	3.52931300
H	-1.80488400	-3.64660200	5.46009900
H	-3.34684400	-4.14149800	1.47529200
H	-3.60465700	-4.43708900	3.93272500
C	1.68830100	0.33431400	1.37637100
C	0.50888800	1.69460800	-0.26049600
H	2.39176100	-0.08713800	0.66185600
H	1.17135000	1.66884600	-1.12694400
H	0.43085800	2.65150800	0.25991900
C	2.16383600	1.56425300	2.14357800
H	2.73118500	1.17297200	3.00492100
H	1.29868900	2.09001800	2.55701200
C	3.05441000	2.53127700	1.38806400
C	4.26611600	2.10740300	0.82127200
C	2.69955900	3.88251900	1.27267700
C	5.09272900	3.00479800	0.14248400
H	4.57138400	1.06722200	0.91661900
C	3.52660000	4.78306300	0.59699700
H	1.76421800	4.22332900	1.70913400
C	4.72400500	4.34771400	0.02700200
H	6.03050000	2.65870200	-0.28571100
H	3.23251900	5.82645300	0.51813700
H	5.36864800	5.04863500	-0.49686500
N	-1.56425100	2.62948300	2.30878400
O	-2.55665000	2.90765300	2.98043500

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B3LYP SCF energy: -1999.168363 a.u.
B3LYP enthalpy: -1998.332808 a.u.
B3LYP free energy: -1998.454223 a.u.
M06 SCF energy in solution: -1998.316265 a.u.
M06 enthalpy in solution: -1997.48071 a.u.
M06 free energy in solution: -1997.602125 a.u.

Cartesian coordinates

Ru	0.47204600	-0.55934600	-0.43231800
O	1.99630400	-3.17620100	0.50795100
O	0.47586300	-2.64278500	-1.00017800
N	1.84746200	1.97530300	-0.27260600
N	-0.22026400	2.51921900	0.21749000
C	0.59400900	1.46832200	-0.12865200
C	1.95285900	3.42079600	-0.06114200
C	2.85775800	1.18706800	-0.98238100
C	2.84968100	1.56464400	-2.48938400
C	3.83040400	0.67081500	-3.26894200
C	5.25036200	0.85224800	-2.69385600
C	5.25717700	0.46384700	-1.20045300
C	4.28644600	1.38497400	-0.42347400
C	4.81685500	-1.00865900	-1.06336800
C	3.38244900	-1.18819800	-1.62981100
C	2.45674100	-0.28356200	-0.80656800
C	3.37736900	-0.79426900	-3.12027500
C	-1.65415700	2.56912200	0.13988800
C	-2.26901900	2.58886700	-1.13463100
C	-3.66204900	2.62927200	-1.20352400
C	-1.45454100	2.61814900	-2.40933700
C	0.50099900	3.81162700	0.26700700
C	-2.42553300	2.73305200	1.30455800
C	-4.46173400	2.68810600	-0.05469600
C	-3.82228600	2.76915800	1.18180100
C	-1.81767500	2.94337400	2.67379700
C	-5.96762100	2.66268900	-0.16149100
H	2.55822200	-0.56114100	0.27089900
H	2.64079800	3.64422900	0.76167500
H	2.32772300	3.92631600	-0.95836600
H	1.83131900	1.44184300	-2.88051700
H	3.12471800	2.62177400	-2.61226800
H	3.81975600	0.96183700	-4.32768500
H	5.57800500	1.89428000	-2.81915200
H	5.96268900	0.22509400	-3.24611400
H	6.26775300	0.58955100	-0.79060300
H	4.29771300	1.14241800	0.64702700
H	4.60431400	2.43309000	-0.52846500
H	4.84188800	-1.32530600	-0.01308400
H	5.51510500	-1.65761400	-1.60997600

H	3.08296100	-2.22937700	-1.51134800
H	2.37260000	-0.92664900	-3.54313300
H	4.05071200	-1.45739900	-3.67987000
H	-4.13832200	2.62150800	-2.18160200
H	-0.81878200	1.73473800	-2.51857900
H	-2.11342700	2.66900800	-3.28122900
H	-0.79664000	3.49593000	-2.44237700
H	0.07410100	4.50917400	-0.46269900
H	0.40377000	4.26711700	1.25810600
H	-4.42092200	2.87118800	2.08505200
H	-1.98044600	3.97795800	3.00369300
H	-2.28456700	2.29380200	3.42226400
H	-0.74305200	2.75537100	2.68941700
H	-6.32510400	1.63726000	-0.32290200
H	-6.44253000	3.04051300	0.74972000
H	-6.32118400	3.26549400	-1.00554400
C	-0.41859900	-1.15872300	1.25421900
H	-0.12652200	-2.19907600	1.42069800
C	-0.46633500	-0.40300700	2.57393500
H	-0.72290100	0.64082400	2.39368900
H	-1.28715900	-0.82973900	3.17604300
C	0.82250600	-0.49715500	3.36807200
C	1.15918200	-1.67252200	4.05378600
C	1.71388200	0.58226400	3.42451700
C	2.35322800	-1.76937800	4.76830700
H	0.48100300	-2.52249000	4.02512200
C	2.90827000	0.49333100	4.14380300
H	1.46915500	1.50296100	2.89996100
C	3.23287600	-0.68532700	4.81683500
H	2.59616700	-2.69202100	5.28847700
H	3.58167200	1.34632500	4.18196100
H	4.16090100	-0.75837100	5.37753200
C	-1.70619800	-1.05909300	0.33895500
C	-1.37814800	-0.71150400	-1.17432900
H	-2.30244800	-0.22785400	0.72566300
H	-1.94112200	0.14930200	-1.52243400
H	-1.48555000	-1.57540300	-1.83386300
C	-2.49914700	-2.39500600	0.43879500
H	-2.62076500	-2.63598800	1.50357700
H	-1.89060000	-3.18792000	-0.00675300
C	-3.86355200	-2.33980200	-0.21575300
C	-4.93105800	-1.68434500	0.41620700
C	-4.09634900	-2.93830800	-1.46161300
C	-6.19107400	-1.62086200	-0.18031900
H	-4.77492100	-1.22803000	1.39197700
C	-5.35507900	-2.87557800	-2.06394800
H	-3.28647200	-3.46864200	-1.95678000
C	-6.40653300	-2.21499900	-1.42672900
H	-7.00839100	-1.12065600	0.33390300
H	-5.51455800	-3.35111800	-3.02832900
H	-7.38820900	-2.17212400	-1.89121600
N	1.19652500	-3.54992100	-0.37032800
O	1.02998900	-4.72370500	-0.69406000

TS30

B3LYP SCF energy: -1999.152963 a.u.
B3LYP enthalpy: -1998.319414 a.u.
B3LYP free energy: -1998.439781 a.u.
M06 SCF energy in solution: -1998.291209 a.u.
M06 enthalpy in solution: -1997.45766 a.u.
M06 free energy in solution: -1997.578027 a.u.

Cartesian coordinates

Ru	-0.93529900	0.20966100	0.57490900
O	-1.10383400	-0.22547800	2.96629900
O	-1.27785500	1.75538900	2.08841100
N	-2.26399100	-1.73217400	-1.11750700
N	-0.16534500	-1.96189100	-1.68330800
C	-1.00417300	-1.30778600	-0.81334700
C	-2.34579000	-2.54954800	-2.32905400
C	-3.41921800	-1.01880000	-0.56405800
C	-3.88163900	0.10965700	-1.52173600
C	-5.01142000	0.92466200	-0.86333400
C	-6.20596400	-0.00876900	-0.58328700
C	-5.75811200	-1.14510600	0.35936200
C	-4.62435200	-1.95744400	-0.31150700
C	-5.25632100	-0.53041300	1.68303400
C	-4.04515200	0.39896200	1.40713300
C	-2.92696400	-0.45850400	0.78081800
C	-4.49158000	1.52876000	0.45753400
C	1.26450100	-2.07373400	-1.68517300
C	2.02114800	-1.30071600	-2.58422500
C	3.41002100	-1.49736400	-2.63038400
C	1.39412300	-0.28848000	-3.51621200
C	1.14987300	0.43423500	1.37489700
C	-0.88083500	-2.93193800	-2.54216800
C	1.88100500	-3.07466200	-0.89906700
C	4.05149100	-2.45161800	-1.84057400
C	3.26425700	-3.23790800	-0.98850100
C	1.07948700	-3.95317900	0.03540900
C	5.54985900	-2.63912100	-1.89207400
H	-2.75537100	-1.32351000	1.44036700
H	-2.99552800	-3.41737100	-2.18553800
H	-2.74337000	-1.96119700	-3.16755700
H	-3.03029700	0.75894500	-1.75312700
H	-4.23669000	-0.32245800	-2.46855300
H	-5.32240700	1.72762500	-1.54540400
H	-6.59165300	-0.42428700	-1.52555700
H	-7.02814100	0.55572500	-0.12291100
H	-6.60477300	-1.81571900	0.55784000
H	-4.31162700	-2.78832700	0.33475000
H	-4.99248100	-2.39273600	-1.25285300
H	-4.96697100	-1.32233700	2.38668800
H	-6.06924800	0.03758800	2.15749000
H	-3.71230400	0.83294700	2.35441200
H	-3.65298600	2.20772600	0.26173600
H	-5.28417900	2.12346600	0.93255300
H	3.99849100	-0.89650700	-3.32126400
H	1.83251900	-0.36754200	-4.51741800
H	0.31407400	-0.42531400	-3.60051500
H	1.56699200	0.73889600	-3.17237500
H	-0.55229200	-2.83618300	-3.58137800
H	-0.66988000	-3.95675300	-2.21279000
H	3.74261500	-3.99527000	-0.37084400
H	0.54345400	-4.74176100	-0.50890400
H	1.73803600	-4.44852800	0.75490800
H	0.33490600	-3.37935300	0.59508000
H	6.01753800	-2.33166500	-0.94800600
H	5.81601700	-3.69033100	-2.05418300
H	6.00090500	-2.04902200	-2.69592600
C	-0.71567200	1.43157300	-0.81646200
C	1.31755400	1.18065000	0.18714700
H	-0.43126100	1.25576000	-1.85944800
H	-0.91555000	2.49004700	-0.61019000
H	1.77448800	0.67637100	-0.66122700
C	1.60504500	2.68047700	0.30496100
H	2.58014700	2.74673300	0.81320700
H	0.87867200	3.13522800	0.98622100
C	1.69190800	3.46412000	-0.98939400
C	2.65698900	3.14253200	-1.95664100
C	0.84211500	4.54990100	-1.23731600
C	2.75323100	3.86838100	-3.14501200
H	3.34912900	2.32336900	-1.77117200
C	0.93667600	5.28171800	-2.42337200
H	0.10239300	4.82855000	-0.49015200
C	1.88948000	4.93999900	-3.38412300
H	3.50958300	3.60412000	-3.87978800
H	0.26681300	6.12056400	-2.59335300
H	1.96564500	5.50878600	-4.30689100
H	1.01234800	1.04877700	2.26407600
C	1.88295500	-0.85917600	1.68769800
H	1.26670500	-1.46566300	2.35960400
H	2.05195300	-1.42686800	0.77503100
C	3.21553100	-0.55964300	2.36022800
C	4.36472300	-0.31033200	1.59551900
C	3.31442900	-0.49061200	3.75632400
C	5.58027400	-0.00292200	2.20895400
H	4.30446300	-0.36466800	0.51037800
C	4.52860300	-0.18264500	4.37359000
H	2.43162700	-0.68115100	4.36293000
C	5.66596700	0.06227300	3.60177500
H	6.46162000	0.18415100	1.60010700
H	4.58519700	-0.13537300	5.45805800
H	6.61169400	0.30105400	4.08106500
N	-1.31255000	1.01865300	3.15530500
O	-1.53193300	1.50151300	4.25394100

TS31

B3LYP SCF energy: -1999.152246 a.u.
B3LYP enthalpy: -1998.318197 a.u.
B3LYP free energy: -1998.43825 a.u.
M06 SCF energy in solution: -1998.290488 a.u.

M06 enthalpy in solution: -1997.456439 a.u.
M06 free energy in solution: -1997.576492 a.u.

Cartesian coordinates

Ru	0.45085400	0.10967600	0.83883600
O	0.74883100	-1.29641100	2.73082100
O	0.66050400	0.86863700	2.89094600
N	1.80059800	-1.19462200	-1.37489000
N	-0.33188500	-1.34471900	-1.89047200
C	0.54739500	-0.88210000	-0.93023000
C	1.81288100	-2.03781000	-2.57289600
C	2.92344900	-1.16881200	-0.42536000
C	3.10327500	-2.56284200	0.23398600
C	4.23251500	-2.51302000	1.28336200
C	5.54786600	-2.07906400	0.60779300
C	5.35917500	-0.68474500	-0.02262900
C	4.25481200	-0.76575500	-1.10255000
C	4.96235200	0.32388900	1.07972800
C	3.62536100	-0.11359900	1.74226700
C	2.55765200	-0.11410600	0.62660400
C	3.84489500	-1.50288400	2.37890600
C	-1.71726100	-1.68687000	-1.74719700
C	-2.08432500	-2.74797200	-0.88988800
C	-3.43312400	-3.11566500	-0.82021600
C	-1.06173000	-3.50924400	-0.07885300
C	0.37479800	-1.88797900	-3.07408200
C	-2.67933500	-1.07927500	-2.58027800
C	-4.41678800	-2.49540800	-1.59679200
C	-4.01338800	-1.49036200	-2.48006300
C	-2.30948800	-0.03544200	-3.60861100
C	-5.87028700	-2.89280100	-1.48574800
H	2.64173100	0.86420100	0.12825500
H	2.55044500	-1.68651400	-3.29986400
H	2.05534700	-3.07816700	-2.31745700
H	2.16183500	-2.86058800	0.71043600
H	3.34425300	-3.31520600	-0.53076700
H	4.35457200	-3.51150700	1.72399800
H	5.84444200	-2.80714000	-0.16146600
H	6.35799400	-2.05003900	1.34904400
H	6.29596100	-0.36237700	-0.49672100
H	4.13077800	0.20384400	-1.60151400
H	4.54861500	-1.49794900	-1.87027000
H	4.86265500	1.33107900	0.65311400
H	5.75922500	0.37267700	1.83549700
H	3.35293900	0.61361500	2.51566400
H	2.94357700	-1.84125300	2.89400200
H	4.64707600	-1.43897700	3.12755300
H	-3.71679700	-3.92574500	-0.15183400
H	-0.59905400	-2.88634500	0.69366600
H	-1.52749400	-4.36745100	0.41460700
H	-0.25036500	-3.88853800	-0.71239600
H	-0.07342100	-2.83539200	-3.38529800
H	0.30641900	-1.18434500	-3.91307900
H	-4.75531700	-1.00995700	-3.11482200
H	-1.99079600	-0.50228100	-4.55055900
H	-3.16758600	0.60278900	-3.84132300
H	-1.49063900	0.60285200	-3.27040700
H	-6.43572700	-2.15905500	-0.89623600
H	-6.34695000	-2.94927400	-2.47087700
H	-5.98350300	-3.86578200	-0.99720500
C	0.02891000	1.81638400	0.12685300
H	0.20649100	2.61754100	0.86170300
C	-0.13668700	2.38694800	-1.26640300
H	-0.29996100	1.58897200	-1.99292300
H	-0.99514900	3.07112400	-1.32116700
C	1.11923000	3.16873500	-1.62515100
C	1.27372300	4.50035300	-1.21429300
C	2.15618100	2.56887100	-2.35257600
C	2.43213300	5.21466900	-1.52288100
H	0.47571300	4.98466900	-0.65519600
C	3.31430700	3.28246700	-2.66813000
H	2.05313300	1.53440100	-2.66964000
C	3.45694900	4.60743800	-2.25213300
H	2.53133600	6.24740600	-1.19915500
H	4.10482300	2.80259500	-3.23956100
H	4.35739700	5.16408200	-2.49719000
C	-1.74945400	1.11264900	1.07768600
C	-1.59188800	-0.27412200	1.42457800
H	-2.12426700	-1.00069200	0.82102300
H	-1.54312600	-0.52302800	2.48062100
H	-1.62784800	1.80142400	1.91147300
C	-2.84985600	1.52649100	0.10061100
H	-2.64152900	2.50754400	-0.33469700
H	-2.90844000	0.80466500	-0.71899100
C	-4.18861800	1.60790500	0.82129900
C	-4.64690800	2.83282900	1.32367600
C	-4.98298100	0.46840300	1.01267400
C	-5.86561000	2.92169400	1.99963700
H	-4.04508000	3.72818100	1.18023600
C	-6.20159700	0.55320100	1.68706800
H	-4.64384600	-0.48989900	0.62837300
C	-6.64765500	1.78060300	2.18323800
H	-6.20331100	3.88223300	2.38000500
H	-6.80475000	-0.34070000	1.82539200
H	-7.59696700	1.84631400	2.70800800
N	0.80810200	-0.26930200	3.49153000
O	0.99374300	-0.34236900	4.69297500

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B3LYP SCF energy: -1999.164451 a.u.
B3LYP enthalpy: -1998.328882 a.u.
B3LYP free energy: -1998.449432 a.u.
M06 SCF energy in solution: -1998.308932 a.u.
M06 enthalpy in solution: -1997.473363 a.u.
M06 free energy in solution: -1997.593913 a.u.

Cartesian coordinates

Ru	-0.46829100	0.86317800	-0.02238600
O	-0.68957300	2.71440200	-1.77885300
O	-0.58698400	2.99622100	0.38172800
N	-1.86084000	-1.53153200	-0.85369400
N	0.22618000	-2.19256900	-0.79531900
C	-0.59621400	-1.10296600	-0.59796900
C	-1.98051900	-2.95535200	-1.16233400
C	-2.94478500	-0.57090500	-1.03650700
C	-3.17646200	-0.31779500	-2.55154700
C	-4.25953200	0.75949200	-2.75217900
C	-5.57341700	0.29858300	-2.09021900
C	-5.33583900	0.06972800	-0.58333200
C	-4.27453600	-1.03727500	-0.39362700
C	-4.84496200	1.38251600	0.06325600
C	-3.51353400	1.83744800	-0.60269500
C	-2.49240700	0.72047000	-0.35693600
C	-3.77227000	2.06956900	-2.10646000
C	1.63784400	-2.20604000	-1.06726100
C	2.11648300	-1.64648200	-2.27524200
C	3.47924100	-1.75185600	-2.56597800
C	1.19497200	-0.96176400	-3.25862900
C	-0.51250400	-3.36888500	-1.31502600
C	2.50364200	-2.92819000	-0.22410700
C	4.37363700	-2.41877000	-1.71940800
C	3.86095300	-3.00941900	-0.56415500
C	2.02862100	-3.65723500	1.01333500
C	5.84775300	-2.48925800	-2.04271100
H	-2.43023400	0.53760900	0.74842200
H	-2.47929800	-3.48584500	-0.34116100
H	-2.56270300	-3.12216700	-2.07409300
H	-2.23172300	0.00441300	-3.00604600
H	-3.47950100	-1.25475900	-3.04067900
H	-4.41922300	0.91130900	-3.82768700
H	-5.93591400	-0.62638300	-2.56146000
H	-6.35335700	1.05779900	-2.23577000
H	-6.27077800	-0.24941200	-0.10442100
H	-4.11328000	-1.24418800	0.67202400
H	-4.62243200	-1.96974700	-0.86233100
H	-4.70189200	1.24407400	1.14333000
H	-5.60337200	2.16748000	-0.06194400
H	-3.17487300	2.76329300	-0.12787200
H	-2.85813400	2.42054500	-2.59262800
H	-4.53164000	2.85417700	-2.22728100
H	3.84972700	-1.31257500	-3.48965900
H	0.76430800	-0.04446400	-2.84406600
H	1.73863900	-0.69808700	-4.17058200
H	0.35674300	-1.60740500	-3.54795900
H	-0.23368800	-3.55081100	-2.36072800
H	-0.26070200	-4.26604800	-0.74185900
H	4.53001800	-3.56065700	0.09415300
H	2.23386500	-4.73180400	0.92916000
H	2.55363800	-3.30189200	1.90773600
H	0.95885700	-3.52951200	1.18325800
H	6.39691500	-1.67586400	-1.55011900
H	6.28918800	-3.43126500	-1.70004200

H	6.02713500	-2.40021400	-3.11918400
C	0.30004400	0.62082800	1.80755100
H	-0.11963000	1.42063300	2.43133800
C	0.37924600	-0.67165800	2.61629000
H	0.71829400	-1.49621100	1.98716700
H	1.12631300	-0.55732700	3.41844100
C	-0.94900800	-1.02766600	3.26016900
C	-1.48141600	-0.23191500	4.28664600
C	-1.67745100	-2.15403600	2.85599400
C	-2.70491200	-0.54434700	4.87982800
H	-0.92807600	0.63973800	4.62957100
C	-2.90018500	-2.47682500	3.45120600
H	-1.27848800	-2.78959200	2.06911400
C	-3.42117300	-1.66945600	4.46332200
H	-3.09574300	0.08685600	5.67375500
H	-3.44180500	-3.36239700	3.12735400
H	-4.37094500	-1.91793500	4.92924000
C	1.62439700	1.20006100	1.09295600
C	1.47999000	1.22092000	-0.46728400
H	2.05893300	0.44863900	-0.96611700
H	1.66913800	2.20472500	-0.89647400
H	1.67122200	2.24425000	1.41018800
C	2.93204100	0.48573600	1.53657200
H	2.90126900	0.34235600	2.62305000
H	2.98779400	-0.50696900	1.07906300
C	4.16861300	1.29341900	1.19476900
C	4.58973800	2.32678500	2.04477700
C	4.90847800	1.05055700	0.02948300
C	5.71114800	3.09884000	1.73960100
H	4.03236000	2.52717600	2.95795000
C	6.03144600	1.82089800	-0.28032400
H	4.60125000	0.25187900	-0.64001300
C	6.43712000	2.84816600	0.57324800
H	6.01896400	3.89409400	2.41364200
H	6.59022800	1.61759600	-1.19066800
H	7.31125100	3.44754100	0.33304200
N	-0.67866700	3.52559700	-0.80691700
O	-0.75547100	4.73706800	-0.93714000

TS32

B3LYP SCF energy: -1999.133859 a.u.
B3LYP enthalpy: -1998.301681 a.u.
B3LYP free energy: -1998.426385 a.u.
M06 SCF energy in solution: -1998.282324 a.u.
M06 enthalpy in solution: -1997.450146 a.u.
M06 free energy in solution: -1997.57485 a.u.

Cartesian coordinates

Ru	0.60036100	-0.59345400	0.31318700
O	1.01087600	-3.92915200	0.79471200
O	0.99701400	-2.02044700	1.90713300
N	1.85368200	1.13997600	-1.63926200
N	-0.23241600	1.79484100	-1.71941600
C	0.62060700	0.90025200	-1.11339200
C	1.89976400	2.17743600	-2.67087600
C	2.93155000	0.16653400	-1.44632300
C	2.94654300	-0.85510200	-2.61668200
C	4.00913900	-1.93956400	-2.35419300
C	5.39455900	-1.27199600	-2.23480400
C	5.38015400	-0.25875300	-1.07065900
C	4.32304800	0.83409100	-1.35075400
C	5.03481900	-0.99834200	0.23789300
C	3.63867400	-1.66591200	0.12030500
C	2.60342100	-0.56077600	-0.14082800
C	3.65879600	-2.67509800	-1.04573800
C	-1.66612700	1.80275100	-1.75182700
C	-2.34531400	0.89815900	-2.59971400
C	-3.74183900	0.94917100	-2.64966000
C	-1.61416600	-0.04035600	-3.53595500
C	0.44153700	2.65620300	-2.71709400
C	-2.37628400	2.82524100	-1.09012600
C	-4.48005200	1.88707200	-1.91849800
C	-3.77505400	2.82868200	-1.16647400
C	-1.68136700	3.96832700	-0.38350300
C	-5.98996100	1.87760500	-1.94917600
H	2.68195100	0.18735100	0.69375500
H	2.59375800	2.97742400	-2.39169500
H	2.23506700	1.76262100	-3.62869500
H	1.95128800	-1.30879100	-2.69506100
H	3.15885300	-0.33943300	-3.56457100
H	4.01188100	-2.64857000	-3.19279600
H	5.65671300	-0.76670200	-3.17577900
H	6.16502300	-2.03380300	-2.05610300
H	6.36610200	0.21636600	-0.98162700
H	4.31944000	1.58042200	-0.54450900
H	4.57177000	1.36081000	-2.28422600
H	5.04626900	-0.29873300	1.08516000
H	5.79714600	-1.76179700	0.44578400
H	3.41622400	-2.17797100	1.05900700
H	2.68351000	-3.16727700	-1.12445200
H	4.40140300	-3.45938700	-0.84585400
H	-4.26675600	0.24738200	-3.29539900
H	-0.62455000	-0.32154900	-3.17315100
H	-2.18821100	-0.95773800	-3.70188100
H	-1.48361600	0.43484400	-4.51834600
H	-0.01880100	2.52144400	-3.70224700
H	0.33644200	3.71096600	-2.44050300
H	-4.32428400	3.60212300	-0.63340000
H	-1.62531100	4.84209900	-1.04741200
H	-2.23576600	4.28183300	0.50695600
H	-0.66309200	3.72031400	-0.07981500
H	-6.38905600	1.09735800	-1.28795500
H	-6.40472600	2.83476900	-1.61755800
H	-6.36983600	1.67233600	-2.95629100
C	-0.68149700	0.18329900	2.04874500
H	0.05035400	-0.18760900	2.76795100
C	-1.02908000	1.65675100	2.18675200
H	-1.31776600	2.06087500	1.21558400
H	-1.92491400	1.73626600	2.82367100
C	0.07653600	2.48412900	2.81389600
C	0.02088200	2.82723200	4.17101900
C	1.18807000	2.90556400	2.06842800
C	1.04277200	3.56659700	4.77038000
H	-0.83323500	2.51055600	4.76594600
C	2.21094700	3.64726900	2.66240200
H	1.25548600	2.64355900	1.01601500
C	2.14243600	3.97985900	4.01693900
H	0.97812200	3.81937600	5.82544500
H	3.06291600	3.96521600	2.06644500
H	2.93882100	4.55589000	4.48029200
C	-1.58293200	-0.76953400	1.57513400
C	-0.56191400	-1.70388600	-0.59490700
H	-1.26833900	-1.40988600	-1.37414100
H	-0.55229000	-2.76471600	-0.32697000
H	-1.40919000	-1.79404000	1.88620300
C	-2.98452700	-0.44775500	1.08671500
H	-3.45118000	0.19460000	1.85247500
H	-2.95655400	0.15789800	0.17724600
C	-3.85194600	-1.67611100	0.88774800
C	-4.19164600	-2.48460500	1.98303200
C	-4.33469000	-2.03254300	-0.37698300
C	-4.98275400	-3.62113300	1.81718200
H	-3.83377900	-2.22085300	2.97633100
C	-5.12943400	-3.16890300	-0.54754000
H	-4.08747500	-1.41132500	-1.23341500
C	-5.45454300	-3.96803700	0.54876400
H	-5.23190800	-4.23530000	2.67845400
H	-5.49281600	-3.42933600	-1.53849600
H	-6.07072200	-4.85344500	0.41792200
N	1.33137400	-3.29207400	1.81169200
O	1.94292600	-3.77997500	2.76098600

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B3LYP SCF energy: -1999.160267 a.u.
B3LYP enthalpy: -1998.324617 a.u.
B3LYP free energy: -1998.445298 a.u.
M06 SCF energy in solution: -1998.310669 a.u.
M06 enthalpy in solution: -1997.475019 a.u.
M06 free energy in solution: -1997.5957 a.u.

Cartesian coordinates

Ru	-0.54396200	0.63646000	-0.47339500
O	-2.13846300	3.22481300	0.40028200
O	-0.69763600	2.66981300	-1.17720800
N	-1.82226000	-1.93847800	-0.13998000
N	0.26700800	-2.40380500	0.32646500
C	-0.57847300	-1.38919500	-0.06009200
C	-1.88704400	-3.37315100	0.14334400
C	-2.87194100	-1.22865700	-0.87194500
C	-2.86356800	-1.67437900	-2.36060900
C	-3.88620200	-0.85516600	-3.16758800
C	-5.29217800	-1.06793300	-2.56943700

C	-5.30064100	-0.61550200	-1.09398400
C	-4.28561100	-1.46113700	-0.28849500
C	-4.91938900	0.87777200	-1.02494600
C	-3.49987200	1.09057400	-1.61654100
C	-2.52844700	0.25966200	-0.76703500
C	-3.49303500	0.63205200	-3.08833800
C	1.69574100	-2.47435100	0.20509500
C	2.26813400	-2.56870400	-1.08542700
C	3.65369000	-2.70744400	-1.19364300
C	1.41378200	-2.59282900	-2.33297300
C	-0.42918900	-3.70101800	0.49873300
C	2.49495000	-2.63789000	1.35224500
C	4.48445900	-2.78687300	-0.06805000
C	3.88137900	-2.77071400	1.18941400
C	1.92086500	-2.74629300	2.74744500
C	5.98449100	-2.87838000	-0.21696300
H	-2.62027400	0.57854500	0.29911700
H	-2.57530400	-3.57621800	0.97070900
H	-2.23952900	-3.93250100	-0.73119100
H	-1.85442300	-1.53092300	-2.76803000
H	-3.09897000	-2.74564000	-2.43284100
H	-3.87396000	-1.19193900	-4.21267400
H	-5.57920100	-2.12650600	-2.64618200
H	-6.03427100	-0.49387400	-3.13996100
H	-6.30125800	-0.76409400	-0.66770600
H	-4.29741900	-1.17237500	0.77047900
H	-4.56052400	-2.52499200	-0.34414100
H	-4.94579700	1.23751400	0.01138700
H	-5.64888300	1.47438700	-1.58990200
H	-3.24534100	2.14769900	-1.55162300
H	-2.49894500	0.78868600	-3.52759600
H	-4.19929900	1.24140300	-3.66808100
H	4.09623100	-2.77430100	-2.18548300
H	0.84231000	-1.66952400	-2.46313800
H	2.03745500	-2.73369200	-3.22073100
H	0.68980600	-3.41718200	-2.30366400
H	0.01140800	-4.45354100	-0.16441400
H	-0.31993300	-4.05881100	1.52800200
H	4.50127200	-2.87422000	2.07780900
H	1.94278700	-3.79037500	3.08792300
H	2.51250100	-2.16574600	3.46339600
H	0.88820200	-2.40047000	2.80619700
H	6.42424600	-1.87952400	-0.33847700
H	6.44897800	-3.33591200	0.66246600
H	6.26577400	-3.46710300	-1.09703000
C	0.37942900	1.39310200	1.14149100
H	-0.07430800	2.36842900	1.33164300
C	0.60350400	0.65290800	2.45259700
H	0.95537700	-0.36046800	2.26014500
H	1.40728000	1.16345600	3.00724200
C	-0.63418000	0.63626200	3.33139200
C	-0.95731400	1.74799200	4.12196700
C	-1.49125200	-0.47175700	3.36603900
C	-2.10288600	1.75636100	4.91806400
H	-0.30444600	2.61819700	4.11208200
C	-2.63583800	-0.47218200	4.16692600
H	-1.26286000	-1.34071700	2.75518700
C	-2.94720400	0.64416100	4.94436600
H	-2.33469400	2.63114900	5.51973300
H	-3.28237700	-1.34639400	4.18546400
H	-3.83729000	0.64693500	5.56777800
C	1.56702400	1.54033200	0.08900900
C	1.25636000	0.83722200	-1.30984400
H	1.89168500	-0.02595000	-1.49770100
H	1.28030200	1.56258900	-2.12602800
H	1.58058300	2.60676600	-0.14476500
C	2.95784200	1.11281700	0.63205900
H	3.04938300	1.45890600	1.66861100
H	3.03823500	0.02245900	0.65176000
C	4.09247300	1.71924800	-0.17120600
C	4.46821800	3.05320800	0.04717100
C	4.78202500	0.98799900	-1.14769100
C	5.49562800	3.64207100	-0.69001600
H	3.94984600	3.63664700	0.80572600
C	5.81280100	1.57275200	-1.88739100
H	4.50923000	-0.04851100	-1.32667100
C	6.17272200	2.90230300	-1.66220500
H	5.76887300	4.67738000	-0.50344900
H	6.33498300	0.98765200	-2.64053900
H	6.97429900	3.35816100	-2.23722700
N	-1.45029400	3.57305300	-0.57845700
O	-1.42966800	4.71330400	-1.03283100

TS33

B3LYP SCF energy: -1999.139884 a.u.
B3LYP enthalpy: -1998.306816 a.u.
B3LYP free energy: -1998.428949 a.u.
M06 SCF energy in solution: -1998.285825 a.u.
M06 enthalpy in solution: -1997.452757 a.u.
M06 free energy in solution: -1997.57489 a.u.

Cartesian coordinates

Ru	0.66135600	-0.55829600	0.49374600
O	2.14851600	-0.20385900	2.99273800
O	1.00514700	-1.88866200	2.17628400
N	1.86109900	0.72214100	-1.82183800
N	-0.23721600	1.32390400	-2.00546200
C	0.63381800	0.58591600	-1.23828300
C	1.85368300	1.45949300	-3.08779000
C	2.90957100	-0.25317800	-1.49786300
C	2.78957300	-1.49015000	-2.42914500
C	3.81088100	-2.56448800	-2.01262600
C	5.23352300	-1.97849800	-2.12007200
C	5.35515200	-0.74834800	-1.19637500
C	4.33476800	0.32961500	-1.63380200
C	5.07610700	-1.18454800	0.25761000
C	3.64118000	-1.76277600	0.36949400
C	2.65615800	-0.65429400	-0.04257800
C	3.51734800	-2.98640600	-0.55966100
C	-1.66899000	1.27190900	-2.05945700
C	-2.29034100	0.16671900	-2.68549900
C	-3.68490000	0.14950000	-2.78100000
C	-1.48967600	-0.92539900	-3.36081400
C	0.43977700	2.04883800	-3.10532100
C	-2.43168000	2.39166600	-1.67323500
C	-4.47637200	1.20587500	-2.31308300
C	-3.82705900	2.32323100	-1.78618400
C	-1.79521400	3.68784300	-1.22339800
C	-5.98333700	1.13522500	-2.38655000
H	2.86193800	0.23585300	0.59007500
H	2.62991600	2.22988400	-3.10151800
H	2.03263700	0.78281200	-3.93342900
H	1.77074300	-1.88965800	-2.35816900
H	2.96181600	-1.19666600	-3.47450900
H	3.71624400	-3.43037900	-2.68173400
H	5.44968200	-1.69732200	-3.16094900
H	5.97615400	-2.73500300	-1.83304800
H	6.36705200	-0.32890600	-1.27135500
H	4.42777100	1.22467900	-1.00421000
H	4.54121400	0.63424100	-2.67092700
H	5.18785400	-0.33393900	0.94279900
H	5.81270100	-1.94057000	0.56404400
H	3.46098700	-2.07263300	1.40063500
H	2.50830400	-3.41125700	-0.48418800
H	4.22268800	-3.76746500	-0.24435300
H	-4.16528600	-0.70172100	-3.25985100
H	-0.60284900	-1.21961800	-2.79760800
H	-2.10453700	-1.81649600	-3.52124300
H	-1.14749000	-0.58857800	-4.34958000
H	-0.08440700	1.88136500	-4.05107300
H	0.43839700	3.12628700	-2.90304700
H	-4.41733800	3.17868100	-1.46399100
H	-1.70755700	4.37963400	-2.07247700
H	-2.40785400	4.18841900	-0.46683200
H	-0.79685100	3.54593900	-0.80611100
H	-6.38940200	0.53688800	-1.56036000
H	-6.43554900	2.13016200	-2.32475800
H	-6.31773400	0.66638400	-3.31880000
C	-0.71211000	0.53378900	1.92140200
H	0.00964000	0.45434000	2.73329500
C	-1.24477900	1.93840600	1.70206400
H	-1.61482000	2.03868900	0.67919100
H	-2.13505600	2.05613100	2.34163800
C	-0.28110800	3.06139500	2.04063900
C	-0.64808100	4.04214400	2.97163100
C	0.97951400	3.16714600	1.43286300
C	0.21059700	5.09695500	3.28875400
H	-1.61871800	3.97699500	3.45911400
C	1.84229300	4.21750400	1.74869500
H	1.29241600	2.41618800	0.71328400
C	1.46122900	5.18839500	2.67743400
H	-0.09725300	5.84222400	4.01769300

H	2.81837400	4.27256200	1.27309800
H	2.13527700	6.00381400	2.92571900
C	-1.51718700	-0.60153500	1.69496900
C	-0.54515000	-1.85488200	-0.04942900
H	-1.28361600	-1.79000400	-0.85067800
H	-0.53535700	-2.81543100	0.48188600
H	-1.29319000	-1.47107500	2.30416400
C	-2.94553400	-0.51595800	1.17811400
H	-3.47394900	0.19655900	1.83406200
H	-2.97908100	-0.07325700	0.17890000
C	-3.69072000	-1.83775800	1.20293000
C	-3.86832600	-2.52954200	2.41091800
C	-4.23274800	-2.38961300	0.03590800
C	-4.55459000	-3.74316700	2.44797100
H	-3.46827400	-2.11385800	3.33343500
C	-4.92379500	-3.60354400	0.06878700
H	-4.11415600	-1.85986100	-0.90550800
C	-5.08464800	-4.28603000	1.27482800
H	-4.67791200	-4.26363500	3.39400300
H	-5.33562000	-4.01485300	-0.84946700
H	-5.62019900	-5.23113300	1.30286300
N	1.78419700	-1.39864000	3.10919900
O	2.11546500	-2.12634400	4.03781400

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B3LYP SCF energy: -1650.227563 a.u.
B3LYP enthalpy: -1649.567684 a.u.
B3LYP free energy: -1649.672378 a.u.
M06 SCF energy in solution: -1649.524977 a.u.
M06 enthalpy in solution: -1648.865098 a.u.
M06 free energy in solution: -1648.969792 a.u.

Cartesian coordinates

Ru	-0.44217700	0.19819800	0.83525400
O	-0.14463800	1.67065200	2.54419700
O	0.98852800	-0.18135600	2.42972900
N	-1.76519500	-1.77150200	-0.79533300
N	0.39609200	-2.16370200	-0.94662100
C	-0.53655000	-1.35673200	-0.37947900
C	-1.68757400	-2.79617900	-1.84069700
C	-2.89320500	-0.86186800	-0.56522100
C	-3.12189800	0.05807200	-1.79174600
C	-4.22167300	1.09215900	-1.47852400
C	-5.53264300	0.35445700	-1.14082000
C	-5.30681200	-0.55924000	0.08154200
C	-4.21213700	-1.60350800	-0.25037400
C	-4.87307700	0.30952500	1.28304700
C	-3.54664200	1.04418700	0.94957500
C	-2.48112900	-0.02472600	0.66565200
C	-3.77466600	1.94959900	-0.27740600
C	1.78936300	-2.22028000	-0.59455600
C	2.73989300	-1.69818000	-1.49003300
C	4.09453400	-1.80120600	-1.15624600
C	2.33707600	-1.01083600	-2.77407000
C	-0.02729800	1.32410400	-0.54033100
C	-0.22922300	-3.27148400	-1.70026900
C	2.18475800	-2.85092800	0.60158200
C	4.52028800	-2.39931300	0.03241000
C	3.54990900	-2.92398100	0.89168800
C	1.17994300	-3.42320100	1.57410700
C	5.98681700	-2.46340200	0.39049500
H	-2.47574100	-0.72127700	1.54018600
H	0.24487900	0.96307200	-1.54294700
H	-2.41136500	-3.59984200	-1.67690600
H	-1.87755500	-2.35882700	-2.83070400
H	-2.18297300	0.56555800	-2.03882400
H	-3.41289500	-0.54676300	-2.66239000
H	-4.37416000	1.73293700	-2.35721100
H	-5.86742000	-0.23860400	-2.00374300
H	-6.32893900	1.07917100	-0.92383100
H	-6.23790500	-1.08730800	0.32537600
H	-4.05755800	-2.28347100	0.59802700
H	-4.53248200	-2.21643100	-1.10619900
H	-4.74229300	-0.31508800	2.17713600
H	-5.66220900	1.03834400	1.51558200
H	-3.23773700	1.65169400	1.80911700
H	-2.85339000	2.49070100	-0.52166000
H	-4.54168900	2.70195400	-0.04746600
H	4.83458900	-1.39776700	-1.84415200
H	3.19207700	-0.93277000	-3.45271100
H	1.53490100	-1.53888800	-3.30030500
H	1.97859500	0.00693200	-2.57759300
H	0.26929300	-3.42301300	-2.66153800
H	-0.15524500	-4.20526900	-1.12706000
H	3.86149100	-3.40456300	1.81672700
H	0.39440200	-4.00076600	1.07439700
H	1.67531900	-4.08379100	2.29214900
H	0.69157900	-2.62363300	2.14220900
H	6.25858200	-1.65269200	1.07917200
H	6.23867000	-3.40700800	0.88727400
H	6.62146900	-2.36589500	-0.49647500
C	0.09417500	2.83354100	-0.41746300
H	-0.60641500	3.28845500	-1.13659100
H	-0.20110800	3.16716100	0.58146200
C	1.50537700	3.30055400	-0.73589400
C	1.89083900	3.58451700	-2.05323300
C	2.46109000	3.41884900	0.28300600
C	3.19810300	3.97684900	-2.34790000
H	1.15684400	3.50976600	-2.85360400
C	3.76796100	3.81249900	-0.00814700
H	2.17314300	3.20870300	1.31024600
C	4.14161000	4.09117800	-1.32502800
H	3.47669200	4.20032000	-3.37482100
H	4.49376100	3.90497900	0.79566700
H	5.15859100	4.40059200	-1.55138400
N	0.74576000	0.92609700	3.08454700
O	1.32362500	1.20147800	4.11108200

TS34

B3LYP SCF energy: -1999.165062 a.u.
B3LYP enthalpy: -1998.331308 a.u.
B3LYP free energy: -1998.452497 a.u.
M06 SCF energy in solution: -1998.300661 a.u.
M06 enthalpy in solution: -1997.466907 a.u.
M06 free energy in solution: -1997.588096 a.u.

Cartesian coordinates

Ru	-0.76794500	-0.00190200	0.70194600
O	-1.11084600	-0.40478900	3.09777700
O	-0.69667000	1.55179200	2.25069100
N	-2.40999600	-1.64632100	-1.02538400
N	-0.36543100	-2.31622500	-1.44355400
C	-1.11370900	-1.47420100	-0.65731300
C	-2.57915400	-2.47034300	-2.22249400
C	-3.42952100	-0.74248900	-0.48602500
C	-3.67720200	0.45646800	-1.43632400
C	-4.65802100	1.44888500	-0.78014200
C	-5.99753200	0.73342700	-0.51046800
C	-5.75706200	-0.46598700	0.42967400
C	-4.78067200	-1.45785800	-0.24699200
C	-5.16436200	0.04739400	1.75998300
C	-3.81016300	0.75606300	1.49469500
C	-2.85825300	-0.28106900	0.86783100
C	-4.05491600	1.94962300	0.54869900
C	0.96748200	-2.79394600	-1.19688300
C	1.99908500	-2.43427100	-2.08484300
C	3.27569100	-2.96783000	-1.87668700
C	1.75909400	-1.49720400	-3.24695700
C	-0.10757300	1.11655700	-0.68851900
C	-1.21964500	-3.17184400	-2.30024900
C	1.20076000	-3.70970600	-0.14939600
C	3.54905700	-3.84848900	-0.82606200
C	2.49519800	-4.21276000	0.01770200
C	0.10104100	-4.13213500	0.79855600
C	4.94543300	-4.37853800	-0.59986300
H	-2.85266600	-1.16437800	1.52459300
H	0.16942400	0.73066100	-1.67609300
H	-3.41352100	-3.16946900	-2.11885300
H	-2.76688700	-1.84064400	-3.10376000
H	-2.72113800	0.94759600	-1.65109700
H	-4.08739200	0.10039800	-2.39276300
H	-4.82254300	2.29665200	-1.45893800
H	-6.44301800	0.39334700	-1.45647100
H	-6.71244800	1.43068200	-0.05328300
H	-6.70794100	-0.98050500	0.62152300
H	-4.62184700	-2.33747200	0.39079500
H	-5.21620000	-1.81098100	-1.19416300
H	-5.01798800	-0.78614500	2.45960100
H	-5.87216100	0.74278800	2.23351900
H	-3.40551000	1.11902600	2.44461500
H	-3.11549600	2.48474400	0.36538300
H	-4.74139600	2.66618100	1.02096700

H	4.07649200	-2.68789300	-2.55790400
H	0.93089600	-1.83013300	-3.88298200
H	1.51063000	-0.48391500	-2.91095900
H	2.65284400	-1.42835800	-3.87437500
H	-0.81927100	-3.23007600	-3.31601300
H	-1.25841400	-4.19037700	-1.89217000
H	2.68216400	-4.91203900	0.82987200
H	-0.78685700	-4.49470300	0.26839100
H	0.44788900	-4.93620300	1.45426700
H	-0.22650700	-3.29991800	1.43252100
H	5.52509600	-3.69727600	0.03677000
H	4.92860500	-5.35403600	-0.10264500
H	5.49197100	-4.48637900	-1.54292100
C	1.58108900	0.41319400	0.37818600
C	1.17971900	-0.59119900	1.32836900
H	2.00051700	0.02017100	-0.54547700
H	1.39321300	-1.62778700	1.10025200
C	2.27308100	1.67288600	0.90392400
H	1.67588500	2.09102900	1.71988100
H	1.28922100	-0.34038700	2.38174500
C	-0.23889800	2.63613900	-0.68256700
H	-0.14355700	3.03037100	0.33314900
H	-1.28690900	2.82625500	-0.96576000
H	2.33653700	2.42553100	0.11514200
C	0.64604400	3.40944000	-1.65005500
C	1.40626600	4.50112000	-1.20734000
C	0.68675100	3.08664100	-3.01527300
C	2.19406100	5.23869600	-2.09394100
H	1.37829300	4.77719700	-0.15577700
C	1.47438500	3.81895500	-3.90457600
H	0.08498800	2.26275000	-3.39301400
C	2.23467400	4.89734700	-3.44630400
H	2.77529700	6.07980200	-1.72509400
H	1.48839000	3.55149500	-4.95822400
H	2.84740900	5.46898800	-4.13812800
C	3.67707200	1.35567400	1.39362100
C	3.93673400	1.12962400	2.75231300
C	4.74406000	1.27114700	0.48776200
C	5.22445100	0.81932000	3.19329900
H	3.12492600	1.20674800	3.47196100
C	6.03265200	0.95932300	0.92408200
H	4.56409500	1.46117400	-0.56865700
C	6.27679300	0.73012800	2.27995200
H	5.40549000	0.65306200	4.25213900
H	6.84723600	0.90282400	0.20623300
H	7.28019600	0.49154200	2.62275800
N	-0.94407900	0.83786600	3.30778400
O	-1.00821400	1.34992300	4.41348700

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B3LYP SCF energy: -1999.173856 a.u.
B3LYP enthalpy: -1998.338186 a.u.
B3LYP free energy: -1998.460413 a.u.
M06 SCF energy in solution: -1998.315245 a.u.
M06 enthalpy in solution: -1997.479575 a.u.
M06 free energy in solution: -1997.601802 a.u.

Cartesian coordinates

Ru	-0.89952800	-0.13356500	-0.62191900
O	-1.39094200	-0.61063400	-3.36502700
O	-0.82609000	-1.97846100	-1.74688600
N	-2.46302600	1.90417200	0.71308600
N	-0.39736900	2.50180800	1.11771600
C	-1.16521200	1.57402700	0.46764600
C	-2.62277300	2.94821500	1.72732000
C	-3.49194100	0.92381400	0.36344700
C	-3.70735900	-0.08022400	1.52759400
C	-4.70027100	-1.17862500	1.10344500
C	-6.04615000	-0.52398700	0.73009000
C	-5.83253900	0.47011600	-0.43034900
C	-4.84741700	1.57703800	0.01381500
C	-5.26002600	-0.28733400	-1.64707100
C	-3.90049500	-0.93878000	-1.27620400
C	-2.93977300	0.19509400	-0.87588900
C	-4.12333100	-1.92865800	-0.11411700
C	1.00833400	2.75382500	0.96461600
C	1.89947200	2.36154900	1.97929300
C	3.26346100	2.64315000	1.81556200
C	1.44502800	1.66532400	3.24283300
C	0.27343400	-0.96680100	0.76000300
C	-1.21538100	3.55561600	1.75816000
C	1.46469000	3.48514900	-0.15592200
C	3.75286400	3.30930900	0.69226700
C	2.83208900	3.73735000	-0.27333600
C	0.51043100	3.99779700	-1.21218600
C	5.23248300	3.54551600	0.50433900
H	-2.86425900	0.91532700	-1.70679100
H	0.40309100	-0.39962300	1.68319500
H	-3.39221100	3.67184400	1.44492200
H	-2.90159600	2.51174000	2.69708600
H	-2.74082300	-0.52459600	1.80150600
H	-4.08568800	0.44910100	2.41383900
H	-4.84723500	-1.87656400	1.93840400
H	-6.46986200	-0.00538300	1.60208700
H	-6.77041700	-1.29443800	0.43391900
H	-6.79006800	0.93487300	-0.69920600
H	-4.70479800	2.31200100	-0.78937900
H	-5.25999700	2.11232100	0.88214500
H	-5.12774000	0.39598300	-2.49626600
H	-5.96906200	-1.06301400	-1.96901300
H	-3.51071200	-1.46683900	-2.14890900
H	-3.17823600	-2.41970900	0.15104600
H	-4.81498300	-2.72168500	-0.42919500
H	3.95777400	2.32784600	2.59219600
H	1.72971600	2.24848400	4.12745300
H	0.36303000	1.52050000	3.26379800
H	1.91573700	0.68012100	3.34438600
H	-0.85375700	3.76263900	2.76944200
H	-1.15589900	4.48481900	1.17732400
H	3.19088800	4.28077800	-1.14482200
H	-0.12218900	4.80771800	-0.82638900
H	1.06390300	4.39767300	-2.06677500
H	-0.15729900	3.21279900	-1.58025900
H	5.65838600	2.79679400	-0.17645800
H	5.43100500	4.53094100	0.06850200
H	5.77454600	3.47693400	1.45309200
C	1.41361000	-0.50419000	-0.29857200
C	0.83544200	0.37012700	-1.47288900
H	2.03710000	0.17964700	0.28204500
H	1.18880800	1.39618300	-1.46028000
C	2.27048900	-1.67279900	-0.84826500
H	1.64685300	-2.30161200	-1.49054200
H	0.94915900	-0.08393600	-2.45773300
C	0.08300200	-2.46001700	1.07720500
H	0.10869100	-3.05685700	0.16361400
H	-0.93443500	-2.57248400	1.47957600
H	2.59980300	-2.28816800	-0.00518800
C	1.05301000	-3.02308900	2.10800900
C	1.88155400	-4.11129300	1.80096000
C	1.11678300	-2.49228600	3.40620900
C	2.75723200	-4.64297300	2.75087400
H	1.83554000	-4.55028200	0.80711800
C	1.99108500	-3.01800300	4.35833200
H	0.46350100	-1.66664400	3.68082000
C	2.81917800	-4.09499300	4.03251300
H	3.38871500	-5.48750400	2.48712200
H	2.01959700	-2.59240800	5.35846900
H	3.49940500	-4.50696100	4.77315500
C	3.49143100	-1.19606700	-1.61065600
C	3.54363000	-1.24710500	-3.01029200
C	4.60561500	-0.69091000	-0.92296200
C	4.66908500	-0.79597600	-3.70424200
H	2.69813300	-1.65264400	-3.56144600
C	5.73266200	-0.24027100	-1.61147700
H	4.59180300	-0.65968700	0.16487200
C	5.76682400	-0.28853300	-3.00766200
H	4.68802100	-0.84749600	-4.78982000
H	6.58989700	0.13593300	-1.05791800
H	6.64508500	0.05782800	-3.54619600
N	-1.08186000	-1.77392200	-3.01917600
O	-1.00464100	-2.72221200	-3.79185600

TS35

B3LYP SCF energy: -1999.146014 a.u.
B3LYP enthalpy: -1998.313557 a.u.
B3LYP free energy: -1998.436257 a.u.
M06 SCF energy in solution: -1998.288837 a.u.
M06 enthalpy in solution: -1997.45638 a.u.
M06 free energy in solution: -1997.57908 a.u.

Cartesian coordinates

Ru	-0.74132500	-0.17139900	-0.48502800

O	-1.21222900	-2.16733100	-3.09740300
O	-0.74548900	-2.29426200	-0.94558500
N	-2.30596100	2.06225200	0.41751600
N	-0.23868000	2.73874400	0.69730400
C	-1.00975800	1.70256600	0.23405800
C	-2.46559800	3.27297200	1.22438100
C	-3.34456200	1.05788400	0.15399900
C	-3.60940600	0.19124000	1.41395500
C	-4.61162500	-0.93234200	1.08274300
C	-5.93546100	-0.29933100	0.60738100
C	-5.67310000	0.56036700	-0.64663200
C	-4.67891700	1.69232100	-0.29253600
C	-5.08753600	-0.33605800	-1.75954300
C	-3.75077200	-0.96521900	-1.28847200
C	-2.76843500	0.18464400	-0.98920100
C	-4.02175200	-1.81913100	-0.03247800
C	1.15430300	2.95394500	0.42108600
C	2.10242000	2.77330800	1.44482000
C	3.45704400	2.98261900	1.14818100
C	1.71665100	2.40382300	2.86024600
C	0.74767700	-0.70904300	1.20970400
C	-1.06651600	3.89488200	1.10809500
C	1.55092100	3.43126000	-0.85025900
C	3.88510700	3.38824100	-0.11578000
C	2.91188500	3.62248700	-1.09580200
C	0.54683000	3.79877300	-1.92206500
C	5.35161400	3.57607700	-0.42719300
H	-2.71572900	0.82303300	-1.88113100
H	0.71861100	0.20393200	1.79513100
H	-3.25286900	3.92173700	0.83188000
H	-2.71558200	3.01942700	2.26499900
H	-2.66041100	-0.24213000	1.76406600
H	-3.99532800	0.81867200	2.23116100
H	-4.79198200	-1.53202200	1.98508800
H	-6.37274500	0.31548300	1.40750100
H	-6.66455200	-1.08695400	0.37489100
H	-6.61438600	1.01122800	-0.98775300
H	-4.50536600	2.33755900	-1.16414700
H	-5.10626600	2.32092400	0.50392400
H	-4.92375600	0.25133500	-2.67323400
H	-5.81073100	-1.12418600	-2.01356000
H	-3.33876200	-1.59013700	-2.08521500
H	-3.09310600	-2.29606200	0.30400200
H	-4.72447200	-2.62891900	-0.27263700
H	4.19287100	2.82681800	1.93479300
H	1.97213200	3.21846400	3.55007200
H	0.64656600	2.20750600	2.95464000
H	2.25581300	1.51350200	3.20359900
H	-0.70137400	4.32055200	2.04704300
H	-1.03119700	4.67748800	0.33878800
H	3.22122900	3.97048200	-2.07944400
H	0.20275500	4.83426800	-1.79226600
H	1.00086100	3.73605200	-2.91597000
H	-0.33574500	3.15522300	-1.91401500
H	5.71249000	2.79753200	-1.11165000
H	5.53728600	4.54114500	-0.91330200
H	5.96342500	3.53051900	0.47917100
C	1.67068100	-0.74093300	0.17427300
C	0.31921800	0.28020200	-1.90716400
H	2.20523300	0.18267800	-0.03064900
H	0.93610500	1.17546100	-2.01827800
C	2.26351400	-1.99570900	-0.43056000
H	1.48918700	-2.75652400	-0.55197400
H	0.35033300	-0.43266600	-2.73860000
C	0.21504700	-1.93780600	1.94562400
H	0.15514700	-2.79373100	1.27115100
H	-0.80990500	-1.73598600	2.28646200
H	2.97170000	-2.38464300	0.32113900
C	1.07684800	-2.26184800	3.15754100
C	1.99467600	-3.32033500	3.12619800
C	0.98113600	-1.49711700	4.32972900
C	2.80010000	-3.60265400	4.23202800
H	2.06805700	-3.93682500	2.23376400
C	1.78480700	-1.77502200	5.43605500
H	0.26084200	-0.68242700	4.37993900
C	2.70033600	-2.82924500	5.38952400
H	3.50079900	-4.43252800	4.18960000
H	1.69027700	-1.17455700	6.33739700
H	3.32400400	-3.05062300	6.25149600
C	3.00379900	-1.79464300	-1.73875600
C	2.60781100	-2.48614600	-2.89178900
C	4.11271000	-0.93879100	-1.81702500
C	3.29342700	-2.31247900	-4.09657200
H	1.76220300	-3.16796000	-2.84596400
C	4.79781700	-0.76338800	-3.01992800
H	4.45063500	-0.41107500	-0.92675200
C	4.38756500	-1.44893200	-4.16619900
H	2.96802900	-2.85525200	-4.98002200
H	5.65773500	-0.09901100	-3.06061700
H	4.92153500	-1.31534600	-5.10342000
N	-0.84823800	-2.85252000	-2.12904700
O	-0.55055300	-4.04938800	-2.20829800

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B3LYP SCF energy: -1999.168432 a.u.
B3LYP enthalpy: -1998.332538 a.u.
B3LYP free energy: -1998.454139 a.u.
M06 SCF energy in solution: -1998.311564 a.u.
M06 enthalpy in solution: -1997.47567 a.u.
M06 free energy in solution: -1997.597271 a.u.

Cartesian coordinates

Ru	-0.94377800	-0.34671300	-0.47503800
O	-1.90431400	-3.10581800	0.25233200
O	-0.88160200	-2.24479400	-1.48786300
N	-2.46236800	1.98731500	0.35337500
N	-0.39035500	2.56192500	0.74870700
C	-1.17878300	1.54478400	0.27496300
C	-2.61282900	3.25225500	1.07647200
C	-3.56362400	1.06062600	0.10150000
C	-4.12404400	0.49840800	1.43459600
C	-5.23681400	-0.52820600	1.15104200
C	-6.36792900	0.14419600	0.34806000
C	-5.80333900	0.67848000	-0.98427900
C	-4.71637500	1.73398100	-0.68242000
C	-5.19502400	-0.48908200	-1.79088100
C	-4.04733900	-1.15537300	-0.98089900
C	-2.97422600	-0.07598500	-0.74991700
C	-4.63483100	-1.69050700	0.34254400
C	1.03364500	2.71421700	0.64087000
C	1.84297900	2.45540600	1.76267800
C	3.22878700	2.62279300	1.63995400
C	1.26738900	2.05314900	3.10145400
C	0.57692800	-0.84574800	0.76382300
C	-1.17144700	3.77108900	1.08672600
C	1.59455300	3.23437500	-0.54759700
C	3.81929400	3.06958000	0.45682700
C	2.98104000	3.38372100	-0.61974800
C	0.74344900	3.68678800	-1.71511500
C	5.31761800	3.21974000	0.33330100
H	-2.69109200	0.34208500	-1.74566100
H	0.77255200	-0.09213700	1.52581900
H	-3.30394100	3.92931300	0.56709100
H	-2.99292100	3.07585300	2.09192100
H	-3.30592800	0.02932300	1.99715900
H	-4.51820500	1.32129500	2.04766000
H	-5.63187300	-0.90225400	2.10474200
H	-6.81404700	0.96600300	0.92666900
H	-7.16929100	-0.58061700	0.15293400
H	-6.60648800	1.15073700	-1.56509300
H	-4.32070200	2.16347900	-1.61265300
H	-5.15413300	2.55835300	-0.10041100
H	-4.81918300	-0.12701100	-2.75781300
H	-5.97223400	-1.23438700	-2.00935400
H	-3.62978300	-1.97985100	-1.56523600
H	-3.85804100	-2.20020900	0.91619200
H	-5.41108000	-2.43494900	0.11846500
H	3.85901400	2.39862100	2.49797900
H	1.23364700	2.91713000	3.77946500
H	0.25144400	1.66252400	3.01213800
H	1.88800400	1.28973600	3.58068200
H	-0.86221600	4.17054600	2.05691600
H	-1.00845900	4.54871900	0.32951700
H	3.41881200	3.75872700	-1.54275600
H	0.50280000	4.75518800	-1.62687200
H	1.28077100	3.55903000	-2.66029200
H	-0.20021400	3.14135200	-1.78619400
H	5.72150900	2.52944000	-0.41794500
H	5.59325000	4.23351200	0.01834400
H	5.82113500	3.01301900	1.28261600
C	1.42071000	-0.48433100	-0.55682000
C	0.52639500	0.10962400	-1.72396200

H	2.05638300	0.34672100	-0.24380700
H	0.78198600	1.13621300	-1.96992800
C	2.29300500	-1.65134900	-1.08437800
H	1.64013800	-2.44545600	-1.45772300
H	0.50417200	-0.53145500	-2.60897600
C	0.69508400	-2.24577100	1.38729700
H	0.80566600	-3.01607100	0.62207200
H	-0.25703700	-2.46343700	1.88235400
H	2.86661900	-2.05633500	-0.24486800
C	1.81277500	-2.37118900	2.41328400
C	2.92393500	-3.19670200	2.19432500
C	1.73519600	-1.68556000	3.63629300
C	3.93662300	-3.31485400	3.15025600
H	2.99094300	-3.76872800	1.27220100
C	2.74284300	-1.79897700	4.59466600
H	0.86326700	-1.06968900	3.84619000
C	3.85363100	-2.61138100	4.35193800
H	4.78633800	-3.96435300	2.95572900
H	2.65456600	-1.26463600	5.53764700
H	4.63827300	-2.70457100	5.09810000
C	3.25868900	-1.22156400	-2.17096200
C	3.03487700	-1.54952300	-3.51509500
C	4.40935100	-0.48504800	-1.85007200
C	3.92546600	-1.14346100	-4.51180800
H	2.15938600	-2.13770500	-3.78050900
C	5.30218900	-0.07796700	-2.84198300
H	4.61034000	-0.23746500	-0.80952000
C	5.06100200	-0.40324300	-4.17928100
H	3.73378400	-1.41253600	-5.54745100
H	6.19302500	0.48404600	-2.57096400
H	5.75753500	-0.09078900	-4.95293700
N	-1.42333100	-3.27813000	-0.88671200
O	-1.42220300	-4.35601900	-1.47390300

TS36

B3LYP SCF energy: -1999.152221 a.u.
B3LYP enthalpy: -1998.318605 a.u.
B3LYP free energy: -1998.440732 a.u.
M06 SCF energy in solution: -1998.286261 a.u.
M06 enthalpy in solution: -1997.452645 a.u.
M06 free energy in solution: -1997.574772 a.u.

Cartesian coordinates

Ru	0.88454700	-0.35843700	0.41273400
O	1.66901000	-2.23102100	-0.72780600
O	0.95873600	-2.37191700	1.31541600
N	2.45868700	1.70386200	-0.86724200
N	0.38551100	2.28589600	-1.27156200
C	1.16874900	1.35285400	-0.62496400
C	2.60585100	2.76558000	-1.86378000
C	3.55771400	0.85299900	-0.40188100
C	4.09247900	-0.05754100	-1.53630400
C	5.20936400	-0.97377200	-0.99185300
C	6.35711200	-0.11882500	-0.42072100
C	5.81180100	0.76267700	0.72091500
C	4.73208500	1.70466200	0.14243000
C	5.21105700	-0.13616600	1.82619100
C	4.04180200	-0.98028500	1.24494700
C	2.97003500	0.02630200	0.75922800
C	4.62918700	-1.86610500	0.12216100
C	-1.00595400	2.56166400	-1.05818300
C	-1.93296300	2.23038500	-2.06828000
C	-3.28441000	2.52362500	-1.86163400
C	-1.49763100	1.62431500	-3.38335100
C	-1.05674500	-0.94845200	-0.69736000
C	1.19396700	3.35824600	-1.88863600
C	-1.42048800	3.26970800	0.08956900
C	-3.73543500	3.15904800	-0.70022700
C	-2.78549500	3.53460800	0.25391900
C	-0.43739000	3.82696200	1.09662000
C	-5.20670700	3.43146200	-0.48772500
H	2.83536800	0.73421200	1.58797500
H	-1.05433800	-0.21447300	-1.49529800
H	3.36656600	3.49322300	-1.56894100
H	2.89266200	2.34592400	-2.83816300
H	3.27291400	-0.66362800	-1.93753200
H	4.48584700	0.56059000	-2.35698100
H	5.58709500	-1.60127800	-1.80994100
H	6.79772500	0.51170400	-1.20693500
H	7.15896300	-0.76955300	-0.04648000
H	6.62484700	1.36978400	1.14138100
H	4.35642400	2.38759500	0.91649500
H	5.18015900	2.32141000	-0.65145200
H	4.85545400	0.48072100	2.66307300
H	5.99362300	-0.79633900	2.22686800
H	3.62345800	-1.61388100	2.03617700
H	3.88003500	-2.53754100	-0.29742200
H	5.42636600	-2.49604100	0.54183000
H	-4.00231800	2.25129700	-2.63274300
H	-1.32091100	2.40992100	-4.13119700
H	-0.57023000	1.05429200	-3.28758800
H	-2.27257500	0.96412700	-3.78417800
H	0.83713400	3.58250300	-2.89812200
H	1.12298900	4.27604600	-1.28932300
H	-3.10995900	4.06479900	1.14712900
H	-0.16016700	4.85599700	0.82904800
H	-0.88218200	3.86854700	2.09622500
H	0.48290600	3.24318600	1.15748200
H	-5.73056000	2.53313500	-0.13517200
H	-5.36525900	4.21732800	0.25779200
H	-5.69454200	3.74258400	-1.41814600
C	-1.60913200	-0.51066800	0.52212700
C	0.00960400	0.41488800	1.86731000
H	-1.98489800	0.50753600	0.54126400
H	-0.47832900	1.38381900	1.99972200
C	-2.26488600	-1.46774200	1.51047500
H	-1.57555100	-2.28058700	1.75714400
H	-0.05037000	-0.20309500	2.77390200
C	-1.17579400	-2.38643800	-1.20093600
H	-1.11512000	-3.09787200	-0.37285200
H	-0.33050900	-2.60033300	-1.86030400
H	-3.10912900	-1.92907600	0.97530900
C	-2.47267300	-2.60823500	-1.96709900
C	-3.53386200	-3.34069300	-1.41760200
C	-2.62806200	-2.09129700	-3.26277400
C	-4.72125900	-3.53302700	-2.12874600
H	-3.42305700	-3.78365000	-0.43083300
C	-3.81129600	-2.28001800	-3.97699000
H	-1.80395000	-1.54944400	-3.72151400
C	-4.86685500	-2.99825200	-3.40900800
H	-5.52825500	-4.10896900	-1.68302200
H	-3.90554200	-1.87762900	-4.98271600
H	-5.78799000	-3.15008900	-3.96530000
C	-2.79611700	-0.83385800	2.78132200
C	-2.36128200	-1.27529700	4.03795300
C	-3.75970900	0.18446300	2.73016000
C	-2.86367200	-0.70910900	5.21180400
H	-1.62159300	-2.07074200	4.09569800
C	-4.26251600	0.75461000	3.90028600
H	-4.12403600	0.53154300	1.76543700
C	-3.81470500	0.31025900	5.14682500
H	-2.51144300	-1.06661700	6.17588100
H	-5.01013300	1.54159700	3.83931800
H	-4.20818400	0.75151800	6.05868300
N	1.47515900	-2.97510300	0.29845900
O	1.75730600	-4.16040100	0.31780600

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B3LYP SCF energy: -1379.854479 a.u.
B3LYP enthalpy: -1379.31082 a.u.
B3LYP free energy: -1379.399895 a.u.
M06 SCF energy in solution: -1379.286394 a.u.
M06 enthalpy in solution: -1378.742735 a.u.
M06 free energy in solution: -1378.83181 a.u.

Cartesian coordinates

Ru	0.29191800	0.89390000	-0.53776200
O	0.80871300	3.10539500	-0.72726900
O	-0.42237000	2.32885600	0.88903300
N	0.78571500	-1.76832400	0.34733800
N	-1.39462000	-1.50943900	0.45290700
C	-0.23475700	-0.90206000	0.09292800
C	0.36024300	-2.90385600	1.16777600
C	2.14298400	-1.21866300	0.22722700
C	2.56578600	-0.47579300	1.52273200
C	3.93006800	0.21158500	1.31559500
C	4.98462300	-0.85845200	0.96398100
C	4.56400000	-1.59220500	-0.32618200
C	3.20162700	-2.29121800	-0.09816100
C	4.45624100	-0.56632400	-1.47715700
C	3.38736100	0.50420300	-1.13155500
C	2.04069300	-0.22254600	-0.95975300

C	3.81216800	1.22941200	0.16222900
C	-2.72181200	-0.99781900	0.26224300
C	-3.28707100	-0.17330800	1.25397900
C	-4.58928200	0.29809600	1.06019000
C	-2.52367700	0.20903600	2.50007800
C	-1.16200600	-2.88935500	0.92925000
C	-3.45708400	-1.37109700	-0.87909300
C	-5.33643400	-0.02890700	-0.07548300
C	-4.75491700	-0.87124700	-1.02731400
C	-2.89494000	-2.30935300	-1.92346600
C	-6.72685800	0.52757500	-0.27602500
H	1.86048300	-0.82229800	-1.85673000
H	0.82859000	-3.83753000	0.84493400
H	0.60688900	-2.74125600	2.22755600
H	1.80203900	0.27110400	1.78820900
H	2.61900800	-1.18336800	2.36293200
H	4.21990700	0.72751900	2.24027000
H	5.09073200	-1.57344600	1.79215500
H	5.96582800	-0.38580100	0.82279900
H	5.31448200	-2.35245100	-0.57912900
H	2.89780800	-2.84626400	-0.99554800
H	3.29321600	-3.01789800	0.72342400
H	4.18994200	-1.07386100	-2.41417100
H	5.43390700	-0.09006100	-1.63717200
H	3.31282000	1.22806900	-1.95228400
H	3.08496300	2.01214800	0.41409300
H	4.77620400	1.73360600	0.00952900
H	-5.03064000	0.93818700	1.82119300
H	-1.97853300	-0.64239700	2.92247300
H	-1.79073100	0.99519000	2.28860300
H	-3.20684300	0.58788100	3.26662600
H	-1.74253300	-3.08806300	1.83439600
H	-1.45897800	-3.61530600	0.16147400
H	-5.32477800	-1.14955100	-1.91174500
H	-3.05960700	-3.36041800	-1.64869400
H	-3.38528100	-2.15183700	-2.88927200
H	-1.81840600	-2.17458900	-2.06346100
H	-6.69326600	1.49560100	-0.79326500
H	-7.34525200	-0.14370300	-0.88140400
H	-7.23566300	0.68919600	0.68032300
C	-0.52541800	0.78548900	-2.14953500
H	-0.37203500	1.62388200	-2.84625200
H	-1.23371700	0.02219300	-2.48640200
N	0.14603000	3.37731200	0.32801400
O	0.03689800	4.48298900	0.80215600

TS37

B3LYP SCF energy: -1999.165519 a.u.
B3LYP enthalpy: -1998.33152 a.u.
B3LYP free energy: -1998.451397 a.u.
M06 SCF energy in solution: -1998.304319 a.u.
M06 enthalpy in solution: -1997.47032 a.u.
M06 free energy in solution: -1997.590197 a.u.

Cartesian coordinates

Ru	-0.90752300	0.10263300	0.68361000
O	-1.44428600	-0.18624000	3.05186800
O	-1.01800200	1.74134700	2.14602300
N	-2.38643700	-1.69401500	-1.03944500
N	-0.33523600	-2.44055300	-1.17949000
C	-1.12537900	-1.49349700	-0.57112700
C	-2.46859900	-2.65129200	-2.14139700
C	-3.44429600	-0.74752100	-0.68333700
C	-3.57949000	0.37062700	-1.74667700
C	-4.60709300	1.41795400	-1.27292000
C	-5.97637400	0.73349500	-1.08714800
C	-5.85003700	-0.38892600	-0.03646900
C	-4.82163500	-1.43640200	-0.52669900
C	-5.38935800	0.22444800	1.30370800
C	-4.00516700	0.90204200	1.12464300
C	-3.00600600	-0.18498400	0.68056800
C	-4.13680100	2.01842100	0.06874400
C	0.96567400	-2.90541300	-0.79624800
C	2.02571700	-2.77822700	-1.71746000
C	3.27208500	-3.31598700	-1.38246300
C	1.83789500	-2.09209200	-3.05152500
C	-0.18914500	1.19341800	-0.69013600
C	-1.13397500	-3.38351200	-1.99748400
C	1.14018200	-3.60585200	0.41429600
C	3.48840200	-3.98484100	-0.17313100
C	2.40936100	-4.12136900	0.70552000
C	0.00269700	-3.81199600	1.38799900
C	4.85449600	-4.53091200	0.17156700
H	-3.07411800	-1.01436200	1.40041200
H	0.24773000	0.80532400	-1.61962200
H	-3.33142300	-3.31470600	-2.03857300
H	-2.55031000	-2.12923200	-3.10570700
H	-2.60034300	0.83614900	-1.90406400
H	-3.89791500	-0.06118900	-2.70697700
H	-4.69114700	2.21121700	-2.02821100
H	-6.32813800	0.32223300	-2.04429200
H	-6.72457700	1.46852700	-0.76094700
H	-6.82218700	-0.88201700	0.09571000
H	-4.73912500	-2.26089100	0.19392100
H	-5.16321000	-1.86490100	-1.48117600
H	-5.32863600	-0.55119500	2.07847400
H	-6.13088700	0.96072100	1.64545000
H	-3.69629100	1.33791000	2.07983200
H	-3.17757200	2.53218600	-0.05774200
H	-4.85959000	2.77203500	0.41129700
H	4.09581500	-3.20673700	-2.08497200
H	1.40938100	-2.77457600	-3.79826500
H	1.16342500	-1.23465000	-2.97334500
H	2.79690200	-1.74437500	-3.44761000
H	-0.64459300	-3.58308900	-2.95395900
H	-1.24154100	-4.33730200	-1.46311600
H	2.55141400	-4.65689300	1.64176800
H	-0.89444800	-4.19958900	0.89169300
H	0.28952600	-4.52572600	2.16588600
H	-0.28790700	-2.87611600	1.87834200
H	5.55040400	-3.72009200	0.42345900
H	4.81058400	-5.20884800	1.02967100
H	5.29141000	-5.07871600	-0.67136600
C	1.42191200	0.77722700	0.63948500
C	1.05087300	-0.28737900	1.52220700
H	1.45221700	-1.27435100	1.31822800
H	0.93401500	-0.05940400	2.57768300
C	-0.39367300	2.70537200	-0.73071200
H	-0.74656500	3.06108700	0.24109100
H	-1.22607900	2.85592400	-1.43730800
C	0.78252900	3.54573000	-1.19803300
C	1.45329700	4.38888300	-0.30196100
C	1.21212700	3.51558700	-2.53380500
C	2.52750600	5.17614900	-0.72479200
H	1.12380900	4.43562600	0.73348900
C	2.28817700	4.29556000	-2.95913200
H	0.69069700	2.88364400	-3.25043100
C	2.95119500	5.12929300	-2.05435900
H	3.02892500	5.82856000	-0.01459100
H	2.60337000	4.26059700	-3.99885900
H	3.78428200	5.74319700	-2.38599800
H	1.41272100	1.77079800	1.08230100
C	2.54275100	0.56166500	-0.38106500
H	2.44802700	-0.43892300	-0.81053200
H	2.46965700	1.28627100	-1.19579800
C	3.90598700	0.71052400	0.28178200
C	4.48548800	-0.34756900	0.99764100
C	4.60697700	1.92073700	0.19474100
C	5.73038000	-0.19896500	1.61013700
H	3.95934200	-1.29548600	1.07246800
C	5.85361500	2.07164600	0.80659500
H	4.17426900	2.75067100	-0.35826100
C	6.41995000	1.01245800	1.51684900
H	6.16325400	-1.03060200	2.16085000
H	6.38193300	3.01833500	0.72603200
H	7.38991600	1.12816800	1.99330900
N	-1.35347800	1.07343100	3.20883100
O	-1.56556300	1.63737700	4.26859100

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B3LYP SCF energy: -1999.175241 a.u.
B3LYP enthalpy: -1998.339196 a.u.
B3LYP free energy: -1998.459945 a.u.
M06 SCF energy in solution: -1998.317604 a.u.
M06 enthalpy in solution: -1997.481559 a.u.
M06 free energy in solution: -1997.602308 a.u.

Cartesian coordinates

Ru	-0.94828800	-0.18212900	-0.61511700
O	-1.47078500	-0.35950900	-3.21482800
O	-0.96749500	-1.97508200	-1.83531400
N	-2.45975100	1.75962500	0.89840700

N	-0.40352900	2.45646800	1.15001600
C	-1.17436400	1.50400600	0.53107600
C	-2.58920100	2.74901700	1.96692800
C	-3.49352100	0.79654800	0.52695000
C	-3.64355100	-0.30626400	1.60840700
C	-4.64494900	-1.37677900	1.13372800
C	-6.01508200	-0.71266800	0.88778200
C	-5.86997700	0.38580500	-0.18556900
C	-4.87280800	1.46004300	0.30757900
C	-5.35353300	-0.24979300	-1.49324000
C	-3.96967800	-0.91158900	-1.25273300
C	-3.00197700	0.19919800	-0.80408800
C	-4.12104100	-2.00433700	-0.17411500
C	0.92655800	2.88819300	0.82763000
C	1.93508000	2.76221100	1.80311200
C	3.20370700	3.28218100	1.52407800
C	1.67210900	2.10130700	3.13663300
C	0.18354000	-1.10104700	0.75146900
C	-1.22934600	3.44399300	1.88641500
C	1.17118700	3.56767200	-0.38367700
C	3.49001300	3.92881700	0.31832800
C	2.45838400	4.06461600	-0.61711600
C	0.08349300	3.77616200	-1.41252600
C	4.88012100	4.44333300	0.02656700
H	-2.98573000	0.99563600	-1.56163600
H	0.44576600	-0.54731300	1.65936900
H	-3.42707600	3.42884900	1.79129200
H	-2.74234900	2.25703900	2.93830400
H	-2.66258800	-0.75864100	1.80259700
H	-3.98689700	0.14340700	2.55140100
H	-4.74249600	-2.15037700	1.90698100
H	-6.40179500	-0.28301500	1.82293200
H	-6.74391900	-1.46427500	0.55630000
H	-6.84373300	0.86081000	-0.36271300
H	-4.77907000	2.26773900	-0.43045800
H	-5.24446400	1.90742000	1.24157200
H	-5.27329300	0.50892100	-2.28282400
H	-6.06925100	-1.00510300	-1.84700400
H	-3.62882800	-1.35649400	-2.18994300
H	-3.15833600	-2.50093100	-0.00207900
H	-4.81843200	-2.77705500	-0.52506700
H	3.98854400	3.17571500	2.27004400
H	1.21342500	2.80111700	3.84873900
H	0.99431700	1.24888900	3.03910500
H	2.60591600	1.75131600	3.58691200
H	-0.79569100	3.66132900	2.86562500
H	-1.27881000	4.38272900	1.31853800
H	2.65478100	4.58382300	-1.55279300
H	-0.79784900	4.26561800	-0.98081000
H	0.44563000	4.40567900	-2.23051800
H	-0.25853000	2.82785900	-1.84077900
H	5.52335000	3.63802600	-0.35216600
H	4.86458300	5.23489000	-0.72968500
H	5.35804500	4.84214200	0.92798200
C	1.30405400	-0.86644400	-0.38086900
C	0.86617300	0.21382200	-1.41605300
H	1.31871000	1.18932200	-1.25622000
H	0.94621100	-0.11040900	-2.45340700
C	-0.11903900	-2.57499100	1.07138900
H	-0.45449900	-3.08594700	0.16396500
H	-0.95951800	-2.59415200	1.77918800
C	1.04660100	-3.33879200	1.67868200
C	1.76177400	-4.27703100	0.92103200
C	1.43781800	-3.12291300	3.00885800
C	2.84123500	-4.97288800	1.47202400
H	1.46273600	-4.46958300	-0.10684600
C	2.51650000	-3.81350800	3.56277000
H	0.88434200	-2.41190000	3.61966700
C	3.22468200	-4.74083400	2.79423600
H	3.37648600	-5.70192500	0.86881000
H	2.80002800	-3.63369200	4.59681200
H	4.06199700	-5.28320300	3.22511000
H	1.40026600	-1.81565400	-0.91280000
C	2.66623100	-0.50408400	0.28501400
H	2.60425000	0.50707500	0.69611600
H	2.82286000	-1.19078800	1.12324700
C	3.83690600	-0.61073600	-0.67231900
C	4.29750700	0.49825600	-1.39670000
C	4.48333400	-1.84160500	-0.85904900
C	5.36645300	0.37957500	-2.28731200
H	3.81743300	1.46347800	-1.25863500
C	5.55264400	-1.96355600	-1.74778700
H	4.14620500	-2.70959900	-0.29691500
C	5.99800500	-0.85257500	-2.46685300
H	5.70726600	1.25169100	-2.84013100
H	6.04029900	-2.92665700	-1.87601300
H	6.83109400	-0.94555800	-3.15861100
N	-1.26719000	-1.59149400	-3.05080900
O	-1.34418000	-2.42174300	-3.94420300

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B3LYP SCF energy: -1999.141123 a.u.
B3LYP enthalpy: -1998.308548 a.u.
B3LYP free energy: -1998.431337 a.u.
M06 SCF energy in solution: -1998.284645 a.u.
M06 enthalpy in solution: -1997.45207 a.u.
M06 free energy in solution: -1997.574859 a.u.

Cartesian coordinates

Ru	0.76708200	0.08324500	-0.57058300
O	1.41611000	1.24376200	-3.58518200
O	1.04253800	2.00299500	-1.54718900
N	2.11766200	-2.02993600	0.85752400
N	0.01007100	-2.39017900	1.32181100
C	0.85838100	-1.58795800	0.60053800
C	2.18878000	-3.01328500	1.93922300
C	3.25351500	-1.24543500	0.36303700
C	3.65782500	-0.15556600	1.39105500
C	4.77021500	0.73667500	0.80678900
C	5.99697800	-0.14117700	0.48606100
C	5.59967100	-1.22737600	-0.53587600
C	4.49100600	-2.12131600	0.06927600
C	5.08698900	-0.54646400	-1.82233600
C	3.84648000	0.32819000	-1.50373400
C	2.74601000	-0.59476500	-0.94343800
C	4.25259400	1.40962500	-0.48071400
C	-1.40901800	-2.53837000	1.17745500
C	-2.25881300	-2.05974300	2.19310700
C	-3.63832100	-2.27417900	2.07065800
C	-1.73383200	-1.36088600	3.42764100
C	-0.60029300	1.13466800	0.85981500
C	0.73220000	-3.48236500	2.01250300
C	-1.92888800	-3.28813500	0.09822100
C	-4.18776200	-2.96414300	0.98925800
C	-3.31219200	-3.47238900	0.02081000
C	-1.03287700	-3.95049500	-0.92594300
C	-5.68093400	-3.14915500	0.85428000
H	2.58724300	-1.40699100	-1.66648500
H	-0.96159500	0.46486100	1.63710200
H	2.88491100	-3.82281700	1.70521300
H	2.51583400	-2.53957900	2.87614000
H	2.77595800	0.45106900	1.64072600
H	3.99918800	-0.62463700	2.32573700
H	5.04592400	1.50057200	1.54619800
H	6.38388800	-0.60517600	1.40494100
H	6.80499800	0.47939900	0.07630000
H	6.47195100	-1.85330900	-0.76630100
H	4.21703100	-2.92092700	-0.63198200
H	4.86578700	-2.60023200	0.98684500
H	4.82782400	-1.30289100	-2.57551400
H	5.88560100	0.07282000	-2.25506300
H	3.49322800	0.79370500	-2.42684000
H	3.39604600	2.05781600	-0.25959600
H	5.03571300	2.05309000	-0.90449400
H	-4.29693000	-1.89280800	2.84861400
H	-1.89891400	-1.97957000	4.31935700
H	-0.66432700	-1.15358400	3.35527500
H	-2.25312200	-0.41087300	3.59860900
H	0.36505700	-3.60172400	3.03580600
H	0.57957800	-4.43093000	1.48107400
H	-3.71624900	-4.04466800	-0.81224600
H	-0.66431500	-4.91624000	-0.55392700
H	-1.58508500	-4.15379300	-1.84870800
H	-0.16058900	-3.34394000	-1.18034300
H	-6.10728800	-2.40865200	0.16483700
H	-5.92799700	-4.14019000	0.45778300
H	-6.18869200	-3.03147600	1.81684600
C	-1.39739100	1.25767800	-0.28347000
C	-0.43051600	-0.54413100	-1.81056400
H	-1.15088400	-1.35548200	-1.68381800
H	-0.42098600	-0.05245000	-2.78944700
C	0.23491900	2.30476800	1.39436000

H	0.59802700	2.91220100	0.56091000
H	1.11310700	1.92190900	1.93116800
C	-0.59050400	3.15151500	2.35164400
C	-1.31644200	4.25581200	1.88428900
C	-0.66735000	2.82933900	3.71350000
C	-2.09980800	5.01581400	2.75425300
H	-1.25658100	4.52758700	0.83275500
C	-1.45098300	3.58606200	4.58689900
H	-0.09899000	1.98317400	4.09547700
C	-2.17165500	4.68205800	4.10866100
H	-2.64886000	5.87378200	2.37488900
H	-1.49231000	3.32403100	5.64118200
H	-2.77887200	5.27564400	4.78680300
H	-1.17161400	2.08262800	-0.95376800
C	-2.79903800	0.68467700	-0.38798600
H	-2.83760900	-0.32351000	0.03207000
H	-3.41600200	1.30991200	0.28041800
C	-3.42056100	0.71280200	-1.77238400
C	-3.93262500	-0.45367400	-2.35450300
C	-3.52934700	1.91533400	-2.48704100
C	-4.52394500	-0.42600200	-3.61985900
H	-3.86647000	-1.39179200	-1.80909000
C	-4.11433300	1.94677500	-3.75284300
H	-3.15543800	2.83905500	-2.05097900
C	-4.61366900	0.77429200	-4.32520300
H	-4.91233800	-1.34396300	-4.05395900
H	-4.18135600	2.88814200	-4.29153200
H	-5.06951000	0.79825500	-5.31127700
N	1.33858900	2.21529400	-2.81456300
O	1.51302200	3.38312200	-3.15764500

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B3LYP SCF energy: -1999.167289 a.u.
B3LYP enthalpy: -1998.331353 a.u.
B3LYP free energy: -1998.454154 a.u.
M06 SCF energy in solution: -1998.313589 a.u.
M06 enthalpy in solution: -1997.477653 a.u.
M06 free energy in solution: -1997.600454 a.u.

Cartesian coordinates

Ru	-1.00026000	-0.34212200	-0.51062100
O	-1.86246200	-3.41551200	-0.08493800
O	-0.97579800	-2.16173300	-1.66203600
N	-2.55000500	1.92532300	0.43450300
N	-0.48831000	2.56035600	0.77856400
C	-1.25429200	1.53421500	0.28466500
C	-2.72106000	3.13730700	1.23652600
C	-3.62514700	0.97154500	0.17657600
C	-4.07361500	0.27594900	1.48968600
C	-5.14596300	-0.78816300	1.18732100
C	-6.35764900	-0.12000900	0.50813000
C	-5.90391400	0.55230500	-0.80438100
C	-4.85702800	1.64173400	-0.47863300
C	-5.28589000	-0.50928600	-1.73925500
C	-4.06008800	-1.17522000	-1.05377900
C	-3.03205400	-0.05890200	-0.79324200
C	-4.53424900	-1.84649200	0.25299500
C	0.90729700	2.83582800	0.58495800
C	1.79312200	2.70588100	1.66972800
C	3.13145800	3.08343700	1.49099500
C	1.35389000	2.19110400	3.02161400
C	0.44896200	-0.84847200	0.80585000
C	-1.30626000	3.71735000	1.20982100
C	1.34175800	3.39677700	-0.63819800
C	3.60252300	3.59462300	0.28186900
C	2.68647300	3.75096200	-0.76733200
C	0.38649600	3.66722100	-1.78021400
C	5.05864100	3.94867000	0.09329100
H	-2.81044000	0.44570500	-1.75990700
H	0.74753500	-0.04048300	1.47858100
H	-3.46584200	3.80901900	0.80127600
H	-3.04196300	2.88396400	2.25624000
H	-3.19898400	-0.18862300	1.96494100
H	-4.46969800	1.02582200	2.18908300
H	-5.46120100	-1.25789600	2.12827600
H	-6.81125300	0.62487500	1.17774300
H	-7.12871800	-0.87242500	0.29654500
H	-6.76484400	1.02331900	-1.29667100
H	-4.54484400	2.16729000	-1.39110100
H	-5.29976900	2.38901000	0.19635000
H	-4.98659900	-0.04939600	-2.69114400
H	-6.03519700	-1.27671000	-1.97728600
H	-3.63899300	-1.92412500	-1.72969300
H	-3.69662800	-2.35462200	0.73661200
H	-5.28070600	-2.61653200	0.01588300
H	3.82130400	2.96857200	2.32469300
H	1.46712600	2.96807400	3.78847800
H	0.31161000	1.86607900	3.01656400
H	1.97174000	1.34087200	3.33277200
H	-0.96835500	4.08362100	2.18343000
H	-1.20914300	4.53641100	0.48602200
H	3.02714000	4.17396500	-1.71046600
H	-0.18725800	4.58782200	-1.60753000
H	0.93547200	3.80340600	-2.71697800
H	-0.33352800	2.85747900	-1.92411100
H	5.58535700	3.15284800	-0.44929000
H	5.17555000	4.87003000	-0.48822900
H	5.56635900	4.08468200	1.05336300
C	1.30600700	-0.81321600	-0.53283200
C	0.59250500	0.02023300	-1.66550200
H	0.98278300	1.02981700	-1.77362000
H	0.54747400	-0.52019300	-2.61348000
C	0.40781000	-2.18179300	1.56285800
H	0.08161200	-2.98534700	0.90195300
H	-0.36803400	-2.09752700	2.33592600
C	1.72565000	-2.54616000	2.22769100
C	2.54936900	-3.54522900	1.68929000
C	2.15088300	-1.89730100	3.39704000
C	3.76679300	-3.87532000	2.29030700
H	2.22515700	-4.07743500	0.79781900
C	3.36683700	-2.22209000	4.00058400
H	1.51210200	-1.14010900	3.84779100
C	4.18248200	-3.21120800	3.44582900
H	4.38559500	-4.65851700	1.85964700
H	3.67329400	-1.71038000	4.90969700
H	5.12764000	-3.46909300	3.91603000
H	1.37255200	-1.84375400	-0.88842900
C	2.74231600	-0.26315400	-0.26562100
H	2.68851400	0.80694300	-0.05783600
H	3.12414000	-0.75153900	0.63653600
C	3.69028300	-0.53266600	-1.41717200
C	3.97651900	0.44709000	-2.37811200
C	4.30121500	-1.78892000	-1.54770800
C	4.83940900	0.17845100	-3.44298100
H	3.52429900	1.43119200	-2.28486600
C	5.16268200	-2.06217200	-2.61058600
H	4.10382200	-2.55491500	-0.80127300
C	5.43371900	-1.07867200	-3.56456500
H	5.04915300	0.95305900	-4.17665500
H	5.62553200	-3.04236000	-2.69187400
H	6.10516300	-1.28936000	-4.39275500
N	-1.50890400	-3.29904700	-1.27458100
O	-1.62191500	-4.18938000	-2.11255300

TS39

B3LYP SCF energy: -1999.144764 a.u.
B3LYP enthalpy: -1998.311897 a.u.
B3LYP free energy: -1998.432754 a.u.
M06 SCF energy in solution: -1998.279071 a.u.
M06 enthalpy in solution: -1997.446204 a.u.
M06 free energy in solution: -1997.567061 a.u.

Cartesian coordinates

Ru	-0.88330100	0.17196800	0.60507900
O	-1.80802800	2.30896500	0.39440500
O	-1.13015900	1.54920300	2.30713900
N	-2.31837400	-1.15957600	-1.52833100
N	-0.21490400	-1.43098100	-2.07501100
C	-1.05074000	-0.91804300	-1.10394900
C	-2.40186400	-1.64104900	-2.90734800
C	-3.47122800	-0.68508700	-0.75682500
C	-4.06400700	0.61060100	-1.36519700
C	-5.24190800	1.10622000	-0.49869500
C	-6.33010000	0.01811600	-0.42242400
C	-5.72914900	-1.25561600	0.20554600
C	-4.58643600	-1.75994200	-0.70519500
C	-5.19180100	-0.93130100	1.61856400
C	-4.07980900	0.15182900	1.52840800
C	-2.94067500	-0.45911400	0.67248000
C	-4.72475200	1.41796300	0.91854200
C	1.16444400	-1.80657100	-1.95186100
C	2.13839500	-1.09598900	-2.67967900

C	3.47216600	-1.51916900	-2.60940800
C	1.78296200	0.07596500	-3.56672900
C	1.03166400	1.26523500	-0.15658000
C	-0.96678900	-2.11013600	-3.15318100
C	1.51323100	-2.97637000	-1.23893000
C	3.85635500	-2.63867900	-1.86974400
C	2.85752100	-3.35969100	-1.20316800
C	0.47383600	-3.86158300	-0.58525300
C	5.30485700	-3.05916000	-1.78024100
H	-2.77047000	-1.46117700	1.08715200
H	1.37037100	0.75331900	-1.05190600
H	-3.13531600	-2.44478700	-3.01216200
H	-2.68912100	-0.82449200	-3.58420000
H	-3.28778700	1.38096100	-1.42025500
H	-4.41372700	0.41245200	-2.38935000
H	-5.65952600	2.01631300	-0.94931000
H	-6.72609300	-0.20450000	-1.42410000
H	-7.17455000	0.37502000	0.18261300
H	-6.49984600	-2.03523700	0.27402600
H	-4.16659400	-2.69944100	-0.32095100
H	-4.99016600	-1.96567700	-1.70817500
H	-4.79879600	-1.84193900	2.09136300
H	-6.01732000	-0.57432800	2.25083400
H	-3.70930800	0.37395300	2.53617400
H	-4.02534100	2.25265200	0.87815000
H	-5.56363400	1.73401100	1.55495400
H	4.22694800	-0.95803100	-3.15667100
H	1.79591600	-0.22429100	-4.62336000
H	0.78796200	0.46704400	-3.34401800
H	2.50526900	0.89111400	-3.45365000
H	-0.57965200	-1.82174300	-4.13486000
H	-0.86723400	-3.19903100	-3.05378500
H	3.12953100	-4.25882400	-0.65302300
H	0.05103400	-4.56785000	-1.31308500
H	0.92214900	-4.45907500	0.21480300
H	-0.35667600	-3.29340000	-0.16147300
H	5.75629700	-2.72262100	-0.83767900
H	5.40910500	-4.14937400	-1.81673500
H	5.89654100	-2.63373000	-2.59703300
C	1.51398800	0.75046100	1.05319100
C	0.03006600	-1.09034600	1.60909100
H	0.67337200	-1.91992600	1.30464900
H	-0.01753300	-0.97644100	2.70315500
C	0.84342500	2.76727300	-0.36700100
H	0.57536600	3.25589300	0.57448200
H	0.02952200	2.96291100	-1.06918700
C	2.13362800	3.37629300	-0.89977600
C	3.22417100	3.61418100	-0.05019200
C	2.26663300	3.70361200	-2.25571200
C	4.41191000	4.15819300	-0.53981500
H	3.13582800	3.38126300	1.00893300
C	3.45439500	4.24707200	-2.75218300
H	1.42529500	3.54326500	-2.92656300
C	4.53252900	4.47417000	-1.89552100
H	5.24152600	4.34191600	0.13820800
H	3.53267000	4.50096400	-3.80638900
H	5.45600900	4.90067100	-2.27796900
H	1.35117500	1.36057600	1.94021300
C	2.72357000	-0.17207200	1.12216500
H	2.67046300	-0.93819200	0.34517500
H	3.57401900	0.47279400	0.84111200
C	3.03403100	-0.79937800	2.46969900
C	3.30992700	-2.16942400	2.57062500
C	3.10254900	-0.02294500	3.63635200
C	3.62979300	-2.75247400	3.79876100
H	3.27443500	-2.78397400	1.67429300
C	3.41687700	-0.60138200	4.86649300
H	2.91086300	1.04639300	3.58809400
C	3.68020300	-1.97041500	4.95322100
H	3.83785700	-3.81819500	3.85223300
H	3.45881400	0.01931300	5.75766700
H	3.92559300	-2.42109500	5.91107200
N	-1.67913100	2.51599700	1.65182400
O	-2.04510500	3.54463100	2.19376600

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B3LYP SCF energy: -1650.223591 a.u.
B3LYP enthalpy: -1649.563811 a.u.
B3LYP free energy: -1649.666507 a.u.
M06 SCF energy in solution: -1649.524048 a.u.
M06 enthalpy in solution: -1648.864268 a.u.
M06 free energy in solution: -1648.966964 a.u.

Cartesian coordinates

Ru	-0.54288800	0.01862200	1.01726100
O	0.94997400	-0.64893600	2.44959400
O	-0.47881800	0.84805800	3.11965700
N	-1.61282100	-1.39517800	-1.25481700
N	0.56539500	-1.68264300	-1.33810300
C	-0.43894100	-1.07397400	-0.64283500
C	-1.42130100	-2.08516600	-2.53167200
C	-2.82064900	-0.68164400	-0.83287600
C	-3.05205700	0.57688800	-1.70718000
C	-4.23885200	1.39105300	-1.15664200
C	-5.50676500	0.51513300	-1.18480000
C	-5.28107800	-0.74149400	-0.31743000
C	-4.09308300	-1.55716500	-0.88632000
C	-4.98515800	-0.30034200	1.13321000
C	-3.70212000	0.57202900	1.16733000
C	-2.54336700	-0.28225800	0.63171100
C	-3.92388500	1.82131400	0.29089000
C	1.92377200	-1.84948600	-0.89984200
C	2.95547400	-1.19591700	-1.59983700
C	4.27678600	-1.39360600	-1.18072000
C	2.69999500	-0.29989800	-2.79163300
C	0.03430400	-2.56289000	-2.40104900
C	2.21795200	-2.73245000	0.16162800
C	4.59666300	-2.22440900	-0.10585800
C	3.55263800	-2.89428200	0.54041700
C	1.14829300	-3.50529400	0.89968000
C	6.02614200	-2.39444600	0.35301200
H	-2.53149000	-1.23025700	1.22361400
H	-2.12766200	-2.91046200	-2.65876200
H	-1.54857900	-1.39069200	-3.37468200
H	-2.14069300	1.18154900	-1.70731100
H	-3.25249600	0.27640200	-2.74594200
H	-4.38948100	2.27951000	-1.78440200
H	-5.74513800	0.22680600	-2.21847800
H	-6.36751900	1.08150600	-0.80441400
H	-6.18164800	-1.36917200	-0.33541700
H	-3.93732000	-2.47188100	-0.29869600
H	-4.31781600	-1.86513200	-1.91837600
H	-4.85728300	-1.17934700	1.77970500
H	-5.84071700	0.26487200	1.52883200
H	-3.49021400	0.87402900	2.20016800
H	-3.03030700	2.45718900	0.30925700
H	-4.75386100	2.41747300	0.69448600
H	5.07546000	-0.88411200	-1.71671800
H	1.64859500	-0.29063800	-3.08544900
H	2.99095900	0.73383900	-2.57100500
H	3.29284100	-0.62537800	-3.65502400
H	0.60897800	-2.45431600	-3.32480400
H	0.09537800	-3.61257000	-2.08204600
H	3.78185400	-3.56840600	1.36333600
H	1.54566200	-4.46369900	1.25009900
H	0.80825500	-2.94813800	1.77984000
H	0.27214200	-3.71070100	0.27779600
H	6.23545000	-1.76656700	1.22898600
H	6.23410700	-3.43056000	0.64276000
H	6.73610700	-2.11158500	-0.43109000
C	-0.21078900	1.64528100	0.27076800
H	-0.38594700	2.46630700	0.98950800
C	0.36213200	2.13030500	-1.03823400
H	-0.39988000	2.74287400	-1.54688800
H	0.58182900	1.28481600	-1.69747900
C	1.60605000	2.98432800	-0.83349300
C	2.75193200	2.43784100	-0.23373200
C	1.63107800	4.32913200	-1.22293100
C	3.89331800	3.21689700	-0.03952300
H	2.74507900	1.39855500	0.08559900
C	2.77222400	5.11097400	-1.02849600
H	0.74961100	4.76859200	-1.68535200
C	3.90772500	4.55646800	-0.43653700
H	4.77091700	2.77725600	0.42743800
H	2.77161100	6.15280800	-1.33877200
H	4.79604800	5.16325800	-0.28241100
N	0.52912500	0.12023100	3.42416800
O	1.05906400	0.11865700	4.51097700

TS40

B3LYP SCF energy: -1999.166864 a.u.
B3LYP enthalpy: -1998.333034 a.u.

B3LYP free energy: -1998.45252 a.u.
M06 SCF energy in solution: -1998.303238 a.u.
M06 enthalpy in solution: -1997.469408 a.u.
M06 free energy in solution: -1997.588894 a.u.

Cartesian coordinates

Ru	0.81846900	-0.12160800	0.70650100
O	1.23644000	0.63096300	2.94286200
O	0.73984100	-1.43106700	2.47730700
N	2.47863400	1.21520000	-1.24286500
N	0.50943400	2.14749500	-1.50657500
C	1.20451900	1.20897000	-0.77163400
C	2.66227500	2.00801800	-2.45631700
C	3.46509400	0.29973900	-0.66111600
C	3.59226300	-1.00567000	-1.48306300
C	4.52717000	-1.99438500	-0.75881200
C	5.92374600	-1.35714800	-0.61722700
C	5.80818300	-0.04820500	0.19056900
C	4.87224700	0.93653600	-0.55364400
C	5.24536700	-0.37446000	1.59127400
C	3.83357600	-1.00426800	1.45682200
C	2.93273200	0.03365500	0.76134600
C	3.94434200	-2.30464900	0.63635700
C	-0.68638400	2.83811600	-1.10886300
C	-1.82917000	2.76601800	-1.92553500
C	-2.97214100	3.48424700	-1.54973900
C	-1.84860100	1.98369900	-3.21831500
C	0.13532200	-1.45985300	-0.44604300
C	1.39869500	2.87626200	-2.44213900
C	-0.66765200	3.68127400	0.02737100
C	-3.00016100	4.28708000	-0.40950300
C	-1.83095600	4.38110300	0.35565100
C	0.56115700	3.82857900	0.89502200
C	-4.25152600	5.03029300	-0.00453900
H	3.03559900	0.97916700	1.31361000
H	3.58228400	2.59784800	-2.42061500
H	2.70613500	1.35959700	-3.34326000
H	2.60143000	-1.45001000	-1.60538800
H	3.98150200	-0.78037000	-2.48710300
H	4.60105500	-2.91908400	-1.34714600
H	6.35132400	-1.15686800	-1.61022100
H	6.60696900	-2.05080500	-0.10879900
H	6.79955900	0.41381300	0.28803500
H	4.80609200	1.88756800	-0.00867000
H	5.28911100	1.15410800	-1.54868400
H	5.19028100	0.53536100	2.20358400
H	5.92536000	-1.06752800	2.10703300
H	3.44791300	-1.23428000	2.45537200
H	2.95678200	-2.77328200	0.54039200
H	4.59140400	-3.02263400	1.15903300
H	-3.86061800	3.41503900	-2.17434400
H	-1.67038000	2.64323700	-4.07893000
H	-1.08116500	1.20762600	-3.23796900
H	-2.82504400	1.51340000	-3.37792200
H	0.93269200	2.97397200	-3.42659400
H	1.59695500	3.88573900	-2.05745200
H	-1.82191200	5.02199600	1.23491600
H	1.46765600	3.99342300	0.30203400
H	0.44759400	4.67771400	1.57559200
H	0.73769200	2.93376800	1.50277100
H	-4.76923900	4.51458600	0.81467500
H	-4.02018200	6.04228400	0.34667000
H	-4.95629700	5.11274100	-0.83818100
C	-1.56036700	-0.56235700	0.49302200
C	-1.15795800	0.53199900	1.31733800
H	-1.96427100	-0.29090300	-0.47993200
H	-1.35223700	1.54004700	0.97469300
H	0.09325800	-2.44044300	0.05243700
C	-0.17647300	-1.56760600	-1.92936200
H	-0.38928600	-0.57874000	-2.34501500
H	0.76164600	-1.89732300	-2.40360500
C	-1.26908800	-2.55466600	-2.30528600
C	-1.08846900	-3.93121500	-2.09862500
C	-2.47749600	-2.12076800	-2.86571900
C	-2.08999000	-4.84412300	-2.42936700
H	-0.15176900	-4.29215400	-1.67859900
C	-3.48233600	-3.03225700	-3.20234400
H	-2.63151800	-1.05987300	-3.04839300
C	-3.29313100	-4.39719200	-2.98153800
H	-1.92896700	-5.90562200	-2.26071900
H	-4.41013200	-2.67421400	-3.64136300
H	-4.07284200	-5.10760100	-3.24203800
H	-1.23095400	0.40004500	2.39463200
C	-2.20500600	-1.79590800	1.13559000
H	-1.60800200	-2.09291600	2.00326700
H	-2.20432200	-2.63175100	0.43013300
C	-3.63665000	-1.50231300	1.55464300
C	-4.68356000	-1.60629400	0.62742400
C	-3.94168300	-1.11297800	2.86609300
C	-5.99844800	-1.31933600	0.99767300
H	-4.46553300	-1.92648100	-0.38930900
C	-5.25582900	-0.82702300	3.24010300
H	-3.14483000	-1.04455500	3.60307900
C	-6.28887400	-0.92636900	2.30584500
H	-6.79755800	-1.41031000	0.26600800
H	-5.47273500	-0.53306000	4.26389400
H	-7.31280700	-0.70701400	2.59702200
N	1.04430200	-0.55316500	3.38048000
O	1.13679900	-0.85370500	4.55827700

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B3LYP SCF energy: -1999.174743 a.u.
B3LYP enthalpy: -1998.339107 a.u.
B3LYP free energy: -1998.459869 a.u.
M06 SCF energy in solution: -1998.315942 a.u.
M06 enthalpy in solution: -1997.480306 a.u.
M06 free energy in solution: -1997.601068 a.u.

Cartesian coordinates

Ru	0.91310400	-0.19062400	0.63200700
O	1.38117700	0.14062300	3.20925400
O	0.93791400	-1.72463800	2.16359500
N	2.40384100	1.42294600	-1.22025700
N	0.36946200	2.21092700	-1.43051000
C	1.13419600	1.28222100	-0.76206100
C	2.52562500	2.30222400	-2.38123700
C	3.44458800	0.54930900	-0.67640500
C	3.59744400	-0.74807300	-1.51198500
C	4.60481900	-1.69736300	-0.83351900
C	5.97367600	-0.99447500	-0.73606100
C	5.82845200	0.30043700	0.09000200
C	4.82272400	1.24772100	-0.60542600
C	5.32566900	-0.05595100	1.50429300
C	3.94504500	-0.75986900	1.41459500
C	2.96598600	0.22804300	0.75757800
C	4.09120700	-2.04778000	0.57831200
C	-0.88330100	2.76750300	-0.99772400
C	-2.00498000	2.67917700	-1.84365800
C	-3.21013900	3.25552300	-1.42443700
C	-1.93364900	2.03789500	-3.21022900
C	-0.10872900	-1.46693100	-0.48871200
C	1.20015200	3.07039100	-2.30803800
C	-0.94872100	3.50558200	0.20619600
C	-3.32303800	3.93721000	-0.21138900
C	-2.17432300	4.06588000	0.57711900
C	0.25458500	3.69592500	1.10131400
C	-4.64450500	4.51048700	0.24309500
H	2.95229500	1.16308800	1.33582900
H	3.39855800	2.95619600	-2.30763500
H	2.61230700	1.71699800	-3.30812400
H	2.62031000	-1.23604200	-1.60248800
H	3.93283300	-0.49664800	-2.52879700
H	4.70028500	-2.61149700	-1.43438600
H	6.35483300	-0.76415400	-1.74121800
H	6.70689000	-1.65981900	-0.26103000
H	6.80045100	0.80633600	0.15797200
H	4.73283600	2.18870300	-0.04639100
H	5.18670100	1.49531400	-1.61368500
H	5.24432200	0.84864900	2.12156200
H	6.05017100	-0.71736700	1.99973100
H	3.61076100	-1.00677700	2.42527700
H	3.12596600	-2.56604200	0.51918800
H	4.79245900	-2.73438000	1.07171500
H	-4.08112500	3.17145700	-2.07141100
H	-1.70393300	2.78554500	-3.98245400
H	-1.16109500	1.26844200	-3.26462400
H	-2.89332000	1.58672200	-3.48287700
H	0.72664900	3.20488100	-3.28401800
H	1.32332400	4.06027000	-1.84811500
H	-2.23079400	4.62257600	1.51016300
H	1.15518000	3.95480200	0.53386200
H	0.06955200	4.49969400	1.82027000

H	0.48524000	2.78694300	1.66873500
H	-5.18254000	3.79632600	0.88020300
H	-4.50446500	5.42567900	0.82843900
H	-5.29464500	4.74511000	-0.60626500
C	-1.35004000	-0.82112800	0.33330800
C	-0.92158400	0.29383000	1.32863400
H	-1.96382300	-0.33833700	-0.43302900
H	-1.33816800	1.27043600	1.10408100
H	0.08310800	-2.47804800	-0.10464800
C	-0.28559500	-1.49211400	-2.00875800
H	-0.50175400	-0.48309400	-2.37111100
H	0.67353400	-1.78782200	-2.45475700
C	-1.36021500	-2.45779200	-2.48205700
C	-1.12577300	-3.84134800	-2.47693500
C	-2.61378400	-2.00090400	-2.91204300
C	-2.11456700	-4.73997800	-2.87834000
H	-0.15599900	-4.21792200	-2.15752600
C	-3.60706000	-2.89667400	-3.31662100
H	-2.81277900	-0.93209400	-2.93730200
C	-3.36152200	-4.27029800	-3.29843800
H	-1.91021600	-5.80744700	-2.86666600
H	-4.57034000	-2.51949700	-3.65094100
H	-4.13205900	-4.96889800	-3.61294800
H	-1.04937500	0.02842500	2.37833700
C	-2.13852300	-1.96054500	1.03825600
H	-1.49134700	-2.39194400	1.80840400
H	-2.33040000	-2.74426000	0.29659500
C	-3.45258300	-1.50851400	1.64093400
C	-4.57358000	-1.30104100	0.82277000
C	-3.58548900	-1.28704500	3.01869500
C	-5.78657100	-0.87161000	1.36215900
H	-4.49432400	-1.49272300	-0.24556500
C	-4.79813500	-0.85825200	3.56312600
H	-2.73446500	-1.46354100	3.67260300
C	-5.90235900	-0.64579000	2.73608900
H	-6.64478700	-0.72206000	0.71140300
H	-4.87984200	-0.69690400	4.63501200
H	-6.84790400	-0.31627700	3.15898800
N	1.19653500	-1.10484400	3.28505800
O	1.25254100	-1.73849500	4.32926100

TS41

B3LYP SCF energy: -1999.139065 a.u.
B3LYP enthalpy: -1998.30678 a.u.
B3LYP free energy: -1998.429769 a.u.
M06 SCF energy in solution: -1998.282774 a.u.
M06 enthalpy in solution: -1997.450489 a.u.
M06 free energy in solution: -1997.573478 a.u.

Cartesian coordinates

Ru	0.76310000	-0.43263700	-0.34469700
O	1.33556800	-2.95325100	-2.47096300
O	1.07194100	-0.76130700	-2.47469500
N	2.01399400	0.27327100	2.12475100
N	-0.11722900	0.44213000	2.62073700
C	0.76693200	0.12003300	1.61374000
C	2.04031300	0.91114800	3.44117000
C	3.17038700	-0.01778000	1.26648700
C	3.62481800	1.24313200	0.48645300
C	4.76149400	0.88134600	-0.49062200
C	5.95125800	0.31284200	0.30964000
C	5.49857600	-0.94521200	1.07950100
C	4.37383500	-0.55836500	2.06924800
C	4.98801200	-2.00025500	0.07392800
C	3.78431600	-1.43483800	-0.72414500
C	2.66483900	-1.10679100	0.28325000
C	4.24750800	-0.17631800	-1.48804300
C	-1.49347600	0.03203900	2.70282200
C	-2.51453400	0.99940600	2.68893700
C	-3.84849200	0.57000400	2.76234600
C	-2.23887700	2.48666000	2.66023200
C	-0.39554400	1.35140400	-1.27475400
C	0.58885800	0.70855200	3.89605000
C	-1.80575900	-1.33355700	2.91324000
C	-4.18901900	-0.77594100	2.88431000
C	-3.14828300	-1.70930600	2.97756800
C	-0.73596300	-2.38115800	3.13931700
C	-5.63072500	-1.22357200	2.94223500
H	2.47131000	-2.00810000	0.88056300
H	2.76429900	0.43587400	4.10751500
H	2.29929300	1.97647400	3.35558200
H	2.76968000	1.65406600	-0.07010000
H	3.95138800	2.02404000	1.18918900
H	5.07621700	1.78546900	-1.02890600
H	6.33879700	1.06874800	1.00807500
H	6.77280200	0.05763100	-0.37279000
H	6.34424900	-1.35222700	1.64945600
H	4.06129100	-1.43250100	2.65640000
H	4.75265800	0.19635600	2.77559900
H	4.69149800	-2.91618700	0.60325700
H	5.80183100	-2.27703100	-0.61126400
H	3.41986500	-2.18608500	-1.42997800
H	3.42047000	0.22486300	-2.08549000
H	5.04866100	-0.44064800	-2.19206100
H	-4.63806700	1.31878100	2.73518300
H	-2.67854700	2.96832500	3.54263500
H	-1.17026900	2.70741800	2.65398300
H	-2.68641100	2.96805700	1.78260100
H	0.16787900	1.58414700	4.39797400
H	0.48872800	-0.15318900	4.56898500
H	-3.38914100	-2.76137700	3.11601900
H	-0.36607200	-2.34123000	4.17316700
H	-1.14283500	-3.38490700	2.98325300
H	0.12467100	-2.26087900	2.47767900
H	-5.86779000	-1.89971700	2.11140900
H	-5.84294300	-1.76960800	3.86971000
H	-6.31758900	-0.37326600	2.88871500
C	-1.46889800	0.47805800	-1.20573100
C	-0.43595900	-1.80794700	-0.19506700
H	-2.11397400	0.51462600	-0.32898400
H	-1.21847800	-1.91458700	0.55953100
H	0.11092700	1.40526300	-2.24084100
C	-0.25084200	2.59578300	-0.41323100
H	-0.72869100	2.42707400	0.55302700
H	0.80753200	2.79998400	-0.21422600
C	-0.85815000	3.81694400	-1.09338700
C	-0.04386600	4.84348200	-1.58675700
C	-2.24750400	3.93701200	-1.24541300
C	-0.59898800	5.96330600	-2.21080200
H	1.03618400	4.76680400	-1.47983800
C	-2.80703100	5.05453600	-1.86469500
H	-2.89672300	3.14476700	-0.87842000
C	-1.98289700	6.07290700	-2.35065800
H	0.05126500	6.74867900	-2.58722900
H	-3.88629200	5.13046800	-1.96955700
H	-2.41704800	6.94301500	-2.83562300
H	-0.37519100	-2.60574800	-0.94252300
C	-2.02974600	-0.19636200	-2.44286400
H	-1.22104100	-0.36138200	-3.15992800
H	-2.69272600	0.55885700	-2.90090100
C	-2.82581300	-1.46964200	-2.24044200
C	-3.94942200	-1.50185600	-1.40084800
C	-2.47095700	-2.63802000	-2.92969400
C	-4.68861500	-2.67439200	-1.23966300
H	-4.25587800	-0.60161600	-0.87147500
C	-3.21030500	-3.81241100	-2.76991800
H	-1.60975400	-2.62712600	-3.59355800
C	-4.31935600	-3.83604400	-1.92282200
H	-5.55966100	-2.67863100	-0.58844000
H	-2.91562300	-4.70823100	-3.30996000
H	-4.89606100	-4.74921000	-1.80025400
N	1.09084000	-1.91344300	-3.10383600
O	0.84160800	-1.89255800	-4.31404200

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B3LYP SCF energy: -1999.170496 a.u.
B3LYP enthalpy: -1998.334619 a.u.
B3LYP free energy: -1998.455513 a.u.
M06 SCF energy in solution: -1998.316084 a.u.
M06 enthalpy in solution: -1997.480207 a.u.
M06 free energy in solution: -1997.601101 a.u.

Cartesian coordinates

Ru	-1.01894500	-0.39021000	-0.47535400
O	-1.85768400	-3.27888900	0.36955200
O	-1.09144700	-2.30982400	-1.45712300
N	-2.48336200	1.95187200	0.37707400
N	-0.40772500	2.59453700	0.62052500
C	-1.19614100	1.53344700	0.24049800
C	-2.62102600	3.24204000	1.05583200
C	-3.58893000	1.02378800	0.14623200
C	-4.08505400	0.40628200	1.47993400

C	-5.19961200	-0.62164900	1.20319500
C	-6.37157900	0.06936900	0.47895600
C	-5.87229200	0.66216600	-0.85512200
C	-4.78148900	1.71560400	-0.55902700
C	-5.29232200	-0.46457800	-1.73725800
C	-4.10636800	-1.15210500	-1.00770200
C	-3.03154100	-0.07768200	-0.77248800
C	-4.62627700	-1.74523500	0.32034800
C	0.99116000	2.78782600	0.36152500
C	1.89429900	2.81597600	1.44172200
C	3.25795200	2.99130400	1.16844600
C	1.43890300	2.73947000	2.88278100
C	0.35175600	-1.19855800	0.74062100
C	-1.20608900	3.80546500	0.91234400
C	1.43214600	3.07996100	-0.94931000
C	3.73637100	3.17109400	-0.13055600
C	2.80163500	3.23953900	-1.17060000
C	0.46595200	3.30769900	-2.09292700
C	5.21423800	3.29121400	-0.41625500
H	-2.76988000	0.38121100	-1.75504000
H	-3.37925300	3.87095400	0.58249000
H	-2.90151300	3.09789900	2.10872500
H	-3.23952900	-0.07576000	1.98799800
H	-4.45750400	1.20263400	2.14044300
H	-5.54776900	-1.03853200	2.15728500
H	-6.79831800	0.86317900	1.10894700
H	-7.17434300	-0.65566000	0.29083800
H	-6.70448800	1.15123800	-1.37830900
H	-4.43282100	2.18719900	-1.48782900
H	-5.20150500	2.50967100	0.07545000
H	-4.96213000	-0.05798600	-2.70329100
H	-6.07296200	-1.20686300	-1.95356000
H	-3.70319600	-1.94628400	-1.64281500
H	-3.81778100	-2.27067900	0.83423100
H	-5.40696900	-2.48741600	0.10443000
H	3.96062600	2.99264600	1.99956000
H	1.46183800	3.73812500	3.33993500
H	0.42133400	2.35491000	2.97498000
H	2.09998400	2.10095100	3.47798700
H	-0.84308100	4.30097900	1.81672600
H	-1.12924800	4.51493800	0.07743700
H	3.14867300	3.43155700	-2.18379800
H	0.10548700	4.34564500	-2.08780900
H	0.95951600	3.14624800	-3.05631300
H	-0.40884500	2.65565900	-2.04773700
H	5.58848500	2.37979200	-0.90004700
H	5.42585100	4.12642400	-1.09392300
H	5.79058600	3.44420600	0.50165600
C	1.32092200	-0.75430000	-0.43972100
C	0.55186500	-0.15291600	-1.67989000
H	1.95271000	0.04470300	-0.04183100
H	0.91014100	0.83296700	-1.95804400
H	0.20939000	-2.28025400	0.73625500
C	0.69922800	-0.71246500	2.14364300
H	0.88944400	0.36064800	2.12908400
H	-0.17665800	-0.88152200	2.78371600
C	1.89219300	-1.44384800	2.74077100
C	1.73926000	-2.72850600	3.28296400
C	3.17182700	-0.87007600	2.73982900
C	2.83182500	-3.42010100	3.80751900
H	0.75367300	-3.18926800	3.29374700
C	4.26781200	-1.55852200	3.26693700
H	3.31172300	0.12356500	2.31961600
C	4.10125900	-2.83696400	3.80202400
H	2.69082200	-4.41440200	4.22327700
H	5.25080200	-1.09379900	3.26181500
H	4.95216100	-3.37392900	4.21253000
H	0.50953900	-0.83812300	-2.52978200
C	2.19032500	-1.97199500	-0.87631200
H	1.53644600	-2.70330900	-1.36171500
H	2.59161100	-2.44000800	0.02918700
C	3.33642100	-1.58821300	-1.78919800
C	3.25288400	-1.74796100	-3.17942900
C	4.51846200	-1.05544500	-1.25176200
C	4.31183200	-1.37426500	-4.01026000
H	2.35569300	-2.18301900	-3.61343600
C	5.58005200	-0.68312200	-2.07779900
H	4.60939600	-0.94926700	-0.17282000
C	5.47824600	-0.83733500	-3.46292600
H	4.22768800	-1.51245900	-5.08526000
H	6.49338100	-0.28739600	-1.63943900
H	6.30564000	-0.55326200	-4.10801500
N	-1.54405800	-3.37672400	-0.83486100
O	-1.62660500	-4.41824900	-1.47950500

TS42

B3LYP SCF energy: -1999.147748 a.u.
B3LYP enthalpy: -1998.314138 a.u.
B3LYP free energy: -1998.433639 a.u.
M06 SCF energy in solution: -1998.2838 a.u.
M06 enthalpy in solution: -1997.45019 a.u.
M06 free energy in solution: -1997.569691 a.u.

Cartesian coordinates

Ru	-0.86104300	-0.07199500	0.64206300
O	-1.88659800	2.01077600	1.16301500
O	-1.21846000	0.62930200	2.69798400
N	-2.16234400	-0.70183200	-1.86194000
N	-0.03667000	-0.75913800	-2.39357200
C	-0.91650400	-0.56276700	-1.34098200
C	-2.19198500	-0.77925200	-3.32267900
C	-3.35404500	-0.55845500	-1.01898300
C	-4.00306300	0.83832800	-1.18034500
C	-5.22203500	0.96140200	-0.24006000
C	-6.25204500	-0.13629500	-0.56868300
C	-5.59572400	-1.51861700	-0.37969200
C	-4.41174600	-1.63734100	-1.36606100
C	-5.10287700	-1.66381000	1.07825900
C	-4.04906600	-0.56556500	1.39345900
C	-2.86343900	-0.79806600	0.42361500
C	-4.74756500	0.80281100	1.21721600
C	1.34598200	-1.13808300	-2.31033100
C	2.33062600	-0.29119400	-2.85901900
C	3.67582700	-0.67294800	-2.76016200
C	1.98980900	0.96797900	-3.62735800
C	0.80843700	1.50969700	0.71394700
C	-0.74408800	-1.15981800	-3.63066300
C	1.70176200	-2.41667200	-1.81988300
C	4.06366800	-1.88066300	-2.17734800
C	3.05702700	-2.74756300	-1.73641200
C	0.66968600	-3.47811400	-1.49889600
C	5.52157600	-2.25459300	-2.04337000
H	-2.63632300	-1.87082400	0.48768500
H	-2.91072200	-1.52328900	-3.67424400
H	-2.46440700	0.19354000	-3.75601000
H	-3.26822800	1.61533600	-0.94389600
H	-4.31901500	0.98169500	-2.22451500
H	-5.67926500	1.95051300	-0.37512900
H	-6.61654800	-0.02894700	-1.60083600
H	-7.12545600	-0.03925800	0.09026800
H	-6.32444500	-2.30939600	-0.60340100
H	-3.94962800	-2.63190700	-1.30226700
H	-4.78797100	-1.51374100	-2.39276600
H	-4.67080800	-2.66219400	1.23280900
H	-5.95774800	-1.57650300	1.76396200
H	-3.70749200	-0.67610500	2.42938000
H	-4.08895300	1.63055200	1.47893700
H	-5.61234900	0.85382800	1.89406300
H	4.43655000	-0.01023800	-3.16862200
H	2.18695700	0.81690300	-4.69704200
H	0.94100900	1.24857200	-3.51700900
H	2.60428700	1.81584100	-3.30603500
H	-0.33453000	-0.63905300	-4.50045100
H	-0.63150900	-2.24039800	-3.79360400
H	3.33200000	-3.72099700	-1.33533200
H	0.43516600	-4.05724600	-2.40285200
H	1.05550300	-4.18721000	-0.75947600
H	-0.26624900	-3.06711400	-1.11760400
H	5.88427500	-2.07862800	-1.02180900
H	5.68501400	-3.31541800	-2.26373600
H	6.15064100	-1.66650700	-2.71930300
C	1.60006700	0.39988700	1.01044200
C	0.15408400	-1.52397600	1.19076100
H	0.84767600	-2.16554000	0.64366200
H	0.53968700	2.12583500	1.57071700
C	0.85628400	2.29109500	-0.58468700
H	1.13934200	1.62426200	-1.39654500
H	-0.14222900	2.68247200	-0.80562900
C	1.83879700	3.44990900	-0.48965900
C	1.38963900	4.74770400	-0.21349100
C	3.21664800	3.23951600	-0.64925800
C	2.29063000	5.80906300	-0.10324500

H	0.32435500	4.92607200	-0.08430100
C	4.12004700	4.29799400	-0.54334700
H	3.58304600	2.23627400	-0.85894800
C	3.65889000	5.58793900	-0.26927900
H	1.92204400	6.80889300	0.11108200
H	5.18388000	4.11639700	-0.67504800
H	4.36090400	6.41328600	-0.18566000
H	0.11771700	-1.76293700	2.26326100
H	2.13116400	-0.09062200	0.19838300
C	2.19237300	0.24851200	2.40794300
H	2.95403000	1.04193200	2.48774200
H	1.42619800	0.49163400	3.15107200
C	2.85270500	-1.07371400	2.74416500
C	3.90646400	-1.57384900	1.96486700
C	2.45573700	-1.80493100	3.87166400
C	4.53243400	-2.77696400	2.29274700
H	4.24460500	-1.01474200	1.09508800
C	3.08144500	-3.00818800	4.20550700
H	1.64901700	-1.42531700	4.49478300
C	4.12069800	-3.50046800	3.41464700
H	5.34899700	-3.14633800	1.67704600
H	2.75656500	-3.55828400	5.08480800
H	4.61058500	-4.43542200	3.67331500
N	-1.78686000	1.75372700	2.41409200
O	-2.19910200	2.50732800	3.27914000

TS43

B3LYP SCF energy: -1999.158681 a.u.
B3LYP enthalpy: -1998.325566 a.u.
B3LYP free energy: -1998.443016 a.u.
M06 SCF energy in solution: -1998.297567 a.u.
M06 enthalpy in solution: -1997.464452 a.u.
M06 free energy in solution: -1997.581902 a.u.

Cartesian coordinates

Ru	-0.80342800	-0.14001100	0.82592200
O	-1.25720100	-1.28994700	2.98354600
O	-1.03044900	0.86153300	2.75703300
N	-2.13514600	-1.31126500	-1.45295500
N	-0.03382300	-1.84985500	-1.76570300
C	-0.89475500	-1.19673200	-0.90928200
C	-2.14776800	-1.86976900	-2.80321700
C	-3.28177000	-0.70967400	-0.76750200
C	-3.60459200	0.70149700	-1.31770600
C	-4.72800900	1.34737400	-0.48316500
C	-5.99384700	0.47172900	-0.56749600
C	-5.67683300	-0.93756200	-0.02565900
C	-4.55912900	-1.57688400	-0.88508300
C	-5.22428400	-0.81832600	1.44538900
C	-3.94241300	0.05153600	1.53496100
C	-2.85048300	-0.65782600	0.71090900
C	-4.25630100	1.45672000	0.98153200
C	1.26156400	-2.38710700	-1.45940200
C	2.36806500	-1.98723900	-2.23046700
C	3.61607500	-2.57226400	-1.97228200
C	2.24771000	-0.98048600	-3.35195700
C	-0.23449600	1.48567800	0.02756500
C	-0.76252900	-2.52025800	-2.86886700
C	1.39248900	-3.40820300	-0.48840200
C	3.78490300	-3.55389300	-0.99547900
C	2.65674800	-3.95951400	-0.26992700
C	0.21205500	-3.90839500	0.31146900
C	5.13391300	-4.18549200	-0.73985600
H	-2.79165500	-1.69892700	1.06156300
H	-2.96020800	-2.58869500	-2.93819000
H	-2.26628500	-1.07485200	-3.55383700
H	-2.70533200	1.32210900	-1.26766000
H	-3.90421000	0.63277300	-2.37400600
H	-4.94398700	2.34765400	-0.88221300
H	-6.34467400	0.41111000	-1.60778700
H	-6.80585200	0.92351700	0.01800900
H	-6.57377800	-1.56788500	-0.08801400
H	-4.34384000	-2.59657400	-0.53847100
H	-4.89847800	-1.64743400	-1.92957800
H	-5.02866100	-1.81276000	1.86792900
H	-6.03096300	-0.36982000	2.04260100
H	-3.64073100	0.13040800	2.58354600
H	-3.36654100	2.09539400	1.04867700
H	-5.03751300	1.93146200	1.59110500
H	4.47430800	-2.25207700	-2.55973300
H	2.18240600	-1.48390300	-4.32634300
H	1.35835700	-0.35609200	-3.24495700
H	3.12788600	-0.32952700	-3.39083900
H	-0.25658900	-2.36123600	-3.82487400
H	-0.80662100	-3.60184400	-2.68104500
H	2.76157500	-4.73788300	0.48323900
H	-0.66043400	-4.10171800	-0.32256400
H	0.46678300	-4.84023900	0.82514500
H	-0.10211200	-3.18166400	1.06917900
H	5.40891200	-4.12648000	0.31996900
H	5.13237800	-5.24884400	-1.01142200
H	5.92190000	-3.69533600	-1.32002700
C	1.40543000	0.77535700	1.09404900
C	1.17452600	-0.59597400	1.48973000
H	1.70563300	-1.36481100	0.93751300
H	1.29031500	1.49707400	1.89960000
H	-0.42160100	2.34850700	0.68212700
C	0.08500600	1.89256800	-1.40461100
H	0.83696700	1.22547700	-1.83439700
H	-0.82885400	1.69822600	-1.98659500
C	0.48432000	3.34418400	-1.61910200
C	-0.32013900	4.38913600	-1.13841500
C	1.64328700	3.67713000	-2.33348800
C	0.02948300	5.72215300	-1.35553000
H	-1.23316000	4.15987100	-0.59349500
C	1.99626600	5.01040100	-2.55534000
H	2.27663500	2.88314300	-2.72348500
C	1.19115100	6.03843400	-2.06414000
H	-0.60833600	6.51481300	-0.97310900
H	2.90118400	5.24304500	-3.11074500
H	1.46378500	7.07667000	-2.23288700
H	1.07391400	-0.80147700	2.55190400
C	2.58629000	1.07980900	0.16814400
H	2.64152600	0.32058700	-0.61833100
H	2.46353400	2.05450300	-0.30976100
C	3.88179200	1.09370800	0.96551500
C	4.28106300	2.25778400	1.63699000
C	4.69175400	-0.04557700	1.06094400
C	5.45620700	2.28340700	2.38934700
H	3.66734900	3.15349500	1.56508000
C	5.86958300	-0.02220700	1.81004000
H	4.40018500	-0.95372900	0.53935300
C	6.25490300	1.14155800	2.47854300
H	5.74905500	3.19583000	2.90224400
H	6.48839000	-0.91408900	1.86971800
H	7.17157200	1.15947000	3.06198900
N	-1.27256300	-0.14676900	3.54068400
O	-1.50309700	0.02063800	4.72650100

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B3LYP SCF energy: -1999.166015 a.u.
B3LYP enthalpy: -1998.330122 a.u.
B3LYP free energy: -1998.450189 a.u.
M06 SCF energy in solution: -1998.310246 a.u.
M06 enthalpy in solution: -1997.474353 a.u.
M06 free energy in solution: -1997.59442 a.u.

Cartesian coordinates

Ru	-0.89713400	-0.00988400	0.75336700
O	-1.43657900	-0.68878400	3.38194500
O	-1.13779800	1.27769000	2.46555600
N	-2.18208700	-1.45081400	-1.38014100
N	-0.07727800	-1.95421900	-1.69880500
C	-0.93340000	-1.24848400	-0.88477300
C	-2.21210700	-2.11894100	-2.67969300
C	-3.31676800	-0.79948500	-0.72676800
C	-3.61077200	0.59101400	-1.34937500
C	-4.72964800	1.29697700	-0.55890200
C	-6.00704800	0.43438000	-0.60835900
C	-5.71798600	-0.94932300	0.01059000
C	-4.60517900	-1.65233000	-0.80046300
C	-5.26651500	-0.76483200	1.47360000
C	-3.97745100	0.09819300	1.52887900
C	-2.88621600	-0.65458700	0.74786200
C	-4.27153700	1.47721200	0.90243700
C	1.24741900	-2.41747600	-1.39608200
C	2.30954800	-2.05811200	-2.24959200
C	3.58455900	-2.57387400	-1.98968200
C	2.10704500	-1.18048700	-3.46416500
C	0.04477800	1.54203500	-0.05737300
C	-0.81146500	-2.73665100	-2.72259300
C	1.44943600	-3.34436900	-0.34913900

C	3.82755700	-3.45096600	-0.92982700
C	2.74296200	-3.83043600	-0.13132100
C	0.31514700	-3.82906200	0.52452200
C	5.22059900	-3.96583800	-0.65178900
H	-2.75684800	-1.65964800	1.17851600
H	-3.00756500	-2.86651500	-2.73435200
H	-2.36744500	-1.39142700	-3.48945400
H	-2.69540800	1.19550300	-1.33073200
H	-3.90184600	0.47170000	-2.40321200
H	-4.92837300	2.27703900	-1.01252300
H	-6.35017800	0.32303200	-1.64691200
H	-6.81678000	0.92905100	-0.05569200
H	-6.62485400	-1.56709800	-0.02411700
H	-4.40736700	-2.65334200	-0.39408300
H	-4.93283500	-1.77712400	-1.84319200
H	-5.08340400	-1.74017500	1.94370800
H	-6.06487300	-0.27720400	2.05016300
H	-3.68099100	0.21480100	2.57299300
H	-3.37649900	2.10941000	0.95236300
H	-5.05430300	1.98779200	1.47960400
H	4.40703600	-2.28499000	-2.64123200
H	2.00618400	-1.78926400	-4.37340500
H	1.21000000	-0.56407000	-3.38074600
H	2.96751400	-0.52081200	-3.61895200
H	-0.33077300	-2.64779300	-3.70009100
H	-0.82028100	-3.79840800	-2.44099600
H	2.90290600	-4.53819500	0.67923800
H	-0.56811000	-4.10183200	-0.06368900
H	0.62317800	-4.71072000	1.09446500
H	-0.00369600	-3.06227800	1.23897700
H	5.80381000	-3.23323900	-0.07827400
H	5.19676800	-4.89332400	-0.07075100
H	5.76973600	-4.15922200	-1.57983200
C	1.24355500	0.97611500	0.88561500
C	0.92832900	-0.43882100	1.47880700
H	1.50038900	-1.24343800	1.02322600
H	1.26245900	1.66547500	1.73138300
H	-0.34245000	2.44997400	0.41917900
C	0.30084900	1.77482000	-1.55018400
H	0.97049300	1.00890300	-1.94642100
H	-0.65620500	1.63775200	-2.07308400
C	0.83420000	3.15663900	-1.90800200
C	0.11579300	4.31338700	-1.56736800
C	2.03341200	3.31039700	-2.61689700
C	0.58590500	5.58006300	-1.91417200
H	-0.82515500	4.22349800	-1.02909200
C	2.50794500	4.57654200	-2.96843000
H	2.60256800	2.42748700	-2.89972700
C	1.78644100	5.71713200	-2.61551800
H	0.01220500	6.46129400	-1.63884200
H	3.44165400	4.66907400	-3.51736200
H	2.15336200	6.70366100	-2.88565000
H	0.96148400	-0.47113800	2.56752000
C	2.62943000	0.98201500	0.18118100
H	2.68288700	0.16003100	-0.53978600
H	2.73302500	1.91768400	-0.37648300
C	3.76982600	0.88021100	1.17558600
C	4.21192200	2.02652200	1.85261300
C	4.39779000	-0.34086700	1.45611500
C	5.24440800	1.95565600	2.78834900
H	3.74247500	2.98522500	1.64113800
C	5.43186100	-0.41606800	2.39196300
H	4.07448400	-1.23919000	0.93678900
C	5.85853400	0.73160400	3.06221000
H	5.57071000	2.85665500	3.30132100
H	5.90493400	-1.37336600	2.59710800
H	6.66324600	0.67370400	3.79030200
N	-1.37803100	0.55646600	3.53451200
O	-1.54194200	1.12240800	4.60680300

TS44

B3LYP SCF energy: -1999.135212 a.u.
B3LYP enthalpy: -1998.302796 a.u.
B3LYP free energy: -1998.425845 a.u.
M06 SCF energy in solution: -1998.28112 a.u.
M06 enthalpy in solution: -1997.448704 a.u.
M06 free energy in solution: -1997.571753 a.u.

Cartesian coordinates

Ru	-0.84063900	-0.06711900	0.63713500
O	-1.57177800	-0.00103200	3.88574900
O	-1.21121600	1.38543000	2.20695300
N	-2.06738600	-1.47798400	-1.52356700
N	0.05643300	-1.84334400	-1.91165200
C	-0.82227400	-1.23655500	-1.04052800
C	-2.08436300	-2.06762600	-2.86150100
C	-3.22490900	-0.94876400	-0.79484000
C	-3.58732400	0.48044800	-1.27684300
C	-4.73951300	1.04945800	-0.42418200
C	-5.97080500	0.13066300	-0.55874600
C	-5.60905700	-1.28737200	-0.07010900
C	-4.46963900	-1.84998900	-0.95098600
C	-5.15647600	-1.22245800	1.40419400
C	-3.91155900	-0.30738600	1.53837900
C	-2.77839800	-0.92248800	0.69091800
C	-4.28983300	1.10821600	1.04929700
C	1.41492300	-2.22669500	-1.64863500
C	2.44949400	-1.67955700	-2.43297400
C	3.76721300	-2.08796200	-2.18867500
C	2.17913800	-0.73553700	-3.58286700
C	0.35067600	1.79317700	-0.15403200
C	-0.65571800	-2.61251600	-2.95938900
C	1.68957600	-3.25855100	-0.72180300
C	4.07919200	-3.04432800	-1.22087300
C	3.02170200	-3.63008900	-0.51405500
C	0.58932800	-4.03016600	-0.02431700
C	5.51175200	-3.43371600	-0.94107400
H	-2.64367200	-1.96629000	1.00306700
H	-2.84360600	-2.84815100	-2.95189000
H	-2.28569000	-1.30166400	-3.62466200
H	-2.70135500	1.12957500	-1.19646400
H	-3.86820800	0.45797500	-2.34039000
H	-4.98966000	2.05735600	-0.78172900
H	-6.31264900	0.09750500	-1.60351200
H	-6.80164900	0.53144000	0.03685500
H	-6.48414400	-1.94411600	-0.16352300
H	-4.21979500	-2.87566000	-0.64735200
H	-4.80304900	-1.88697700	-1.99936800
H	-4.92446900	-2.23059900	1.77428100
H	-5.97724800	-0.83637400	2.02507300
H	-3.60130900	-0.27269600	2.58589600
H	-3.43860100	1.78779200	1.16573100
H	-5.10272600	1.51065200	1.66900100
H	4.56746200	-1.65244800	-2.78409400
H	2.27687500	-1.26567400	-4.53994300
H	1.17510600	-0.31172100	-3.53830400
H	2.90189000	0.08751300	-3.60457400
H	-0.19824400	-2.45094100	-3.93920700
H	-0.61011900	-3.68612100	-2.73264000
H	3.23705700	-4.41435400	0.20886300
H	0.14288500	-4.76720800	-0.70620700
H	0.99058900	-4.58485600	0.82936200
H	-0.21771000	-3.39019300	0.33881300
H	5.94024200	-2.80757800	-0.14713400
H	5.58738000	-4.47526500	-0.61102700
H	6.14187800	-3.31026300	-1.82814000
C	1.27105200	1.42171300	0.80533900
C	0.30275400	-1.06795400	1.64899600
H	1.07870800	-1.74105000	1.27492200
H	1.03259300	1.67445300	1.83307100
H	-0.47211500	2.41465300	0.20881500
C	0.64738200	1.91159500	-1.63863900
H	1.43237900	1.20738100	-1.91787600
H	-0.24673700	1.63730400	-2.21230400
C	1.07019100	3.32552400	-2.01384000
C	0.13029500	4.36601000	-2.05072500
C	2.40504800	3.62293100	-2.31856300
C	0.51435300	5.66679400	-2.37590900
H	-0.91332900	4.15520100	-1.82546700
C	2.79389100	4.92390300	-2.64655700
H	3.14679200	2.82712400	-2.30731500
C	1.84951600	5.95062600	-2.67409000
H	-0.22949000	6.45885900	-2.39918000
H	3.83421100	5.13277100	-2.88241300
H	2.14938300	6.96348500	-2.92886200
H	0.23710200	-0.94649700	2.73623000
C	2.69629000	0.97894100	0.53704500
H	2.72702400	0.16671200	-0.19614600
H	3.20688000	1.83272700	0.06230500
C	3.46256500	0.58868100	1.78682400
C	3.70415800	1.53474200	2.79403900
C	3.95302700	-0.71112000	1.96048400

C	4.40727000	1.18806400	3.94774300
H	3.33989700	2.55310100	2.67458900
C	4.66024000	-1.06116800	3.11355400
H	3.77575100	-1.45525200	1.18840100
C	4.88824700	-0.11328000	4.11159500
H	4.58041700	1.93464900	4.71822000
H	5.02963100	-2.07680500	3.23195700
H	5.43576200	-0.38451100	5.01017000
N	-1.56323300	1.16577900	3.45842700
O	-1.85842300	2.14933500	4.13427000

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B3LYP SCF energy: -1999.161441 a.u.
B3LYP enthalpy: -1998.325139 a.u.
B3LYP free energy: -1998.444562 a.u.
M06 SCF energy in solution: -1998.306574 a.u.
M06 enthalpy in solution: -1997.470272 a.u.
M06 free energy in solution: -1997.589695 a.u.

Cartesian coordinates

Ru	0.95921200	0.24985600	-0.64386200
O	1.91202800	3.28208900	-0.47438100
O	1.13589600	1.90811300	-2.01871000
N	2.33617300	-1.86916600	0.76160000
N	0.24432000	-2.40389500	1.09245900
C	1.06280300	-1.47885100	0.48573200
C	2.43821400	-2.96086300	1.73078800
C	3.47315500	-1.07400700	0.30483200
C	3.99688400	-0.14154200	1.42823900
C	5.14689400	0.73561700	0.89364800
C	6.29064700	-0.16247400	0.38169000
C	5.76229300	-1.06963200	-0.74826500
C	4.63946600	-1.96836000	-0.18452500
C	5.21472400	-0.19926900	-1.89957900
C	4.05868600	0.69972400	-1.38093100
C	2.94966200	-0.23864900	-0.87379000
C	4.60993200	1.60469900	-0.25787000
C	-1.13736400	-2.68535100	0.82772400
C	-2.08014700	-2.52953400	1.86186800
C	-3.41722600	-2.86251400	1.60557600
C	-1.68640800	-2.09110900	3.25499900
C	-0.32458900	1.37013600	0.41656100
C	1.00987800	-3.50692700	1.71787100
C	-1.50845600	-3.28051400	-0.39944800
C	-3.82995800	-3.37889700	0.37668200
C	-2.85339900	-3.60042000	-0.60333100
C	-0.48523300	-3.64545300	-1.45300300
C	-5.28347300	-3.68371100	0.10267100
H	2.66892700	-0.92981800	-1.70074800
H	3.17908700	-3.70414800	1.42554100
H	2.72577200	-2.57591200	2.71899500
H	3.17169200	0.48953100	1.78440300
H	4.34156300	-0.74575900	2.27979400
H	5.51424000	1.37738700	1.70500700
H	6.69576000	-0.77521300	1.19999800
H	7.11568700	0.45937500	0.01007900
H	6.57351600	-1.70894600	-1.12063800
H	4.27163900	-2.66045700	-0.95418700
H	5.03856900	-2.57555800	0.64095300
H	4.86316700	-0.83671800	-2.72270800
H	6.01861300	0.43022900	-2.30513700
H	3.67790800	1.31051600	-2.20438100
H	3.82705200	2.27958300	0.09653300
H	5.41674100	2.23198200	-0.66082200
H	-4.15071100	-2.72226900	2.39705100
H	-1.59537100	-2.96291800	3.91769400
H	-0.73176700	-1.56246800	3.26753300
H	-2.44602500	-1.43684900	3.69533200
H	0.62367700	-3.72884600	2.71622900
H	0.92057700	-4.41541300	1.10777700
H	-3.14467600	-4.05183200	-1.54972800
H	0.15297600	-4.47173800	-1.11255900
H	-0.98098500	-3.97634100	-2.37049700
H	0.17456900	-2.81170400	-1.70636800
H	-5.75562500	-2.86101400	-0.45031200
H	-5.39655600	-4.58944500	-0.50339900
H	-5.84723300	-3.82204800	1.03076000
C	-1.27946500	0.98622900	-0.81370400
C	-0.64880000	-0.10977800	-1.76635900
H	-1.15225500	-1.07257500	-1.71076000
H	-0.00642300	2.40558100	0.30585300
C	-0.75588200	1.08663200	1.85454800
H	-1.33288800	0.16266900	1.91236600
H	0.15615700	0.92113800	2.44527200
C	-1.53722500	2.22403600	2.50274000
C	-0.97787300	3.50748000	2.60681900
C	-2.81728700	2.01446300	3.03288700
C	-1.68057400	4.54700200	3.21610400
H	0.01624900	3.69625100	2.20777000
C	-3.52365800	3.05270200	3.64592300
H	-3.26895600	1.02702000	2.96340400
C	-2.95758200	4.32424300	3.73803000
H	-1.22866800	5.53319500	3.28404600
H	-4.51618900	2.86587200	4.04830000
H	-3.50472000	5.13494700	4.21175100
H	-0.54048400	0.25382200	-2.79064600
H	-1.30871500	1.89464800	-1.41769900
C	-2.72559200	0.59818000	-0.39735900
H	-2.74299900	-0.41811800	0.00584900
H	-3.04715600	1.27220200	0.40301400
C	-3.69762600	0.72427200	-1.55493300
C	-4.17482400	1.98811100	-1.93423500
C	-4.13449700	-0.39352200	-2.27844800
C	-5.05468900	2.13250100	-3.00712200
H	-3.85476900	2.86781500	-1.37939200
C	-5.01737100	-0.25416100	-3.35208800
H	-3.78141500	-1.38128000	-1.99418700
C	-5.47924400	1.00986000	-3.72173800
H	-5.41107600	3.12153100	-3.28309700
H	-5.34439800	-1.13489600	-3.89956600
H	-6.16553500	1.11991500	-4.55717400
N	1.63882600	3.07426900	-1.67519100
O	1.80984100	3.90140900	-2.56499300

TS45

B3LYP SCF energy: -1999.141677 a.u.
B3LYP enthalpy: -1998.307708 a.u.
B3LYP free energy: -1998.426559 a.u.
M06 SCF energy in solution: -1998.277488 a.u.
M06 enthalpy in solution: -1997.443519 a.u.
M06 free energy in solution: -1997.56237 a.u.

Cartesian coordinates

Ru	-0.94227400	0.30892100	0.64033100
O	-1.97417100	2.40605900	0.10121600
O	-1.25632900	1.92374600	2.09271900
N	-2.32667400	-1.34141400	-1.28182000
N	-0.22755900	-1.77319100	-1.73445600
C	-1.05908600	-1.06513200	-0.88031500
C	-2.41174900	-2.05587900	-2.55486800
C	-3.48854400	-0.81077500	-0.56288200
C	-4.13463400	0.37908100	-1.31298800
C	-5.32324700	0.93111200	-0.49451600
C	-6.36930400	-0.17824900	-0.27480100
C	-5.71546300	-1.34426500	0.49274200
C	-4.56426400	-1.91127100	-0.36761700
C	-5.17494500	-0.83875100	1.85031600
C	-4.10707700	0.26708100	1.61725200
C	-2.95401900	-0.39513900	0.82112000
C	-4.80948400	1.42576800	0.87149900
C	1.10874800	-2.22926900	-1.47801000
C	2.13477200	-1.89334400	-2.38424500
C	3.42729000	-2.38246500	-2.14987600
C	1.87201100	-1.09610600	-3.64334600
C	0.78243800	1.65379100	-0.09847300
C	-0.99693300	-2.61736300	-2.67898800
C	1.35142600	-3.16159900	-0.44155100
C	3.71763700	-3.22745300	-1.07789400
C	2.65760500	-3.62323600	-0.25239200
C	0.23209400	-3.75559600	0.38686200
C	5.12531800	-3.70767500	-0.81476300
H	-2.72514300	-1.33139400	1.34991400
H	-3.17748800	-2.83484900	-2.53152400
H	-2.65396700	-1.36092100	-3.37103600
H	-3.38877500	1.16471900	-1.47038700
H	-4.48478300	0.04582500	-2.30138100
H	-5.77792200	1.76605000	-1.04360800
H	-6.76425000	-0.53482500	-1.23731500
H	-7.22145500	0.21810900	0.29353700
H	-6.45536100	-2.13795000	0.66339000
H	-4.10704800	-2.78427800	0.11766800
H	-4.97246600	-2.24613700	-1.33276500

H	-4.74189300	-1.67393500	2.41806000
H	-6.00553300	-0.44104000	2.45069600
H	-3.73475900	0.62159600	2.58548600
H	-4.15024600	2.28039000	0.72715100
H	-5.65654700	1.77705700	1.47768900
H	4.22245500	-2.10370600	-2.83870300
H	1.79910200	-1.76939100	-4.50850400
H	0.94284700	-0.52737000	-3.58348200
H	2.68875100	-0.39704300	-3.85137500
H	-0.58928500	-2.54022800	-3.69039800
H	-0.94365300	-3.66955600	-2.36867300
H	2.84696200	-4.33645200	0.54773700
H	-0.31118100	-4.51501500	-0.19206800
H	0.63280000	-4.25546300	1.27425100
H	-0.49698700	-3.01262500	0.71440900
H	5.59942700	-3.11661300	-0.02010500
H	5.13826500	-4.75423800	-0.49028300
H	5.75265600	-3.62069900	-1.70763600
C	1.44488100	1.08997800	1.00273000
C	0.12671900	-0.65984700	1.81407300
H	0.82978500	-1.47423800	1.62331500
H	0.26583300	2.58717800	0.09401000
C	1.24819900	1.51766900	-1.53557800
H	1.73050800	0.55201000	-1.67978300
H	0.37023700	1.54280000	-2.19233700
C	2.19941100	2.63774300	-1.93527100
C	1.73069900	3.95277700	-2.07751500
C	3.55849100	2.38655200	-2.16819200
C	2.59674400	4.98591300	-2.43477600
H	0.67670600	4.16591600	-1.91148100
C	4.42894300	3.41886100	-2.52817800
H	3.93790700	1.37135400	-2.07368100
C	3.95079600	4.72262800	-2.66028900
H	2.21365500	5.99749400	-2.54124500
H	5.47910100	3.20172800	-2.70664500
H	4.62511300	5.52750300	-2.94028200
H	0.09975400	-0.36299900	2.87370000
H	1.27922200	1.58939900	1.95332800
C	2.75758700	0.31946900	0.90485900
H	2.64582800	-0.58835000	0.30693900
H	3.44865400	0.96647000	0.34329300
C	3.39046300	-0.00025900	2.24688900
C	3.75358400	1.03475000	3.12240800
C	3.65564700	-1.31975400	2.63349400
C	4.35015500	0.75800400	4.35255100
H	3.57416800	2.06900700	2.83582900
C	4.25598100	-1.60153900	3.86326000
H	3.39116600	-2.13234200	1.96214500
C	4.60298500	-0.56356900	4.72853100
H	4.62218000	1.57513900	5.01550800
H	4.45160300	-2.63350200	4.14393200
H	5.06922800	-0.78044900	5.68585500
N	-1.84452400	2.77657200	1.32012500
O	-2.24888500	3.84941200	1.73328500

TS46

B3LYP SCF energy: -1728.80523 a.u.
B3LYP enthalpy: -1728.087871 a.u.
B3LYP free energy: -1728.193963 a.u.
M06 SCF energy in solution: -1728.074157 a.u.
M06 enthalpy in solution: -1727.356798 a.u.
M06 free energy in solution: -1727.46289 a.u.

Cartesian coordinates

Ru	-0.70546100	-0.64083200	0.35348300
O	-0.46011000	-1.96168900	-1.55770300
O	-0.81794900	-2.84173200	0.39411100
N	-2.14658400	1.79749300	-0.20766700
N	-0.06266300	2.44292200	0.00485500
C	-0.88654800	1.34323500	0.01310800
C	-2.26191600	3.25530700	-0.18022200
C	-3.26772700	0.85730800	-0.11913200
C	-3.89529500	0.85982000	1.29759800
C	-4.97601000	-0.23499400	1.39019300
C	-6.08297000	0.06134400	0.35862700
C	-5.47004400	0.07686500	-1.05701700
C	-4.38747900	1.18080700	-1.13753000
C	-4.84888200	-1.30656300	-1.34668400
C	-3.72227900	-1.60441600	-0.32169100
C	-2.64970300	-0.50931100	-0.48361200
C	-4.32914900	-1.60485400	1.09584800
C	1.36036800	2.45073900	-0.17681800
C	2.17789000	2.92995000	0.86329000
C	3.56316900	2.96467500	0.66411200
C	1.59141600	3.41504500	2.16966700
C	-0.85085500	-0.40151600	2.20390200
C	-0.79783800	3.67756600	-0.35274800
C	1.91516600	2.07221700	-1.41845400
C	4.14756100	2.55686400	-0.53740000
C	3.30346600	2.13037000	-1.56912300
C	1.05233700	1.58669800	-2.56120900
C	5.64716400	2.54789900	-0.71667000
H	-2.39224900	-0.45771100	-1.55173900
H	-0.79819100	0.51108400	2.81287900
H	-2.90725600	3.62611200	-0.98127000
H	-2.67681100	3.59512500	0.77936700
H	-3.11334900	0.68412400	2.04379900
H	-4.33703800	1.84503700	1.50844000
H	-5.40477200	-0.23467900	2.40155300
H	-6.55852500	1.02760900	0.58043800
H	-6.86924700	-0.70336900	0.41700100
H	-6.25252800	0.29411300	-1.79619800
H	-3.96110300	1.22778400	-2.14841600
H	-4.84650800	2.15890000	-0.92772900
H	-4.44295800	-1.33723700	-2.36654400
H	-5.62976900	-2.07840900	-1.29022300
H	-3.29635100	-2.59028800	-0.53485700
H	-3.55143700	-1.82304500	1.83813300
H	-5.08437800	-2.39876500	1.17844400
H	4.20011500	3.31663700	1.47279000
H	1.15233300	4.41655400	2.06577400
H	0.79445900	2.75712500	2.53070600
H	2.36368000	3.47976900	2.94220700
H	-0.50816100	4.50737700	0.29748600
H	-0.57097400	3.96111600	-1.38938700
H	3.73803200	1.82932800	-2.52020100
H	0.20931600	2.25883700	-2.75615600
H	1.64061000	1.51378700	-3.48084800
H	0.62680400	0.59742400	-2.35497400
H	6.04242000	1.52900300	-0.61267800
H	5.93438600	2.90841000	-1.71100600
H	6.14570200	3.17479800	0.02953900
C	1.30392800	-0.51223900	1.69787100
C	1.59231200	-0.90285200	0.38191300
H	1.44366600	0.52019100	1.99266600
H	1.40430700	-1.24898400	2.49230900
H	1.90345700	-0.11808000	-0.29876400
C	2.17174600	-2.27463500	0.06659200
H	1.78889200	-3.01699000	0.77395700
H	1.86405900	-2.58418400	-0.93642700
C	3.69196800	-2.23063200	0.12548300
C	4.44066200	-1.88588200	-1.00816800
C	4.37752900	-2.50269300	1.31730200
C	5.83390500	-1.80828800	-0.95241900
H	3.92595000	-1.68601400	-1.94558700
C	5.76982600	-2.42805500	1.37858500
H	3.81449200	-2.78438500	2.20474000
C	6.50387700	-2.07746900	0.24324300
H	6.39651400	-1.55059600	-1.84644200
H	6.28200200	-2.65059800	2.31130800
H	7.58852400	-2.02463000	0.28731900
H	-1.00501300	-1.29920400	2.82139000
N	-0.66850000	-3.02951900	-0.87376400
O	-0.71870700	-4.13740300	-1.37648900

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B3LYP SCF energy: -1728.819296 a.u.
B3LYP enthalpy: -1728.099174 a.u.
B3LYP free energy: -1728.206012 a.u.
M06 SCF energy in solution: -1728.095256 a.u.
M06 enthalpy in solution: -1727.375134 a.u.
M06 free energy in solution: -1727.481972 a.u.

Cartesian coordinates

Ru	0.73907800	0.60279000	0.36671200
O	0.98001600	2.69710200	-1.32550000
O	1.05920000	2.67743800	0.85700800
N	1.93757600	-1.93306500	-0.30737900
N	-0.15673700	-2.45802900	0.05550300
C	0.71993200	-1.40527700	-0.01777300
C	1.98502900	-3.39361900	-0.22670000
C	3.10776500	-1.05670400	-0.24750300

C	3.73155500	-1.05583600	1.17456700
C	4.88840200	-0.04025700	1.24110100
C	5.96750900	-0.43424900	0.21219800
C	5.35214600	-0.43820800	-1.20268900
C	4.20053900	-1.46799600	-1.26144800
C	4.81195300	0.97038800	-1.52223600
C	3.71951100	1.36794000	-0.49340200
C	2.57485200	0.34477300	-0.61304800
C	4.33810100	1.36344500	0.91946400
C	-1.58953900	-2.41585300	-0.04291900
C	-2.36777700	-2.76813400	1.07462900
C	-3.76251000	-2.76074600	0.94542900
C	-1.73667400	-3.17349100	2.38664400
C	0.20190400	0.33355800	2.25251200
C	0.49409600	-3.74650400	-0.27849500
C	-2.19466600	-2.13045600	-1.28581900
C	-4.39349300	-2.43855800	-0.25807600
C	-3.58924600	-2.14535200	-1.36533000
C	-1.37239200	-1.78571800	-2.50720600
C	-5.89859600	-2.37758800	-0.36228100
H	2.22102900	0.32186500	-1.65592800
H	0.16998700	-0.65389200	2.71572900
H	2.55326200	-3.82663800	-1.05450500
H	2.45069100	-3.71622700	0.71499000
H	2.95735900	-0.80022700	1.90899400
H	4.09824400	-2.06297800	1.42056200
H	5.31948400	-0.05075200	2.25100300
H	6.37750000	-1.42576000	0.45249800
H	6.80437300	0.27566200	0.25356000
H	6.11714000	-0.71952500	-1.93826200
H	3.76931600	-1.50718900	-2.27067000
H	4.58914500	-2.47099400	-1.02988800
H	4.39687500	1.00022500	-2.53844800
H	5.63383900	1.69925200	-1.49141600
H	3.36003500	2.36779200	-0.74253600
H	3.58466300	1.65950600	1.65975400
H	5.14747400	2.10432500	0.97287900
H	-4.36910700	-3.01397200	1.81221800
H	-1.28877600	-4.17438600	2.32447900
H	-0.94043500	-2.48749900	2.68866300
H	-2.48553100	-3.20280800	3.18376300
H	0.20879200	-4.52219600	0.43729800
H	0.18366100	-4.07606000	-1.27854500
H	-4.06080400	-1.91433800	-2.31822300
H	-0.62793700	-2.55698000	-2.73659000
H	-2.01616800	-1.67649100	-3.38498000
H	-0.82333000	-0.84668600	-2.37179000
H	-6.24317300	-1.33582600	-0.32640400
H	-6.25420100	-2.80608300	-1.30622000
H	-6.38183900	-2.91570600	0.45940200
C	-1.20178100	0.77837400	1.64617900
C	-1.24890300	0.93411700	0.07936400
H	-1.92227700	0.00033300	1.90610800
H	-1.47471800	1.73521700	2.09420300
H	-1.77026800	0.09961300	-0.38215300
C	-1.80984200	2.26088300	-0.44045000
H	-1.37253100	3.10213300	0.10337800
H	-1.52099000	2.37221600	-1.49067600
C	-3.32493300	2.31367500	-0.31640800
C	-4.14585600	1.68863600	-1.26650800
C	-3.93988800	2.97641500	0.75507600
C	-5.53634700	1.71890900	-1.14817100
H	-3.68850500	1.18388500	-2.11471800
C	-5.33036500	3.00755200	0.88044100
H	-3.32307900	3.48809500	1.49068800
C	-6.13465200	2.37681300	-0.07031000
H	-6.15364800	1.24152400	-1.90554000
H	-5.78462200	3.53344200	1.71642500
H	-7.21726300	2.40738300	0.02059000
N	1.13660600	3.35070800	-0.26157400
O	1.35144100	4.55469900	-0.22670200
H	0.61452500	1.09118300	2.92568600

TS47

B3LYP SCF energy: -1728.809864 a.u.
B3LYP enthalpy: -1728.090989 a.u.
B3LYP free energy: -1728.196915 a.u.
M06 SCF energy in solution: -1728.087331 a.u.
M06 enthalpy in solution: -1727.368456 a.u.
M06 free energy in solution: -1727.474382 a.u.

Cartesian coordinates

Ru	-0.59225400	0.44693600	-0.43793500
O	-0.02462400	4.15242500	-1.14365700
O	-1.00602000	2.24409600	-1.62137900
N	-1.77389900	-1.73807100	1.04285300
N	0.24634800	-2.44204400	0.57320800
C	-0.61341700	-1.39212700	0.41147600
C	-1.80856600	-3.13607000	1.47921100
C	-2.96917400	-0.94418800	0.75653500
C	-3.72687800	-1.52233900	-0.47134600
C	-4.90664500	-0.60724800	-0.84719100
C	-5.86935600	-0.50470200	0.35400600
C	-5.11749700	0.07551200	1.57062200
C	-3.94727000	-0.86220800	1.95077500
C	-4.57766200	1.47520400	1.20779900
C	-3.60391200	1.37557400	0.00263100
C	-2.44849000	0.45947400	0.42468700
C	-4.35738800	0.78654000	-1.20641200
C	1.57148100	-2.61176100	0.05028600
C	1.72221800	-3.18207000	-1.23327600
C	3.01254400	-3.36080100	-1.73596200
C	0.52788000	-3.65460600	-2.03234400
C	0.46532100	0.02070800	-2.07901500
C	-0.32304400	-3.51351300	1.41747900
C	2.69476000	-2.32957500	0.84833500
C	4.15121400	-3.02322200	-0.99264700
C	3.96889000	-2.52833800	0.29951000
C	2.57939600	-1.87145700	2.28560900
C	5.53404100	-3.19082200	-1.57744500
H	-1.95918200	0.88539700	1.33600700
H	0.70154800	-1.00352000	-2.35402200
H	-2.22812100	-3.23332300	2.48422800
H	-2.41483700	-3.74418300	0.79368500
H	-3.02677800	-1.60608700	-1.31303600
H	-4.09267800	-2.53335200	-0.24240300
H	-5.43470700	-1.03779200	-1.70840000
H	-6.28052600	-1.49506400	0.59723700
H	-6.72075700	0.14035500	0.09943000
H	-5.80170400	0.15066000	2.42586300
H	-3.41810600	-0.48019100	2.83411000
H	-4.33658300	-1.85889400	2.20658100
H	-4.06434600	1.92082400	2.07109300
H	-5.41252100	2.14316700	0.95531200
H	-3.22749300	2.36702100	-0.25564500
H	-3.68222800	0.72481200	-2.06902400
H	-5.17944900	1.45620000	-1.49171400
H	3.13347500	-3.78573100	-2.73024100
H	0.10099900	-4.56793000	-1.59574200
H	-0.27392400	-2.91231300	-2.06772300
H	0.81951500	-3.89236200	-3.05972700
H	-0.14415500	-4.49456700	0.96840500
H	0.14749800	-3.50111400	2.40933400
H	4.84038400	-2.29000100	0.90575300
H	2.77061500	-2.70716800	2.97230400
H	3.32008400	-1.09632100	2.50818700
H	1.58991000	-1.47099200	2.51786800
H	5.77620100	-2.36527400	-2.25931400
H	6.30046300	-3.20563200	-0.79610900
H	5.61623600	-4.11963400	-2.15296700
C	1.58126600	0.70864700	-1.20077700
C	1.20268700	0.88115800	0.33291000
H	2.45239200	0.04867500	-1.22188100
H	1.80669300	1.69060000	-1.61618300
H	1.66784000	0.10024100	0.93060700
C	1.42703500	2.25693300	0.96646300
H	0.87942800	3.02292600	0.41312800
H	1.02317400	2.22058300	1.98781400
C	2.89939400	2.63197600	1.02408100
C	3.73833000	2.12956100	2.02940100
C	3.45322700	3.47956300	0.05371000
C	5.09598200	2.45269000	2.06018800
H	3.31855300	1.49336700	2.80693100
C	4.81115100	3.80408200	0.08137000
H	2.80657800	3.89843700	-0.71329800
C	5.63823500	3.28919000	1.08178600
H	5.72820400	2.05995600	2.85299700
H	5.22085500	4.46827600	-0.67551900
H	6.69407600	3.54612100	1.10577500
H	0.16647700	0.63680000	-2.92863200
N	-1.07691800	3.53220800	-1.36369000
O	-2.18524800	4.07180400	-1.39787500

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B3LYP SCF energy: -1728.816307 a.u.
B3LYP enthalpy: -1728.096443 a.u.
B3LYP free energy: -1728.204541 a.u.
M06 SCF energy in solution: -1728.0928 a.u.
M06 enthalpy in solution: -1727.372936 a.u.
M06 free energy in solution: -1727.481034 a.u.

Cartesian coordinates

Ru	0.66166700	0.53368400	0.26561100
O	-0.47712500	3.40497300	1.82766300
O	1.19335000	2.59721000	0.62302200
N	1.96759800	-1.90227000	-0.55819700
N	-0.04512800	-2.56836100	-0.01212500
C	0.75259900	-1.46100200	-0.12516400
C	2.09913700	-3.36086500	-0.54621400
C	3.10205200	-0.97813400	-0.52775700
C	3.85487700	-1.06715700	0.82867000
C	4.97617200	-0.01092300	0.88154600
C	5.96390400	-0.26225400	-0.27636400
C	5.21625900	-0.16816200	-1.62307700
C	4.10734200	-1.24464700	-1.67090800
C	4.59162100	1.23650500	-1.75913900
C	3.59558300	1.49087400	-0.59726700
C	2.49310500	0.42435100	-0.68594700
C	4.35037400	1.39046100	0.74327500
C	-1.46653300	-2.62449800	0.18065600
C	-1.97779100	-2.95782500	1.44931100
C	-3.36711400	-3.03427700	1.61013000
C	-1.08185500	-3.27832100	2.62481200
C	-0.20770900	0.34747000	2.04572700
C	0.63137100	-3.79560400	-0.48372100
C	-2.33041400	-2.45570900	-0.92346400
C	-4.24968500	-2.81330700	0.55081400
C	-3.70842200	-2.53892400	-0.71033600
C	-1.80846600	-2.23720900	-2.32736700
C	-5.74557100	-2.85596100	0.75698300
H	2.00690600	0.49036100	-1.68551800
H	-0.25350800	-0.62796900	2.52841500
H	2.61368700	-3.72764100	-1.43836400
H	2.66264600	-3.69344000	0.33683800
H	3.13933100	-0.90562400	1.64613200
H	4.27874100	-2.07369200	0.95538100
H	5.50289800	-0.09439100	1.84133900
H	6.43176800	-1.25154700	-0.16998000
H	6.77345000	0.47899300	-0.24584000
H	5.91817800	-0.34527000	-2.44849100
H	3.58268700	-1.21650900	-2.63540900
H	4.55704700	-2.24364300	-1.57038000
H	4.07800400	1.33122700	-2.72607300
H	5.38327300	1.99846700	-1.74326500
H	3.15239900	2.48417000	-0.69194300
H	3.66110600	1.59109400	1.57172800
H	5.13458100	2.15816400	0.78677700
H	-3.76636500	-3.27501200	2.59339000
H	-1.01928000	-4.36436200	2.77810500
H	-0.06576700	-2.90544400	2.48271900
H	-1.47971300	-2.84881300	3.55044100
H	0.45311900	-4.62517200	0.20625100
H	0.24600800	-4.08144100	-1.47127600
H	-4.37830500	-2.38737300	-1.55420000
H	-1.62082700	-3.19658000	-2.82882800
H	-2.54362400	-1.69893200	-2.93384800
H	-0.87383300	-1.67090800	-2.34514100
H	-6.15589200	-1.84357500	0.86531300
H	-6.25433800	-3.32125900	-0.09452800
H	-6.01047200	-3.41620900	1.65938100
C	-1.47582600	0.66619900	1.15629100
C	-1.20129200	0.83077000	-0.40093300
H	-2.17080700	-0.16652900	1.26300000
H	-1.88666900	1.60670600	1.51693700
H	-1.65870900	0.01083900	-0.95261500
C	-1.55529600	2.17928300	-1.03956800
H	-1.06442100	2.98758100	-0.49811600
H	-1.16378700	2.17844800	-2.06586900
C	-3.05552600	2.42095100	-1.07417200
C	-3.86364700	1.81942500	-2.04960200
C	-3.66514900	3.23850800	-0.11164000
C	-5.24445200	2.02203300	-2.06224200
H	-3.40305700	1.19752700	-2.81553700
C	-5.04654200	3.44312000	-0.12153300
H	-3.04638700	3.72310200	0.63988200
C	-5.84125200	2.83416500	-1.09485900
H	-5.85340400	1.55393300	-2.83201200
H	-5.50054200	4.08552600	0.62879400
H	-6.91579000	2.99764500	-1.10554500
N	0.69118300	3.52619700	1.40783900
O	1.41234900	4.48318700	1.67568200
H	0.02102900	1.15753700	2.73986200

TS48

B3LYP SCF energy: -1728.81349 a.u.
B3LYP enthalpy: -1728.094871 a.u.
B3LYP free energy: -1728.202422 a.u.
M06 SCF energy in solution: -1728.092841 a.u.
M06 enthalpy in solution: -1727.374222 a.u.
M06 free energy in solution: -1727.481773 a.u.

Cartesian coordinates

Ru	0.64353400	0.51782400	0.22836400
O	0.68122300	3.18875500	2.48631700
O	1.02395400	2.64867900	0.37393100
N	1.85834000	-1.96107300	-0.61113500
N	-0.17224900	-2.54967600	-0.03939800
C	0.66721600	-1.47651300	-0.15948300
C	1.93292700	-3.42372500	-0.60664300
C	3.02394700	-1.07519100	-0.57569700
C	3.76378300	-1.19113900	0.78618600
C	4.91114600	-0.16496700	0.85539700
C	5.90067200	-0.43578700	-0.29663000
C	5.16601900	-0.31444400	-1.64826900
C	4.02957100	-1.36276200	-1.71252200
C	4.58259200	1.10888000	-1.77928900
C	3.58356700	1.38388600	-0.62452300
C	2.45655200	0.34472500	-0.73396100
C	4.32337400	1.25323800	0.72201300
C	-1.59017100	-2.54170600	0.18761100
C	-2.08848800	-2.84902000	1.46679700
C	-3.47720400	-2.85541100	1.65857200
C	-1.18714700	-3.21898700	2.62351000
C	-0.16097800	0.32452800	2.03533300
C	0.44927500	-3.80214200	-0.52134300
C	-2.47012000	-2.33051800	-0.89784600
C	-4.37080200	-2.59352600	0.61946000
C	-3.84456400	-2.34715600	-0.65493500
C	-1.96439400	-2.12518100	-2.30932300
C	-5.86271000	-2.56654800	0.85526600
H	1.98258800	0.42985200	-1.73704100
H	-0.29647400	-0.66830200	2.46159800
H	2.41808300	-3.80668200	-1.50850500
H	2.49729200	-3.78176700	0.26573700
H	3.04609100	-1.01626200	1.59903600
H	4.16042500	-2.20910500	0.91004000
H	5.42789100	-0.26851400	1.81857700
H	6.34120600	-1.43772300	-0.19168100
H	6.72961700	0.28318800	-0.25615900
H	5.86942900	-0.50527300	-2.46931000
H	3.51407000	-1.31418100	-2.68108400
H	4.45252100	-2.37373400	-1.61482300
H	4.07934800	1.22517500	-2.74917900
H	5.39560600	1.84747500	-1.75202900
H	3.16645700	2.38915500	-0.71434300
H	3.63558400	1.46285500	1.55089900
H	5.12437700	2.00171200	0.78034400
H	-3.86551000	-3.07583400	2.65096100
H	-1.23437900	-4.29903500	2.81760000
H	-0.14410200	-2.96006000	2.43275200
H	-1.50168800	-2.71646000	3.54468000
H	0.25009900	-4.62398800	0.17214600
H	0.03871800	-4.07349500	-1.50251900
H	-4.52469400	-2.16204800	-1.48368600
H	-1.71842400	-3.08425900	-2.78501400
H	-2.73152100	-1.64884000	-2.92748400
H	-1.06516600	-1.50411300	-2.34577900
H	-6.24070300	-1.53616000	0.86238900
H	-6.40259700	-3.10239900	0.06614400
H	-6.12540900	-3.02169600	1.81535700
C	-1.41806600	0.84375500	1.22503400
C	-1.23987500	0.89655000	-0.35025500
H	-2.23512800	0.14480600	1.41763200
H	-1.64682400	1.84810500	1.58154200

H	-1.76666100	0.07046000	-0.82370000
C	-1.58333400	2.22307200	-1.03860600
H	-1.04829500	3.04217200	-0.55486600
H	-1.22053300	2.17068300	-2.07415000
C	-3.08023500	2.48490200	-1.04953600
C	-3.91104900	1.87226700	-1.99929100
C	-3.67031900	3.32692500	-0.09633700
C	-5.28983500	2.08757200	-1.99514100
H	-3.46842500	1.23001000	-2.75870000
C	-5.04961100	3.54475900	-0.08734600
H	-3.04118500	3.82661200	0.63670400
C	-5.86496600	2.92402300	-1.03549700
H	-5.91436000	1.61013200	-2.74639300
H	-5.48532000	4.20669200	0.65674300
H	-6.93787000	3.09755700	-1.03292300
N	1.30738100	3.38231300	1.42916700
O	2.17248100	4.24763600	1.29572500
H	0.19413300	1.07134500	2.74599600

44

B3LYP SCF energy: -1728.821331 a.u.
B3LYP enthalpy: -1728.10141 a.u.
B3LYP free energy: -1728.208412 a.u.
M06 SCF energy in solution: -1728.094194 a.u.
M06 enthalpy in solution: -1727.374273 a.u.
M06 free energy in solution: -1727.481275 a.u.

Cartesian coordinates

Ru	-0.50173600	-0.48630800	0.52958600
O	-1.92410600	-0.83712300	2.68697700
O	-0.74405900	-2.34461300	1.64296600
N	-1.59238200	1.46457600	-1.31322700
N	0.40307200	2.23136100	-0.84579100
C	-0.47943700	1.22603500	-0.56355200
C	-1.57704900	2.75463500	-2.00796800
C	-2.81230200	0.70856900	-1.03336000
C	-3.74091800	1.49727600	-0.07098700
C	-4.98319800	0.65445300	0.27813200
C	-5.74769500	0.29954600	-1.01272500
C	-4.82254700	-0.50270300	-1.95055000
C	-3.60088700	0.36736500	-2.32183600
C	-4.35576800	-1.78894800	-1.23538800
C	-3.57687000	-1.42323600	0.05980800
C	-2.35553800	-0.59540300	-0.36711100
C	-4.52193200	-0.63116100	0.98798500
C	1.66017900	2.52963100	-0.22316800
C	1.65366000	3.27426500	0.97912100
C	2.87478100	3.59988300	1.56925300
C	0.35714700	3.72928700	1.60992500
C	0.76964600	0.07845200	1.99399400
C	-0.10336700	3.16328600	-1.87535600
C	2.86985500	2.19629000	-0.85541100
C	4.09858400	3.23239400	0.99198700
C	4.07187100	2.54709100	-0.22208200
C	2.93030400	1.50756000	-2.20092700
C	5.40395900	3.57296600	1.67213800
H	-1.78137400	-1.19348600	-1.12049200
H	1.03771000	1.12270700	2.12057900
H	-1.89260600	2.65232500	-3.05026300
H	-2.24899700	3.47180500	-1.51768600
H	-3.18178300	1.74570500	0.83973400
H	-4.04835100	2.44154300	-0.54216800
H	-5.63318000	1.23525100	0.94567500
H	-6.09692300	1.21247300	-1.51624800
H	-6.64013100	-0.29216600	-0.76894900
H	-5.36322200	-0.76621800	-2.86908300
H	-2.94303200	-0.16506000	-3.02190600
H	-3.93944000	1.28555000	-2.82430500
H	-3.72213900	-2.38659700	-1.90519200
H	-5.22528600	-2.41039100	-0.98069000
H	-3.24903100	-2.34439800	0.55169800
H	-4.01181000	-0.39290700	1.92443100
H	-5.39141900	-1.25459300	1.23829900
H	2.87358300	4.16066300	2.50164100
H	-0.20187100	4.39672300	0.94147500
H	-0.30188400	2.88721500	1.84552500
H	0.55129200	4.27752800	2.53650600
H	0.02827900	4.20049900	-1.55309200
H	0.45115300	3.02763400	-2.81283000
H	5.01080800	2.27560300	-0.70069300
H	3.34123000	2.18432300	-2.96145200
H	3.58498300	0.62935400	-2.16476200
H	1.94684300	1.17690700	-2.54119400
H	5.56230200	2.94607100	2.55908500
H	6.25651000	3.41957600	1.00320500
H	5.41999800	4.61606300	2.00889700
C	1.76346400	-0.72442700	1.09677400
C	1.17134900	-1.14460000	-0.33265800
H	2.62826700	-0.08808300	0.89634800
H	2.06225400	-1.63653700	1.61640900
H	1.61803500	-0.53649600	-1.11971200
C	1.28329800	-2.63638900	-0.67995200
H	0.82352900	-3.24033100	0.10781100
H	0.70601400	-2.81211500	-1.59881500
C	2.72078500	-3.07382100	-0.90460100
C	3.38774800	-2.75936800	-2.09883300
C	3.42672600	-3.77390100	0.08340200
C	4.72017500	-3.12354100	-2.29690900
H	2.85086100	-2.23412700	-2.88682700
C	4.76067200	-4.14048600	-0.10976500
H	2.92161400	-4.04412200	1.00806400
C	5.41340800	-3.81397800	-1.29951100
H	5.21506500	-2.87644700	-3.23301300
H	5.28718200	-4.68712500	0.66853400
H	6.45006000	-4.10217100	-1.45262400
N	-1.53178800	-2.03594900	2.63802500
O	-1.85029100	-2.88857900	3.45335100
H	0.55598900	-0.40412300	2.94769200

TS49

B3LYP SCF energy: -1728.80732 a.u.
B3LYP enthalpy: -1728.089617 a.u.
B3LYP free energy: -1728.196731 a.u.
M06 SCF energy in solution: -1728.073622 a.u.
M06 enthalpy in solution: -1727.355919 a.u.
M06 free energy in solution: -1727.463033 a.u.

Cartesian coordinates

Ru	0.41148400	0.41305000	0.56446500
O	1.73379400	0.26624100	2.48642600
O	0.83087700	2.14268600	1.87879400
N	1.54756400	-1.55997300	-1.22692700
N	-0.46534200	-2.30658100	-0.80061800
C	0.41113100	-1.28664900	-0.52911800
C	1.55753200	-2.89304700	-1.83406500
C	2.75836600	-0.76978600	-0.97689400
C	3.64072200	-1.44453800	0.10581400
C	4.87489700	-0.56843200	0.40407000
C	5.69123700	-0.36164400	-0.88666600
C	4.80564000	0.33200900	-1.94186800
C	3.60212700	-0.58565300	-2.26091100
C	4.32057800	1.69194900	-1.38897300
C	3.48063600	1.46986900	-0.10000200
C	2.26016800	0.60972300	-0.50449700
C	4.39916100	0.79372000	0.94300500
C	-1.79610100	-2.51134600	-0.31203500
C	-1.97201200	-3.28561700	0.85664900
C	-3.26949100	-3.52436400	1.31259000
C	-0.78807700	-3.87422500	1.59139500
C	-1.07317300	-0.17317900	2.15517400
C	0.07060700	-3.26199000	-1.79144400
C	-2.90769600	-2.05892800	-1.04575400
C	-4.39491900	-3.03776600	0.63438300
C	-4.19122400	-2.32166400	-0.54557000
C	-2.77164100	-1.34318000	-2.37136600
C	-5.78554300	-3.27846100	1.17376100
H	1.84409900	1.09750900	-1.39865000
H	-1.17660100	-1.24963700	2.16498900
H	1.95727400	-2.86807700	-2.85122400
H	2.17042300	-3.58698300	-1.24206200
H	3.04877500	-1.58390700	1.01795100
H	3.96429000	-2.43756100	-0.23966300
H	5.49607400	-1.06972300	1.15824800
H	6.05453700	-1.32557200	-1.27215500
H	6.57737200	0.25223100	-0.67541200
H	5.38310700	0.49280300	-2.86220300
H	2.97536500	-0.14486500	-3.04816500
H	3.97256200	-1.55117600	-2.63813100
H	3.72209800	2.21585400	-2.14724900
H	5.18977000	2.32957400	-1.17257800
H	3.13972900	2.44008100	0.28183200
H	3.88353000	0.65256000	1.89403900

H	5.26737000	1.43993200	1.13477200
H	-3.40727000	-4.10976700	2.21932600
H	-0.26865000	-4.62163300	0.97776100
H	-0.04574800	-3.11548700	1.85984900
H	-1.11327800	-4.37219200	2.50961300
H	-0.11059600	-4.29310500	-1.47466800
H	-0.42009800	-3.11402000	-2.76330500
H	-5.05259600	-1.95961900	-1.10387400
H	-3.09685000	-1.99219100	-3.19515900
H	-3.40273600	-0.44764400	-2.40324200
H	-1.74272600	-1.03882300	-2.57216800
H	-6.02731200	-2.56592700	1.97332500
H	-6.54433100	-3.16441100	0.39296700
H	-5.88233300	-4.28401200	1.59803200
C	-1.88729500	0.59332200	1.31833300
C	-0.79829700	1.27341000	-0.59027400
H	-2.60466900	0.10680400	0.66657100
H	-2.09510100	1.62833400	1.57006600
H	-1.48279600	0.77811600	-1.28930100
C	-0.86792200	2.78315200	-0.72009500
H	-0.31860400	3.26807300	0.09198900
H	-0.30659800	3.00091200	-1.64714300
C	-2.27004300	3.35337700	-0.84149400
C	-3.03297800	3.15733400	-2.00226900
C	-2.83860200	4.07529500	0.21648500
C	-4.33075700	3.66063000	-2.09983400
H	-2.60077000	2.61774000	-2.84301100
C	-4.13715000	4.58146400	0.12212800
H	-2.25356200	4.25038700	1.11681000
C	-4.88866200	4.37328700	-1.03541100
H	-4.90358400	3.50503000	-3.01062900
H	-4.55804900	5.14256100	0.95243000
H	-5.89774100	4.76927300	-1.11170900
N	1.58236800	1.51623600	2.72424500
O	2.10595200	2.07970000	3.66854100
H	-0.68351600	0.26911300	3.06621600

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B3LYP SCF energy: -1728.807177 a.u.
B3LYP enthalpy: -1728.088601 a.u.
B3LYP free energy: -1728.198783 a.u.
M06 SCF energy in solution: -1728.072774 a.u.
M06 enthalpy in solution: -1727.354198 a.u.
M06 free energy in solution: -1727.46438 a.u.

Cartesian coordinates

Ru	0.36599100	0.38314500	0.50590200
O	1.69291100	0.54241000	2.42834400
O	0.76825900	2.29298500	1.54685400
N	1.59244100	-1.91405500	-0.73562200
N	-0.44255500	-2.58228100	-0.26887700
C	0.40515000	-1.50144700	-0.22396300
C	1.66384300	-3.36024500	-0.95494300
C	2.75449800	-1.01613100	-0.71722500
C	3.66896700	-1.30374500	0.50115900
C	4.84171300	-0.30093100	0.52477000
C	5.65819000	-0.42334500	-0.77663700
C	4.74198100	-0.12031100	-1.97971600
C	3.59815100	-1.16045900	-2.00740700
C	4.17245900	1.31006700	-1.84042100
C	3.33519400	1.42167100	-0.53637600
C	2.16635700	0.41404800	-0.66745400
C	4.27947700	1.12833600	0.65052700
C	-1.86857800	-2.56910800	-0.12523500
C	-2.44782400	-3.11184200	1.03837700
C	-3.84205600	-3.09917700	1.16154600
C	-1.61160800	-3.75017300	2.12516300
C	-1.09814000	-0.10668800	2.35158800
C	0.17992100	-3.74715900	-0.93209800
C	-2.68074100	-2.11303900	-1.18604500
C	-4.66998300	-2.58884400	0.15859800
C	-4.06835600	-2.11542900	-1.01267000
C	-2.10346900	-1.70583800	-2.52467600
C	-6.17002300	-2.54221700	0.33314300
H	1.74668500	0.58544100	-1.66743700
H	-1.08271200	-1.18685000	2.41307600
H	2.15056600	-3.60159800	-1.90356500
H	2.22739300	-3.84704500	-0.14684900
H	3.08828000	-1.22365900	1.42598700
H	4.05939600	-2.33055400	0.43851300
H	5.48412800	-0.52303100	1.38702200
H	6.08451800	-1.43279500	-0.87012200
H	6.50198100	0.27975200	-0.75810900
H	5.31619300	-0.19945000	-2.91263000
H	2.95414600	-1.00626100	-2.88384800
H	4.03069800	-2.16914100	-2.09074200
H	3.55022200	1.55507400	-2.71239100
H	5.00023200	2.03362600	-1.82606000
H	2.93797800	2.44044300	-0.44673100
H	3.77058200	1.23810200	1.60868700
H	5.10662400	1.85239800	0.64301000
H	-4.29024300	-3.50130100	2.06793600
H	-1.54469000	-4.83641700	1.97346600
H	-0.59072400	-3.36146200	2.14231400
H	-2.06027900	-3.59295400	3.11145500
H	-0.01773200	-4.66545700	-0.37153200
H	-0.22857500	-3.86941400	-1.94440000
H	-4.69697300	-1.75003900	-1.82250400
H	-2.01140200	-2.57934600	-3.18498200
H	-2.76081200	-0.99221200	-3.03180300
H	-1.11278300	-1.25525000	-2.43775200
H	-6.49027700	-1.57309700	0.73797200
H	-6.68917200	-2.68191300	-0.62121400
H	-6.51754300	-3.31551900	1.02605100
C	-1.95466300	0.54304400	1.50781000
C	-0.77812100	1.09896300	-0.77207200
H	-2.62494400	-0.00430200	0.85437000
H	-2.13177900	1.60971700	1.60076100
H	-1.63539300	0.59495100	-1.23873300
C	-0.66674700	2.53696500	-1.23663600
H	0.15113400	3.04874200	-0.72183400
H	-0.39598700	2.48654300	-2.30626400
C	-1.96450400	3.31200100	-1.08080000
C	-2.97399100	3.24431300	-2.05061200
C	-2.18580700	4.08642500	0.06752300
C	-4.17790100	3.92987600	-1.87839600
H	-2.81083100	2.65968600	-2.95416100
C	-3.38857200	4.77421400	0.24077700
H	-1.40522200	4.15122400	0.82211600
C	-4.38937400	4.69645900	-0.73036800
H	-4.94692900	3.87214400	-2.64467600
H	-3.54129100	5.37488500	1.13375100
H	-5.32422900	5.23432900	-0.59697800
H	-0.60443000	0.42177500	3.15905100
N	1.52382800	1.81253500	2.47682800
O	2.03657200	2.51797600	3.32734900

TS50

B3LYP SCF energy: -1728.797833 a.u.
B3LYP enthalpy: -1728.080053 a.u.
B3LYP free energy: -1728.186182 a.u.
M06 SCF energy in solution: -1728.068906 a.u.
M06 enthalpy in solution: -1727.351126 a.u.
M06 free energy in solution: -1727.457255 a.u.

Cartesian coordinates

Ru	0.72734300	0.65721300	0.46605500
O	0.53705900	2.28957200	-1.25342300
O	1.08965200	2.80398700	0.78354400
N	2.02218300	-1.80602100	-0.30558400
N	-0.05652100	-2.41765600	0.00824900
C	0.78233600	-1.32777200	-0.02138000
C	2.11868200	-3.26568600	-0.28943600
C	3.18037800	-0.91090000	-0.23638000
C	3.88326000	-1.00471400	1.14197700
C	5.01571100	0.03764000	1.22082000
C	6.05043200	-0.25612200	0.11581200
C	5.36198200	-0.18077600	-1.26250300
C	4.22937100	-1.23282200	-1.32969100
C	4.78450900	1.23706100	-1.45652400
C	3.73320000	1.53356300	-0.35495600
C	2.60416300	0.49364400	-0.49751800
C	4.41632300	1.44545700	1.02409700
C	-1.48263900	-2.44289000	-0.14909900
C	-2.28217700	-2.87998200	0.92256400
C	-3.66478200	-2.99079800	0.72403100
C	-1.67926400	-3.25836500	2.25597900
C	0.82253500	0.18583600	2.27805800
C	0.64417600	-3.67080100	-0.35971700
C	-2.04930800	-2.17637100	-1.41385800
C	-4.26014000	-2.70916000	-0.50858300
C	-3.43164800	-2.31536500	-1.56593600

C	-1.20068900	-1.72411500	-2.58005200
C	-5.75636500	-2.80050500	-0.69535200
H	2.27135600	0.50629800	-1.54710300
H	0.67165300	-0.79032600	2.75748500
H	2.70365700	-3.64129500	-1.13358800
H	2.59653800	-3.61068900	0.63773400
H	3.14912700	-0.82918900	1.93579900
H	4.29252100	-2.01542500	1.28592600
H	5.49865300	-0.02880200	2.20516200
H	6.49463300	-1.25060800	0.26707900
H	6.87183900	0.47151400	0.16411900
H	6.09295400	-0.39632200	-2.05314700
H	3.74710000	-1.21634700	-2.31600700
H	4.65484400	-2.23772100	-1.18729200
H	4.32180600	1.32857100	-2.44826100
H	5.59783800	1.97538400	-1.41409500
H	3.34538400	2.54578900	-0.50247800
H	3.68963300	1.66452800	1.81558900
H	5.21042100	2.20152100	1.09684300
H	-4.28817100	-3.31723000	1.55384700
H	-1.16520100	-4.22735300	2.20248500
H	-0.93943800	-2.52670900	2.59392000
H	-2.45528600	-3.34492800	3.02258300
H	0.38342000	-4.47724300	0.33139400
H	0.34960300	-3.98240500	-1.37006900
H	-3.87456700	-2.10051900	-2.53615700
H	-0.41206100	-2.44653300	-2.82165500
H	-1.81584900	-1.59376500	-3.47513900
H	-0.70422700	-0.77069400	-2.36777400
H	-6.21508900	-1.80356300	-0.66183000
H	-6.01289300	-3.24113900	-1.66520600
H	-6.22333800	-3.40631300	0.08781000
C	-1.26551000	0.63490700	1.83462900
C	-1.39709900	1.42491500	0.67387300
H	-1.70627100	-0.35594700	1.85772100
H	-1.19454400	1.13851100	2.79533300
H	-1.24123400	2.49219300	0.81986200
C	-2.35366400	1.10859800	-0.46125200
H	-2.50375400	0.03239700	-0.53682700
H	-1.91567700	1.45916900	-1.40158700
C	-3.69354800	1.79900700	-0.24571200
C	-3.92159700	3.08896600	-0.74282600
C	-4.71832600	1.16872800	0.47441300
C	-5.14126900	3.73381000	-0.52672200
H	-3.13770400	3.59013600	-1.30679800
C	-5.93969400	1.80900400	0.69043000
H	-4.55643900	0.16549200	0.86330500
C	-6.15493200	3.09547700	0.19024100
H	-5.29957900	4.73408800	-0.92156800
H	-6.72419300	1.30331300	1.24830600
H	-7.10548700	3.59531600	0.35698700
H	1.07874800	0.96874400	3.00633400
N	0.88306400	3.20634500	-0.42886800
O	1.01312000	4.37460000	-0.74994500

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B3LYP SCF energy: -1728.811919 a.u.
B3LYP enthalpy: -1728.091618 a.u.
B3LYP free energy: -1728.198719 a.u.
M06 SCF energy in solution: -1728.091089 a.u.
M06 enthalpy in solution: -1727.370788 a.u.
M06 free energy in solution: -1727.477889 a.u.

Cartesian coordinates

Ru	0.72956400	0.54571700	0.47359200
O	1.23879500	3.28339000	-0.67207400
O	1.26243500	2.43422400	1.35931700
N	1.76207000	-1.87497600	-0.69690600
N	-0.30282900	-2.44354600	-0.25743400
C	0.57801500	-1.39325800	-0.22516100
C	1.78193700	-3.32750300	-0.89105800
C	2.98110300	-1.08001500	-0.52272100
C	3.66554100	-1.41823000	0.83062000
C	4.89673500	-0.51553200	1.04262000
C	5.89390100	-0.74163800	-0.11228800
C	5.21640200	-0.39871000	-1.45539400
C	3.99460700	-1.32121600	-1.66507300
C	4.75802100	1.07286300	-1.43231000
C	3.75078600	1.29947700	-0.27367600
C	2.53283400	0.39298600	-0.52358000
C	4.43783600	0.95554500	1.06309600
C	-1.72330700	-2.46291800	-0.05268000
C	-2.24329700	-2.83403800	1.20191100
C	-3.63438800	-2.91439400	1.35271300
C	-1.36415300	-3.20760900	2.37441000
C	-0.00485900	0.19704500	2.28361900
C	0.28937900	-3.66400100	-0.84870800
C	-2.58394600	-2.26340900	-1.15601000
C	-4.51165800	-2.67729600	0.29351100
C	-3.96289100	-2.36660800	-0.95670700
C	-2.05544800	-1.97284100	-2.54369500
C	-6.00875100	-2.74781300	0.48558700
H	2.09199400	0.63516500	-1.51115400
H	-0.15463900	-0.81992200	2.64170000
H	2.25114700	-3.59973900	-1.84031500
H	2.33823700	-3.81957000	-0.08169500
H	2.94228100	-1.27300900	1.64445300
H	3.96841200	-2.47496100	0.84346400
H	5.37218300	-0.77451200	1.99790800
H	6.24085100	-1.78502000	-0.11681000
H	6.78152800	-0.11096000	0.02943600
H	5.92589300	-0.55637200	-2.27831100
H	3.51409800	-1.11365100	-2.63050600
H	4.32219000	-2.37134800	-1.67895300
H	4.29496600	1.34462200	-2.39046000
H	5.62722200	1.73191300	-1.30001800
H	3.44268600	2.34488900	-0.28392500
H	3.74631500	1.13336300	1.89547200
H	5.30187500	1.61605600	1.21706600
H	-4.03774900	-3.18932200	2.32545700
H	-1.51647000	-4.26040500	2.64453100
H	-0.30462600	-3.06413900	2.15651600
H	-1.61196400	-2.61359500	3.26153500
H	0.05822700	-4.53740300	-0.23178100
H	-0.12189300	-3.83661100	-1.85080600
H	-4.62688500	-2.19966600	-1.80250200
H	-1.88761400	-2.90224800	-3.10469000
H	-2.77644000	-1.38060700	-3.11540900
H	-1.11056700	-1.42430300	-2.51964500
H	-6.44092100	-1.74474200	0.59748900
H	-6.50112300	-3.21620900	-0.37377000
H	-6.27143900	-3.31924400	1.38150300
C	-1.30222500	0.80449000	1.59208900
C	-1.04349300	1.45114600	0.18127700
H	-2.06752700	0.03253900	1.50646400
H	-1.63301100	1.61981500	2.24208000
H	-0.87098300	2.52312300	0.27120600
C	-2.04521700	1.18721500	-0.93341900
H	-2.34266100	0.13906700	-0.94318800
H	-1.55191500	1.40734600	-1.88899100
C	-3.27684600	2.07130200	-0.79841600
C	-3.22472400	3.42308300	-1.16984000
C	-4.47471700	1.56752100	-0.27461000
C	-4.33978700	4.24826000	-1.02182800
H	-2.30111000	3.82957300	-1.57687900
C	-5.59341700	2.39089700	-0.12648800
H	-4.53152400	0.52003100	0.01328800
C	-5.52936300	3.73433200	-0.49935800
H	-4.28016000	5.29277800	-1.31645800
H	-6.51578400	1.98161500	0.27866100
H	-6.39901400	4.37610900	-0.38542600
H	0.40633900	0.85881500	3.04959900
N	1.41654300	3.46198900	0.55291900
O	1.73259800	4.53865400	1.04840500

TS51

B3LYP SCF energy: -1728.804798 a.u.
B3LYP enthalpy: -1728.086194 a.u.
B3LYP free energy: -1728.193219 a.u.
M06 SCF energy in solution: -1728.084576 a.u.
M06 enthalpy in solution: -1727.365972 a.u.
M06 free energy in solution: -1727.472997 a.u.

Cartesian coordinates

Ru	0.67073400	0.51076700	0.52193400
O	0.04352200	3.85097000	1.63273900
O	1.45146200	2.15428500	1.71909000
N	1.60599800	-1.58909200	-1.22486300
N	-0.44252000	-2.22112600	-0.76937000
C	0.48196500	-1.23730100	-0.53250600
C	1.54042600	-2.91643800	-1.84230200
C	2.87454600	-0.93561000	-0.88813800

C	3.59487000	-1.71072700	0.25028000
C	4.86577900	-0.95652200	0.68585100
C	5.81120300	-0.82520800	-0.52628800
C	5.09975600	-0.04988700	-1.65470100
C	3.83345500	-0.82175600	-2.09568600
C	4.70799600	1.35041200	-1.13780300
C	3.75317700	1.22206300	0.07842400
C	2.50307500	0.46361600	-0.38688500
C	4.46844000	0.44155800	1.19901000
C	-1.68968900	-2.45046000	-0.09961100
C	-1.67292500	-2.99381300	1.20492800
C	-2.89124400	-3.21656900	1.85075000
C	-0.38319900	-3.42636300	1.86874500
C	0.05340600	-3.26631800	-1.69185200
C	-2.90664100	-2.27886700	-0.78663800
C	-4.11966700	-2.96605000	1.22665500
C	-4.10260800	-2.52538000	-0.09772700
C	-2.97192500	-1.91795600	-2.25500400
C	-5.42035600	-3.17760500	1.96503900
H	2.02231600	1.02614000	-1.22567100
H	1.86032800	-2.88430200	-2.88791400
H	2.18779700	-3.62635500	-1.31124400
H	2.90500800	-1.81741700	1.09818400
H	3.85794700	-2.72211700	-0.09047300
H	5.36379100	-1.52327000	1.48378800
H	6.11530300	-1.82049000	-0.88120500
H	6.72811900	-0.29725900	-0.23260700
H	5.77238900	0.04619200	-2.51701700
H	3.32865900	-0.29784100	-2.91846000
H	4.11501200	-1.81901100	-2.46524800
H	4.22618000	1.93014400	-1.93739100
H	5.60989700	1.90455500	-0.84365900
H	3.80883100	0.36013800	2.07188100
H	5.36204300	0.99193500	1.52222600
H	-2.88144000	-3.61718100	2.86231700
H	0.01456300	-4.32990100	1.38617500
H	0.39798400	-2.66433300	1.82011300
H	-0.55491900	-3.67075000	2.92136800
H	-0.11308700	-4.26024900	-1.26521200
H	-0.48154500	-3.21545600	-2.64740100
H	-5.04503600	-2.37723300	-0.62143100
H	-3.16541800	-2.81561900	-2.85785000
H	-3.78731200	-1.21505500	-2.45477700
H	-2.04469900	-1.46929000	-2.61627400
H	-5.66348500	-2.30908900	2.59120700
H	-6.25554600	-3.32627000	1.27305500
H	-5.36806400	-4.04829900	2.62790900
C	-0.37829200	0.10737400	2.17251700
C	-1.45492300	0.93172500	1.36052400
C	-0.95391800	1.53147400	-0.01968500
H	-1.71849200	1.79754500	1.97119000
H	-2.31145700	0.28492600	1.16586000
H	-0.71252800	-0.90042100	2.40339200
H	3.47271600	2.21130900	0.44414200
H	-0.72822000	2.59426800	0.10234400
C	-1.82167900	1.27102500	-1.24302100
H	-1.22689600	1.49315600	-2.13946100
H	-2.09230800	0.21713100	-1.28405800
C	-3.07710300	2.13022600	-1.25242200
C	-4.30633800	1.61955300	-0.81309800
C	-3.02305900	3.46632400	-1.67438400
C	-5.45071600	2.42015400	-0.79682200
H	-4.36850000	0.58563900	-0.48033800
C	-4.16329800	4.26972000	-1.65814200
H	-2.07732000	3.88073600	-2.01717600
C	-5.38276200	3.74853700	-1.21922200
H	-6.39534500	2.00470800	-0.45449600
H	-4.09939800	5.30314300	-1.98854500
H	-6.27192000	4.37321300	-1.20684000
H	-0.00221500	0.64579700	3.04335800
N	1.21904700	3.44813800	1.68362500
O	2.19498800	4.19871800	1.72575600

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B3LYP SCF energy: -1728.807616 a.u.
B3LYP enthalpy: -1728.087761 a.u.
B3LYP free energy: -1728.195828 a.u.
M06 SCF energy in solution: -1728.08708 a.u.
M06 enthalpy in solution: -1727.367225 a.u.
M06 free energy in solution: -1727.475292 a.u.

Cartesian coordinates

Ru	0.70111000	0.57057400	0.41930000
O	-0.24160900	3.31261200	2.26248300
O	1.47123900	2.43906200	1.16393100
N	1.73383900	-1.73777800	-0.97925400
N	-0.29872300	-2.37496300	-0.48313400
C	0.57495700	-1.32319600	-0.38829500
C	1.74591300	-3.15586600	-1.34853300
C	2.96188000	-0.96465700	-0.77951900
C	3.73582700	-1.47506900	0.46851800
C	4.97253900	-0.59110400	0.72293400
C	5.89363900	-0.64345100	-0.51335200
C	5.12822400	-0.12983900	-1.75103000
C	3.89981100	-1.03266600	-2.00688300
C	4.66700000	1.32021300	-1.49767500
C	3.73717900	1.37371000	-0.25763200
C	2.51822000	0.48439100	-0.54197700
C	4.50964500	0.85712700	0.97284700
C	-1.62836100	-2.50194400	0.03694400
C	-1.80845800	-2.90715300	1.37709900
C	-3.11208900	-3.03260400	1.86659000
C	-0.64586700	-3.30516800	2.26041800
C	0.26561700	-3.53025200	-1.21263000
C	-2.73555100	-2.36704800	-0.82476400
C	-4.23339100	-2.82204400	1.05703500
C	-4.02113500	-2.51614400	-0.29000300
C	-2.58098800	-2.14122300	-2.31336700
C	-5.63006100	-2.92742800	1.62295000
H	2.00356400	0.85333700	-1.46147500
H	2.12545200	-3.30129600	-2.36388700
H	2.38163200	-3.73123900	-0.66238900
H	3.06553600	-1.45243400	1.33833900
H	4.04585600	-2.51878700	0.31776800
H	5.51064400	-0.97160000	1.60122400
H	6.24469400	-1.67152600	-0.68311500
H	6.78524800	-0.02573400	-0.34281100
H	5.78365900	-0.16479700	-2.63117200
H	3.35616700	-0.70161400	-2.90204700
H	4.23124400	-2.06589400	-2.18759100
H	4.14337600	1.71170000	-2.38106100
H	5.54099400	1.96596400	-1.33426100
H	3.86856900	0.91121000	1.86083700
H	5.37808600	1.50172700	1.16412400
H	-3.25478500	-3.32275000	2.90558600
H	-0.42737400	-4.37547100	2.13808400
H	0.26960200	-2.75786200	2.02958900
H	-0.88345700	-3.14722500	3.31714500
H	0.10513800	-4.45359200	-0.64775100
H	-0.22383700	-3.64021100	-2.18797800
H	-4.87749500	-2.39777200	-0.95108400
H	-2.64326200	-3.09615900	-2.85302300
H	-3.38175100	-1.50280000	-2.70014600
H	-1.62507200	-1.67845100	-2.56853100
H	-5.94859700	-1.97464000	2.06595300
H	-6.35877100	-3.18684000	0.84800800
H	-5.68669500	-3.68539000	2.41160700
C	-0.26526700	0.25420700	2.13563100
C	-1.44512600	0.84148100	1.26108600
C	-0.99516000	1.48430300	-0.10996600
H	-1.84842300	1.67072400	1.84445200
H	-2.18390400	0.06298100	1.07216900
H	-0.46456700	-0.75774300	2.47868400
H	3.40691500	2.39770500	-0.07721800
H	-0.83419500	2.55866800	0.00813400
C	-1.84822500	1.18534200	-1.33580500
H	-1.25018700	1.39558200	-2.23268900
H	-2.10732300	0.12758400	-1.35631600
C	-3.11201700	2.03143500	-1.37434300
C	-4.33345800	1.53044000	-0.90403700
C	-3.07228600	3.34764000	-1.85609200
C	-5.48394400	2.32205900	-0.91485700
H	-4.38412100	0.51093900	-0.52809300
C	-4.21884000	4.14233500	-1.86691900
H	-2.13297400	3.75257100	-2.22738000
C	-5.43035100	3.63125000	-1.39580700
H	-6.42284400	1.91467400	-0.54798800
H	-4.16638900	5.16018700	-2.24448300
H	-6.32467800	4.24855600	-1.40423700
H	0.02870200	0.92592200	2.94240200
N	0.95610900	3.37921400	1.93144600
O	1.70898700	4.28667600	2.27466100

TS52

B3LYP SCF energy: -1728.805034 a.u.
B3LYP enthalpy: -1728.085981 a.u.
B3LYP free energy: -1728.192295 a.u.
M06 SCF energy in solution: -1728.085616 a.u.
M06 enthalpy in solution: -1727.366563 a.u.
M06 free energy in solution: -1727.472877 a.u.

Cartesian coordinates

Ru	0.67146000	0.58033900	0.32483600
O	0.76040400	2.98681700	2.94038900
O	1.29515500	2.60824200	0.83204000
N	1.65499800	-1.79138000	-0.99495300
N	-0.38074800	-2.37375200	-0.44358200
C	0.51138900	-1.33570600	-0.40435700
C	1.63811500	-3.22384400	-1.30406000
C	2.89728600	-1.03338000	-0.81955500
C	3.65010100	-1.50827600	0.45521700
C	4.89763300	-0.63501700	0.69196000
C	5.82944800	-0.74631400	-0.53246900
C	5.08369500	-0.26666400	-1.79547000
C	3.84490500	-1.16197400	-2.03307600
C	4.64263700	1.19884000	-1.59724200
C	3.70187700	1.31217000	-0.36894400
C	2.47396000	0.42942200	-0.64000100
C	4.45548400	0.82797500	0.88590600
C	-1.71852400	-2.44737200	0.06774200
C	-1.92502500	-2.81879300	1.41323600
C	-3.23815300	-2.89892500	1.88872300
C	-0.78774100	-3.23159600	2.32249600
C	0.15170500	-3.56247500	-1.14345700
C	-2.81202100	-2.29884000	-0.81013700
C	-4.34332700	-2.67611100	1.06146100
C	-4.10705700	-2.40218800	-0.28896500
C	-2.62932600	-2.10386100	-2.29993100
C	-5.74917400	-2.73498700	1.61150200
H	1.97485500	0.77506900	-1.57665100
H	2.00850700	-3.41947200	-2.31428600
H	2.26663500	-3.78140600	-0.59689600
H	2.97026700	-1.44299200	1.31553700
H	3.94487900	-2.56162800	0.34664400
H	5.42086500	-0.99300800	1.58844000
H	6.16642300	-1.78504300	-0.66091200
H	6.72857500	-0.13596300	-0.37586700
H	5.74725400	-0.34194300	-2.66692300
H	3.31634500	-0.85700300	-2.94628000
H	4.16338600	-2.20598400	-2.17076200
H	4.13360300	1.56736500	-2.49884200
H	5.52541700	1.83583700	-1.44809100
H	3.81224100	0.92409300	1.76939800
H	5.33040600	1.46719600	1.06234000
H	-3.40049800	-3.16389200	2.93160900
H	-0.65380600	-4.32189500	2.28616900
H	0.16366100	-2.77528500	2.04465900
H	-1.00162600	-2.97166800	3.36415100
H	-0.02368800	-4.46497000	-0.55027200
H	-0.34899800	-3.68914500	-2.11098600
H	-4.95198500	-2.27320700	-0.96250100
H	-2.64995800	-3.07190400	-2.81914100
H	-3.43944700	-1.49901600	-2.71924700
H	-1.68190300	-1.61745200	-2.54323900
H	-6.04752300	-1.76732400	2.03596300
H	-6.47515900	-2.98707200	0.83161500
H	-5.83572300	-3.47861700	2.41100800
C	-0.22118400	0.28976600	2.07595100
C	-1.39027200	1.02742600	1.29394800
C	-1.02605500	1.52268100	-0.16121200
H	-1.61149000	1.92218000	1.87949100
H	-2.24608400	0.35377400	1.22968800
H	-0.49410500	-0.71563600	2.38441000
H	3.38456700	2.34621200	-0.22566800
H	-0.78784200	2.58952600	-0.15607700
C	-1.99316700	1.17677100	-1.28527200
H	-1.46318700	1.27747100	-2.24194900
H	-2.31226200	0.13936700	-1.19279500
C	-3.21021200	2.08985000	-1.29364800
C	-4.43447800	1.66657500	-0.75927500
C	-3.12376900	3.38819800	-1.81694500
C	-5.54284900	2.51646800	-0.74672600
H	-4.52112200	0.66037800	-0.35501200
C	-4.22791600	4.24062300	-1.80486000
H	-2.18228500	3.73245600	-2.24036000
C	-5.44292900	3.80687500	-1.26888400
H	-6.48509900	2.16875400	-0.33044600
H	-4.14050400	5.24285000	-2.21631200
H	-6.30434500	4.46932300	-1.26022700
H	0.17646600	0.90898900	2.87970200
N	1.56531100	3.14115000	2.00632200
O	2.60354000	3.79616000	2.10128500

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B3LYP SCF energy: -1728.813271 a.u.
B3LYP enthalpy: -1728.09331 a.u.
B3LYP free energy: -1728.200153 a.u.
M06 SCF energy in solution: -1728.087856 a.u.
M06 enthalpy in solution: -1727.367895 a.u.
M06 free energy in solution: -1727.474738 a.u.

Cartesian coordinates

Ru	0.57142900	0.49563100	0.67505800
O	2.14207800	0.21856500	2.80437800
O	1.11727200	2.02123700	2.11087800
N	1.39732900	-1.18077200	-1.53235100
N	-0.62474300	-1.90172500	-1.10766400
C	0.32795600	-0.99358500	-0.71382200
C	1.22203800	-2.21911500	-2.54931800
C	2.68735900	-0.57156600	-1.21386900
C	3.60035700	-1.59608600	-0.48613100
C	4.93148900	-0.93067100	-0.08517000
C	5.64213200	-0.39590400	-1.34440800
C	4.73501200	0.63663000	-2.04476600
C	3.42130700	-0.05308600	-2.47539100
C	4.42825200	1.79473000	-1.07165200
C	3.70165000	1.25017700	0.19115300
C	2.38946500	0.61035100	-0.28568000
C	4.62902900	0.22781800	0.88262800
C	-1.80021300	-2.31544700	-0.39526200
C	-1.65987300	-3.11128000	0.76522400
C	-2.81460900	-3.52716100	1.43146600
C	-0.30202400	-3.55330800	1.26579500
C	-0.14960700	-2.80431700	-2.18050200
C	-3.07397900	-2.06010300	-0.93662600
C	-4.09738800	-3.21170700	0.96545500
C	-4.20238300	-2.49953400	-0.22975000
C	-3.26965800	-1.40479200	-2.28630700
C	-5.32605200	-3.63848400	1.73381700
H	1.82687700	1.38002600	-0.87384100
H	1.23084300	-1.78221800	-3.55504100
H	2.02323000	-2.96416800	-2.50001200
H	3.07904500	-1.96701900	0.40476100
H	3.79026000	-2.45630800	-1.14392300
H	5.56799000	-1.67442300	0.41175400
H	5.87823400	-1.22029800	-2.03271000
H	6.59647000	0.07102100	-1.06681300
H	5.23958700	1.02840900	-2.93771500
H	2.77180400	0.65058600	-3.01350400
H	3.64666700	-0.88222200	-3.16236100
H	3.80959300	2.55483300	-1.56865300
H	5.36334500	2.28901300	-0.77448200
H	4.15792100	-0.14612700	1.79486900
H	5.56343800	0.72590800	1.17554500
H	-2.70992700	-4.12566100	2.33397200
H	0.22549700	-4.15073100	0.51126300
H	0.34561000	-2.70844400	1.51825200
H	-0.40842800	-4.17499800	2.15961900
H	-0.08334200	-3.83224100	-1.80348700
H	-0.84890400	-2.80286700	-3.02232600
H	-5.18865300	-2.28825200	-0.63888200
H	-3.59528000	-2.14923800	-3.02519600
H	-4.04556600	-0.63262600	-2.25025500
H	-2.35305700	-0.94472000	-2.65945000
H	-5.55496100	-2.92662000	2.53787100
H	-6.20661600	-3.69365600	1.08551900
H	-5.18567900	-4.61901400	2.20179300
C	-0.70052200	-0.13875900	2.11057200
C	-1.62969400	0.89385900	1.39378800
C	-0.94521500	1.68543400	0.18609500
H	-1.93350000	1.64569200	2.12699100
H	-2.49520200	0.36312600	0.99326300
H	-1.09496800	-1.14909500	2.09040700
H	3.48499400	2.08243400	0.86765800

H	-0.67207900	2.69750800	0.50957600
C	-1.73672900	1.73518700	-1.11765300
H	-1.06322500	2.08760600	-1.91094900
H	-2.05339300	0.72793200	-1.39267100
C	-2.93728800	2.66452100	-1.04239600
C	-4.20977000	2.18736600	-0.69628700
C	-2.78788000	4.03814800	-1.28298000
C	-5.29900800	3.05500400	-0.59168100
H	-4.35042000	1.12584400	-0.50492000
C	-3.87264500	4.90946700	-1.17855300
H	-1.80969700	4.42721300	-1.55877600
C	-5.13395600	4.42016000	-0.83177200
H	-6.27718800	2.66322900	-0.32411100
H	-3.73351200	5.97014700	-1.37129100
H	-5.98068400	5.09660600	-0.75189100
H	-0.40399300	0.16501700	3.11419900
N	1.90201000	1.44397800	2.98306100
O	2.36271500	2.09731900	3.90799500

TS53

B3LYP SCF energy: -1728.800772 a.u.
B3LYP enthalpy: -1728.083199 a.u.
B3LYP free energy: -1728.189631 a.u.
M06 SCF energy in solution: -1728.070328 a.u.
M06 enthalpy in solution: -1727.352755 a.u.
M06 free energy in solution: -1727.459187 a.u.

Cartesian coordinates

Ru	0.42513400	0.34865900	0.80775800
O	1.74243800	-0.74966800	2.36880500
O	1.11059500	1.30507400	2.67395600
N	1.22771000	-0.71925200	-1.76666600
N	-0.77520300	-1.55961900	-1.41488400
C	0.19699300	-0.74399600	-0.87499800
C	1.06666000	-1.65008800	-2.88652500
C	2.54523300	-0.24973200	-1.30975400
C	3.36627000	-1.43455200	-0.73374300
C	4.71577200	-0.92757900	-0.18672900
C	5.50767500	-0.24388400	-1.31753300
C	4.68928800	0.94341300	-1.86596300
C	3.35844800	0.40950400	-2.44760100
C	4.41461700	1.94357000	-0.71923100
C	3.59801300	1.25001400	0.40624300
C	2.25922700	0.79758600	-0.22109700
C	4.44519100	0.07759900	0.94843200
C	-1.83273000	-2.24068900	-0.72578400
C	-1.50841800	-3.27438400	0.18395300
C	-2.54953200	-3.96596600	0.80861600
C	-0.07513400	-3.65569400	0.47525800
C	-0.41174700	-2.04324800	-2.76571800
C	-3.17517100	-1.98511000	-1.06224800
C	-3.89520000	-3.68642000	0.54237900
C	-4.18301700	-2.70522700	-0.40722500
C	-3.55968700	-1.01089200	-2.15133600
C	-4.99750600	-4.42569600	1.26384200
H	1.87482400	1.67952200	-0.75457800
H	1.29362900	-1.16612300	-3.84068400
H	1.73566300	-2.51417400	-2.77683000
H	2.79461300	-1.91429200	0.06874500
H	3.54512700	-2.18820100	-1.51432900
H	5.28787000	-1.78094500	0.20122100
H	5.72303900	-0.96070000	-2.12342300
H	6.47551700	0.10994600	-0.93737300
H	5.25173300	1.44359000	-2.66576900
H	2.77252800	1.22723100	-2.88895400
H	3.57464300	-0.30968400	-3.25244600
H	3.86725600	2.81612300	-1.10201100
H	5.36986900	2.31523900	-0.32150800
H	3.93795700	-0.42560900	1.77408600
H	5.39788200	0.46458500	1.33697800
H	-2.30074400	-4.75381000	1.51654000
H	0.48997000	-3.83341300	-0.44760200
H	0.45606000	-2.87343000	1.02856200
H	-0.03741600	-4.57239300	1.07125200
H	-0.57636600	-3.12204700	-2.84235400
H	-1.03074000	-1.54998100	-3.52558900
H	-5.22099700	-2.49525200	-0.65813600
H	-3.67447100	-1.52726900	-3.11429600
H	-4.52016200	-0.53241300	-1.93243700
H	-2.80853300	-0.23106600	-2.29131100
H	-5.19624700	-3.97741200	2.24627800
H	-5.93451300	-4.40175500	0.69796800
H	-4.73059300	-5.47419500	1.43606500
C	-1.11234800	-0.51601000	2.14496700
C	-1.84294400	0.52438700	1.52905400
C	-0.63159900	1.81624900	0.27273800
H	-2.07594300	1.41220000	2.11146000
H	-2.55389400	0.27689600	0.74786200
H	-1.31752400	-1.53849200	1.85736400
H	3.40475300	1.97108800	1.20950800
H	-0.52028000	2.66312000	0.97039600
C	-1.41848800	2.21834800	-0.95152900
H	-0.66020600	2.66956100	-1.61636700
H	-1.79068900	1.33647500	-1.47803400
C	-2.52808700	3.22549400	-0.70789700
C	-3.87222800	2.83129400	-0.68838400
C	-2.22528000	4.57368100	-0.46637100
C	-4.88724600	3.75518900	-0.43028000
H	-4.12825400	1.79235500	-0.88239300
C	-3.23581000	5.49969100	-0.20637800
H	-1.18793400	4.90197700	-0.48824200
C	-4.57198400	5.09275500	-0.18684800
H	-5.92418500	3.42916000	-0.42212000
H	-2.98007400	6.54016200	-0.02416600
H	-5.36039800	5.81331500	0.01282700
H	-0.76930700	-0.37352300	3.16605400
N	1.77229900	0.29065000	3.12212100
O	2.38091900	0.32366400	4.17581100

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B3LYP SCF energy: -1728.803459 a.u.
B3LYP enthalpy: -1728.085041 a.u.
B3LYP free energy: -1728.19499 a.u.
M06 SCF energy in solution: -1728.071437 a.u.
M06 enthalpy in solution: -1727.353019 a.u.
M06 free energy in solution: -1727.462968 a.u.

Cartesian coordinates

Ru	-0.02936100	-0.14024600	0.96729200
O	0.03833600	-2.15665800	2.05351400
O	0.85350400	-0.37703700	2.98685400
N	0.18042600	-0.88171800	-1.83684400
N	-1.89947600	-0.24118700	-1.56738500
C	-0.70220500	-0.39658700	-0.91676800
C	-0.45015600	-1.26658600	-3.10239000
C	1.43323200	-1.47376800	-1.34761800
C	1.24598200	-2.98062600	-1.03126700
C	2.55139700	-3.56317500	-0.45103800
C	3.69887200	-3.37649300	-1.46252000
C	3.88478600	-1.87237600	-1.74875500
C	2.58087300	-1.32308900	-2.37325400
C	4.20673600	-1.13644500	-0.42708800
C	3.03443200	-1.31267000	0.57836700
C	1.78744000	-0.67098700	-0.08066700
C	2.88736900	-2.82486100	0.85897200
C	-3.18271700	0.08389600	-1.02183800
C	-3.96799600	-0.95548000	-0.47732900
C	-5.24502900	-0.64825400	-0.00133100
C	-3.45988900	-2.37912100	-0.42959400
C	-1.80172700	-0.54806300	-3.00905900
C	-3.69920800	1.38661000	-1.14332300
C	-5.76898800	0.64875900	-0.06663100
C	-4.98467100	1.64597100	-0.64983900
C	-2.92105100	2.48949700	-1.82163500
C	-7.13930200	0.95739200	0.48964000
H	2.13679700	0.29935700	-0.44852100
H	0.14216100	-0.93970500	-3.96148700
H	-0.56912600	-2.35719400	-3.16389600
H	0.42909600	-3.10079900	-0.31118400
H	0.97137000	-3.52750800	-1.94528200
H	2.40753100	-4.63271100	-0.24800200
H	3.48031800	-3.91538100	-2.39608700
H	4.62781800	-3.80112300	-1.05850100
H	4.70874200	-1.73009000	-2.46111600
H	2.69414700	-0.26396500	-2.64197600
H	2.36137000	-1.87327100	-3.30122300
H	4.38350000	-0.06948300	-0.61884600
H	5.13587600	-1.54192800	-0.00134200
H	3.27248900	-0.78378500	1.50897900
H	2.11183900	-3.02448300	1.59930100
H	3.83143900	-3.21039700	1.26961200
H	-5.85016300	-1.44486800	0.42658600

H	-2.53002600	-2.46967300	0.14217900
H	-4.20317300	-3.03852100	0.02840900
H	-3.25118300	-2.76405000	-1.43583100
H	-2.64395200	-1.16708800	-3.33180700
H	-1.81623000	0.38044900	-3.59559600
H	-5.38161300	2.65602900	-0.73115900
H	-3.14607900	2.52719800	-2.89637300
H	-3.18372000	3.46821700	-1.40658600
H	-1.84372400	2.34698900	-1.71747700
H	-7.10464300	1.07725100	1.58047200
H	-7.54302300	1.88481000	0.07078900
H	-7.84947300	0.15069200	0.27650800
C	0.40956400	1.65436400	0.75820400
C	-1.99894100	1.10918500	2.11491000
C	-2.10309800	-0.21590700	2.38650900
H	-2.53182200	1.56514400	1.28925300
H	-2.74168300	-0.86234000	1.79770700
H	-1.71023300	-0.62532300	3.31008600
H	-1.49302000	1.77768600	2.80545800
H	0.62966800	2.15679600	1.71828500
C	0.66816800	2.59168200	-0.39741000
H	0.67637300	2.04595400	-1.34632900
H	-0.19520200	3.27822000	-0.43388000
C	1.93860400	3.41314600	-0.23919600
C	2.00917100	4.45363700	0.69858100
C	3.07246400	3.13474500	-1.01325100
C	3.18209200	5.19051800	0.86324100
H	1.13567500	4.69334200	1.30188400
C	4.24771900	3.87219200	-0.85342200
H	3.03360500	2.33544100	-1.74937600
C	4.30730400	4.90088000	0.08764800
H	3.21608200	5.99398600	1.59441800
H	5.11603500	3.64105100	-1.46497900
H	5.22133000	5.47457400	0.21465700
N	0.61935900	-1.63995000	3.08118100
O	0.92405800	-2.29463000	4.06059100

TSB1

B3LYP SCF energy: -2152.997185 a.u.
B3LYP enthalpy: -2152.097851 a.u.
B3LYP free energy: -2152.227182 a.u.
M06 SCF energy in solution: -2152.089218 a.u.
M06 enthalpy in solution: -2151.189884 a.u.
M06 free energy in solution: -2151.319215 a.u.

Cartesian coordinates

Ru	0.20415300	0.43677600	-0.19447600
O	0.53822100	-3.23604700	2.32384000
O	-0.67292600	2.30965300	-1.32679900
O	-1.40045000	1.86882800	0.67696200
N	-0.59041100	-1.26370100	-2.45721100
N	-2.48949800	-0.41463500	-1.77936000
C	-1.15646000	-0.44666300	-1.55950400
C	-1.54983800	-1.86122700	-3.39717500
C	0.84609600	-1.56223300	-2.42927500
C	1.07150700	-2.93960700	-1.75420400
C	2.57602700	-3.26864500	-1.71036300
C	3.15054700	-3.28573500	-3.14086500
C	2.93719300	-1.90443400	-3.79206700
C	1.42240400	-1.61487600	-3.86593100
C	3.64350600	-0.82429600	-2.94564800
C	3.03553700	-0.79705900	-1.51706200
C	1.53267400	-0.41356900	-1.64210000
C	3.28679300	-2.18270300	-0.88271300
C	-3.52139200	0.26300200	-1.04258700
C	-3.99593100	-0.29855600	0.15526400
C	-5.05390600	0.33907500	0.81062200
C	-3.38984000	-1.55285500	0.73724000
C	0.78036600	-0.70572200	1.27977200
C	-0.02700300	-0.94549900	2.50969800
C	-0.72763800	0.07277100	3.17601000
C	1.07864200	-5.44118500	1.66915400
C	-2.89589000	-1.35575300	-2.84836000
C	0.68450000	-4.56590400	2.85403000
C	-0.12304300	-2.26331500	3.03044300
C	-4.11076900	1.41556000	-1.59739100
C	-5.64689600	1.49820100	0.30408600
C	-1.48492100	-0.17830800	4.31909400
C	1.72544300	-4.59263900	3.97431700
C	-0.88718600	-2.51805200	4.17610300
C	-1.56219900	-1.47733400	4.81734200
C	-5.16644100	2.01298600	-0.90366800
C	-3.62473500	2.01290700	-2.89806500
C	-6.76600000	2.19111300	1.04611600
H	1.51346800	0.45517800	-2.32414400
H	1.48740300	-1.51455000	1.12432400
H	-1.35487300	-1.50791900	-4.41557200
H	-1.47588700	-2.95354400	-3.39622700
H	0.65758000	-2.91594900	-0.74007800
H	0.53448000	-3.71973100	-2.31387200
H	2.71974200	-4.25174100	-1.24178000
H	2.66096500	-4.06725900	-3.73949200
H	4.22154000	-3.52861600	-3.11314600
H	3.35070400	-1.90759400	-4.80927400
H	1.23568000	-0.65748800	-4.37025100
H	0.93329800	-2.40078300	-4.46108200
H	3.53581200	0.15974000	-3.42101900
H	4.72087100	-1.04068400	-2.89782500
H	3.57436400	-0.04354600	-0.93142900
H	2.94037900	-2.21749100	0.15501600
H	4.36831300	-2.38062800	-0.85840300
H	-5.42189300	-0.08522900	1.74234700
H	-3.99137900	-1.91667400	1.57563100
H	-3.32225400	-2.36051300	-0.00244300
H	-2.37747100	-1.36864000	1.11051700
H	-0.69177000	1.08025300	2.77469600
H	2.03088200	-5.10469600	1.24469300
H	1.19010400	-6.48340300	1.98727800
H	0.31606100	-5.39484900	0.88559300
H	-3.50683600	-2.15831000	-2.41783300
H	-3.49633800	-0.84372100	-3.60481300
H	-0.28788000	-4.90744600	3.23297900
H	-2.00955800	0.63533200	4.81121300
H	1.45268000	-3.92071600	4.79330200
H	1.82245300	-5.60576300	4.38090100
H	2.70166000	-4.28111900	3.58623200
H	-0.95993000	-3.52097300	4.57968000
H	-2.14685000	-1.69263200	5.70791700
H	-5.61673400	2.91318600	-1.31610200
H	-3.83543600	1.35842000	-3.75481100
H	-4.12310500	2.96760400	-3.08848100
H	-2.54627700	2.19364600	-2.87346500
H	-6.40348000	3.10161000	1.54110900
H	-7.57277200	2.49237800	0.36735400
H	-7.19610700	1.54476100	1.81855800
C	1.79349800	0.72948600	1.35203600
C	1.43677600	1.92413600	0.50194200
H	1.64932000	0.96627600	2.40564000
H	2.78891500	0.34594500	1.13887500
H	0.83579000	2.66024200	1.04181800
C	2.47517700	2.61146200	-0.37518600
H	3.11053000	1.87835600	-0.87567800
H	1.92792200	3.15658100	-1.15418000
C	3.33710200	3.58250300	0.41646400
C	2.85151700	4.85290600	0.75931700
C	4.62231400	3.22286800	0.84337300
C	3.62705400	5.73652600	1.51081800
H	1.85970100	5.15307800	0.42728200
C	5.40285000	4.10484000	1.59365700
H	5.02020100	2.24551100	0.57721600
C	4.90636900	5.36494700	1.93146400
H	3.23408800	6.71816800	1.76299400
H	6.39981500	3.80835500	1.91002400
H	5.51250200	6.05404100	2.51360700
N	-1.40572100	2.66436000	-0.32813500
O	-2.05941400	3.69612600	-0.34433700

TSB2

B3LYP SCF energy: -2152.998433 a.u.
B3LYP enthalpy: -2152.099781 a.u.
B3LYP free energy: -2152.228733 a.u.
M06 SCF energy in solution: -2152.090402 a.u.
M06 enthalpy in solution: -2151.19175 a.u.
M06 free energy in solution: -2151.320702 a.u.

Cartesian coordinates

Ru	-0.04435000	0.17888300	-0.13588200
O	0.50466800	-1.96604000	0.43241300
O	-1.09293600	-0.96806900	1.51438900
N	-0.40533300	-0.82042400	-2.88410200
N	-2.17045100	-1.54415300	-1.80956600
C	-1.02571100	-0.83219200	-1.69165600

C	-1.03222800	-1.72159600	-3.86085000
H	-1.12301500	-1.24809400	-4.84169100
H	-0.43865600	-2.63857000	-3.97373000
C	-2.39505200	-1.99194500	-3.20211700
H	-2.68613700	-3.04490900	-3.22802900
H	-3.20023900	-1.40150700	-3.65843600
C	0.97827500	-0.32517200	-2.95504200
C	1.97055200	-1.48305700	-2.67543400
H	1.74306800	-1.92744200	-1.70064200
H	1.85241000	-2.26937900	-3.43582000
C	3.41429000	-0.94701800	-2.69594500
H	4.11052200	-1.77342600	-2.49949800
C	3.72065400	-0.32609500	-4.07236600
H	3.63964000	-1.08776000	-4.86127800
H	4.75281700	0.04986700	-4.09692200
C	2.73278700	0.82706700	-4.34253100
H	2.94582800	1.27609800	-5.32190100
C	1.29206300	0.26786000	-4.34740600
H	0.56994000	1.06223300	-4.58001900
H	1.20250800	-0.49722600	-5.13377100
C	2.88312600	1.89314000	-3.23612000
H	2.21505600	2.74216200	-3.43696000
H	3.91071700	2.28567500	-3.24195100
C	2.55036500	1.26908700	-1.85534300
H	2.68521100	2.04313500	-1.08709800
C	1.07516100	0.78765600	-1.87580900
H	0.49914900	1.62651800	-2.29443600
C	3.54883300	0.12051400	-1.59445600
H	3.36924000	-0.34141900	-0.61961200
H	4.57449100	0.51845800	-1.58040300
C	-3.16935300	-1.79493700	-0.80755800
C	-3.18714400	-3.04572800	-0.16399500
C	-4.18157200	-3.28273700	0.79030500
H	-4.18895200	-4.23959500	1.30750500
C	-5.14856800	-2.32587200	1.10785100
C	-5.12347200	-1.10822800	0.42052400
H	-5.88179300	-0.35829600	0.63707000
C	-4.15202200	-0.82465700	-0.54324800
C	-2.18369900	-4.12820700	-0.49157300
H	-2.15671400	-4.87742300	0.30355700
H	-2.44782000	-4.64652800	-1.42456800
H	-1.17260000	-3.73029200	-0.60842300
C	-6.17814400	-2.59090000	2.18143400
H	-6.45019600	-3.65113100	2.22460600
H	-5.79163900	-2.31466500	3.17134400
H	-7.09244500	-2.01137600	2.01418100
C	-4.18353000	0.48670000	-1.29197700
H	-4.39737700	0.34132100	-2.35930100
H	-4.96142300	1.14330400	-0.88992500
H	-3.22479300	1.00762900	-1.22430900
C	1.48089100	0.80114700	1.31600300
H	2.42176100	0.72684200	0.78781600
C	-0.95873600	1.84736500	0.03939700
C	0.70293900	1.99244000	1.00352100
H	1.20183800	2.71147800	0.36095600
H	-1.70206800	1.82420300	0.85423700
C	-1.13802100	3.11995500	-0.78086200
H	-2.01557800	2.92755300	-1.41817700
H	-0.29505200	3.27154600	-1.45998500
C	-1.38544400	4.37538000	0.03637500
C	-0.40875100	5.37567600	0.13059600
C	-2.59113900	4.55508900	0.73132100
C	-0.62456700	6.52067400	0.90065200
H	0.52840900	5.25988300	-0.41012600
C	-2.81039200	5.69635200	1.50326700
H	-3.36890800	3.79727800	0.66034300
C	-1.82609200	6.68382400	1.59174800
H	0.14606300	7.28508500	0.95774100
H	-3.75257500	5.81745600	2.03163500
H	-1.99663300	7.57405600	2.19105300
N	-0.37551300	-2.01760700	1.38143000
O	-0.51302200	-3.00954700	2.07752100
H	0.19670900	2.45396300	1.84935400
C	1.51355100	0.19726000	2.66533900
C	2.58943100	-0.65850300	3.02509600
C	0.53026100	0.44813300	3.63632200
C	2.65610400	-1.20295300	4.31479900
C	0.59126800	-0.09731400	4.91469300
H	-0.31635300	1.07609500	3.37719300
C	1.66081800	-0.92509700	5.25120000
H	3.47819900	-1.84730500	4.60042600
H	-0.19170300	0.11694500	5.63590700
H	1.72880800	-1.36173900	6.24401900
O	3.52111200	-0.89552300	2.05225000
C	4.65323700	-1.74774800	2.31002700
H	4.32127300	-2.60060800	2.91463800
C	5.11494700	-2.27116000	0.95436600
H	4.29937900	-2.79912900	0.45133200
H	5.44502600	-1.44741200	0.31277100
H	5.95362300	-2.96402800	1.08568600
C	5.74861400	-0.97083600	3.04268700
H	6.09176500	-0.13447600	2.42345800
H	5.38794900	-0.56579000	3.99279300
H	6.60600600	-1.62157000	3.24986500

8'

B3LYP SCF energy: -1650.212886 a.u.
B3LYP enthalpy: -1649.552646 a.u.
B3LYP free energy: -1649.657806 a.u.
M06 SCF energy in solution: -1649.514533 a.u.
M06 enthalpy in solution: -1648.854293 a.u.
M06 free energy in solution: -1648.959453 a.u.

Cartesian coordinates

Ru	0.46434300	0.56888000	0.43682900
O	1.15416100	-0.28444400	2.52318000
O	-0.94276400	-0.02289100	2.05003200
N	1.90525900	-1.21118200	-1.27838000
N	-0.13497900	-2.01582500	-1.03880700
C	0.68929500	-0.98969100	-0.70054200
C	2.01689500	-2.57302000	-1.80726600
H	2.54779400	-2.59323700	-2.76293500
H	2.55007900	-3.22529700	-1.10095100
C	0.53568300	-2.97238600	-1.94219300
H	0.33670800	-4.00115700	-1.62986100
H	0.17102900	-2.84534900	-2.96988300
C	3.01581900	-0.38049500	-0.78736600
C	3.65337100	-1.00740700	0.47988400
H	2.87843500	-1.22438300	1.22161600
H	4.13520200	-1.96120700	0.21846300
C	4.69745800	-0.04202600	1.07303500
H	5.13659900	-0.49348900	1.97220400
C	5.79990800	0.21236000	0.02582400
H	6.31109900	-0.72906100	-0.22150100
H	6.56131500	0.89213700	0.43203300
C	5.16981800	0.82781400	-1.24099600
H	5.95043400	1.00979800	-1.99152100
C	4.12902200	-0.15825500	-1.83304600
H	3.69470400	0.24813800	-2.75612000
H	4.62784300	-1.10425600	-2.09295800
C	4.49917600	2.16713100	-0.85743800
H	4.08158200	2.65421600	-1.74919900
H	5.25646400	2.84922300	-0.44496100
C	3.37562100	1.91367400	0.18338300
H	2.90207800	2.87098200	0.44362000
C	2.34298600	0.98161800	-0.48367300
H	2.11122500	1.41882000	-1.46104000
C	4.00054500	1.28373800	1.44598700
H	3.23264300	1.09880900	2.20567600
H	4.73120500	1.97785900	1.88462800
C	-1.52386200	-2.15428500	-0.70351100
C	-1.88134100	-2.76286300	0.51438300
C	-3.24104200	-2.90227100	0.81148200
H	-3.52273600	-3.35684100	1.75903900
C	-4.24070200	-2.47181600	-0.06371700
C	-3.85187300	-1.90066300	-1.27929400
H	-4.61485200	-1.56818300	-1.98052200
C	-2.50698900	-1.73571100	-1.62181000
C	-0.85538700	-3.30035600	1.48524400
H	-1.19271700	-3.16673500	2.51736700
H	-0.69742700	-4.37679500	1.32951200
H	0.11382200	-2.80884500	1.38314900
C	-5.70113000	-2.59432300	0.30395200
H	-6.32719400	-2.75193200	-0.58106300
H	-5.87240500	-3.42645500	0.99495000
H	-6.05981600	-1.68152000	0.79772900
C	-2.15212500	-1.15505800	-2.97220600
H	-2.08672200	-1.94067200	-3.73782700
H	-2.91951500	-0.44827400	-3.30372700
H	-1.19248800	-0.63198700	-2.95918300
C	-0.56054700	1.50857200	-0.74462700
H	-0.99454700	1.20363100	-1.70566500

C	-0.95128900	2.91803700	-0.33516200
H	-0.50504200	3.17864200	0.63900100
H	-0.52061700	3.62132000	-1.06545500
N	-0.05825200	-0.38163400	2.92439000
O	-0.36865400	-0.78637900	4.02707400
C	-2.46049200	3.10503800	-0.27757100
C	-3.12349000	3.89468900	-1.22481500
C	-3.21457500	2.46711400	0.71900700
C	-4.51041000	4.05402700	-1.17659700
H	-2.54932400	4.39605000	-2.00128600
C	-4.59953100	2.62830400	0.76932200
H	-2.71513300	1.83841400	1.45243100
C	-5.25220800	3.42205700	-0.17760700
H	-5.00822900	4.67593400	-1.91630400
H	-5.16943000	2.13191900	1.55051400
H	-6.33093400	3.54800100	-0.13553900

TSB3

B3LYP SCF energy: -1999.149459 a.u.
B3LYP enthalpy: -1998.315187 a.u.
B3LYP free energy: -1998.435897 a.u.
M06 SCF energy in solution: -1998.287204 a.u.
M06 enthalpy in solution: -1997.452932 a.u.
M06 free energy in solution: -1997.573642 a.u.

Cartesian coordinates

Ru	-0.23137500	0.36447000	-0.23931600
O	-1.27750000	0.08916400	-2.33149900
O	-0.08921300	-1.51990000	-1.48120100
N	-2.86844100	1.31807100	0.71341200
N	-3.15590200	-0.82248700	0.35833900
C	-2.26092700	0.19200900	0.31566300
C	-4.32022600	1.15521200	0.87352800
H	-4.67748600	1.63541000	1.78758100
H	-4.85031900	1.59700000	0.01968000
C	-4.45558000	-0.37546900	0.90930600
H	-5.28188700	-0.75007500	0.30036100
H	-4.57901100	-0.75759000	1.93099200
C	-2.16206500	2.59977700	0.59364500
C	-2.50465600	3.26515300	-0.76259100
H	-2.23509800	2.58267100	-1.57751300
H	-3.58711300	3.44861100	-0.82815800
C	-1.73723300	4.59321800	-0.90117000
H	-1.99213000	5.06090400	-1.86137100
C	-2.10888300	5.54136800	0.25473600
H	-3.18194800	5.77888300	0.22508200
H	-1.56811700	6.49183800	0.15016900
C	-1.74837200	4.87201200	1.59593400
H	-2.00614500	5.54287800	2.42619100
C	-2.56067300	3.56491700	1.73500300
H	-2.36426700	3.08682400	2.70410200
H	-3.63488100	3.80226900	1.69784300
C	-0.23460600	4.56712700	1.62337500
H	0.04630100	4.13295900	2.59246100
H	0.33001400	5.50495600	1.51670200
C	0.12530800	3.58419200	0.47715100
H	1.20759100	3.39419700	0.51302200
C	-0.65091000	2.25971400	0.71300800
H	-0.50294400	2.02678900	1.78057600
C	-0.23123600	4.27976800	-0.85911700
H	0.01827000	3.65185700	-1.71961200
H	0.35044400	5.20745400	-0.95727600
C	-2.91803100	-2.22240300	0.14007300
C	-3.31886800	-2.80029600	-1.07901500
C	-3.09861800	-4.16877000	-1.26170000
H	-3.38646700	-4.62039600	-2.20835000
C	-2.51194700	-4.96548000	-0.27415000
C	-2.16988100	-4.36644900	0.94180300
H	-1.73918400	-4.97560900	1.73401700
C	-2.37390000	-3.00323900	1.17573700
C	-3.99810500	-1.99127800	-2.16036200
H	-4.00101500	-2.54109600	-3.10497000
H	-5.04499000	-1.78086100	-1.89865000
H	-3.50011000	-1.03385500	-2.33123900
C	-2.24165500	-6.43111900	-0.52227700
H	-2.18968200	-6.99487800	0.41519700
H	-3.01919000	-6.88222600	-1.14842900
H	-1.28521900	-6.57075500	-1.04300400
C	-2.06736100	-2.41481900	2.53395300
H	-2.98425900	-2.27510800	3.12340300
H	-1.41565300	-3.08076500	3.10767800
H	-1.58062600	-1.43862600	2.46043900
C	1.25470400	1.22114200	-1.38063600
H	1.32731700	2.30069400	-1.39685800
H	1.27893200	0.77520000	-2.37535500
C	1.05057500	0.05651400	1.16078300
C	2.05122600	0.51826300	-0.34197800
H	1.28564300	0.85624200	1.87619900
H	2.62096800	1.24615400	0.23927600
C	1.42043800	-1.30798400	1.73642100
H	0.61283100	-1.52692400	2.45038100
H	1.35639100	-2.08800700	0.97141100
C	2.91936600	-0.64945700	-0.84595300
H	3.33448500	-1.19703400	0.00213700
H	2.29149300	-1.34172000	-1.41400100
N	-0.79308400	-1.09274500	-2.47046900
O	-0.99161700	-1.76887700	-3.46738700
C	4.06876900	-0.15505700	-1.70636700
C	5.21018700	0.40250900	-1.11114000
C	4.01937100	-0.23703600	-3.10446100
C	6.26714900	0.87516800	-1.88993800
H	5.27487200	0.45565600	-0.02598600
C	5.07635300	0.23200600	-3.88746100
H	3.14987100	-0.68149000	-3.58362100
C	6.20277100	0.79259000	-3.28283700
H	7.14406300	1.30130200	-1.40898100
H	5.02008900	0.15464900	-4.97027000
H	7.02656800	1.15655500	-3.89117900
C	2.73727300	-1.41475000	2.49816500
C	3.61545900	-2.48060200	2.25469100
C	3.08188400	-0.49125100	3.49699800
C	4.80590300	-2.61481200	2.97261800
H	3.36239000	-3.21502400	1.49296800
C	4.27162800	-0.61962300	4.21509300
H	2.41071400	0.33319800	3.72522900
C	5.14085600	-1.68134000	3.95416200
H	5.47038300	-3.44874900	2.76190900
H	4.51716600	0.10877500	4.98383900
H	6.06716400	-1.78130200	4.51344400

TSB4

B3LYP SCF energy: -1999.144783 a.u.
B3LYP enthalpy: -1998.31152 a.u.
B3LYP free energy: -1998.432832 a.u.
M06 SCF energy in solution: -1998.27879 a.u.
M06 enthalpy in solution: -1997.445527 a.u.
M06 free energy in solution: -1997.566839 a.u.

Cartesian coordinates

Ru	0.11020400	0.24474900	-0.15347700
O	0.78792800	-0.48387100	-2.23163600
O	0.63352000	-1.92967900	-0.61631300
N	2.19003600	2.33737600	-0.17867800
N	3.30632500	0.45378700	-0.15994200
C	2.07134100	1.00073800	-0.16828100
C	3.58114200	2.79552400	-0.05108800
H	3.82653800	3.53316300	-0.81988800
H	3.74432600	3.25793700	0.93030300
C	4.36904300	1.48265100	-0.21563000
H	5.10153300	1.31555800	0.57992800
H	4.89123800	1.43104900	-1.17711300
C	1.01003400	3.17858800	0.06361500
C	0.91840500	3.52640900	1.57246700
H	0.88907700	2.59736800	2.15212400
H	1.81352400	4.08239000	1.88685000
C	-0.33844100	4.37508000	1.84434900
H	-0.38837400	4.61853400	2.91425500
C	-0.26837700	5.67529200	1.01868800
H	0.60660600	6.26984900	1.31809400
H	-1.15580400	6.29271400	1.21342900
C	-0.18682900	5.32438000	-0.48146500
H	-0.14285700	6.24734300	-1.07471400
C	1.09269400	4.49789600	-0.73915000
H	1.19637800	4.26898600	-1.80790300
H	1.97310700	5.08884200	-0.44344400
C	-1.43287800	4.50623200	-0.88134800
H	-1.40931800	4.28163400	-1.95605600
H	-2.33899100	5.10228800	-0.69814200
C	-1.48055500	3.18739900	-0.06288200
H	-2.38852100	2.64011100	-0.34707500
C	-0.21431000	2.35348300	-0.40584200
H	-0.15805000	2.35728100	-1.51001400

C	-1.58200100	3.56743500	1.43005200
H	-1.67898200	2.67633900	2.05936100
H	-2.48760800	4.16873500	1.59635200
C	3.66788400	-0.93619200	-0.11718100
C	3.68173700	-1.59340800	1.12770800
C	4.08792800	-2.92911700	1.16826100
H	4.09664000	-3.44545600	2.12607900
C	4.48468000	-3.61595300	0.01622400
C	4.48709900	-2.92381600	-1.19646700
H	4.79415900	-3.43975500	-2.10343900
C	4.08963900	-1.58570100	-1.29146700
C	3.28118700	-0.88266300	2.39926100
H	3.45077000	-1.52474100	3.26901700
H	3.85427700	0.04105600	2.54969500
H	2.22250900	-0.60244800	2.38561000
C	4.87571000	-5.07394400	0.07716300
H	4.00899700	-5.71986800	-0.11552700
H	5.63501500	-5.31813300	-0.67362000
H	5.27162100	-5.34350900	1.06229800
C	4.12751900	-0.88503900	-2.63056200
H	5.03436400	-0.27362000	-2.73966700
H	4.12867800	-1.61758700	-3.44205400
H	3.25990600	-0.23553400	-2.77237100
C	-0.41401400	0.14407100	1.64811900
H	-0.82265100	0.91276900	2.31572900
C	-1.90524200	-0.07880800	-0.92469000
C	-2.07294500	-0.36686100	0.47818200
H	-2.25404800	0.90279400	-1.23270500
H	-2.59426900	0.41085800	1.03455700
C	-2.38479300	-1.79516600	0.93876200
H	-3.27407600	-2.11348400	0.37628900
H	-1.57145700	-2.46276200	0.63791200
C	-2.12043700	-1.13219400	-2.01020900
H	-1.55310800	-0.82518500	-2.89564800
H	-1.72162200	-2.10256600	-1.70496400
H	-0.25934800	-0.79606000	2.19593800
C	-3.58927700	-1.28434000	-2.38354600
C	-4.26470400	-2.49568000	-2.17989200
C	-4.30063200	-0.21849500	-2.95652000
C	-5.61114400	-2.63757000	-2.52557600
H	-3.72584000	-3.34199300	-1.75976200
C	-5.64499900	-0.35472600	-3.30164400
H	-3.79259300	0.72472900	-3.14608000
C	-6.30762500	-1.56578700	-3.08411400
H	-6.11203000	-3.58820300	-2.36088900
H	-6.17476400	0.48317100	-3.74790600
H	-7.35462000	-1.67346100	-3.35473400
C	-2.67157300	-1.95446900	2.41867100
C	-1.88303300	-2.79111700	3.21992800
C	-3.75362300	-1.28971400	3.01532600
C	-2.15539500	-2.94878500	4.58083500
H	-1.04927700	-3.32672200	2.77076000
C	-4.02733400	-1.44116200	4.37509000
H	-4.39613900	-0.65528100	2.40767200
C	-3.22664800	-2.27065700	5.16411700
H	-1.53044800	-3.60310700	5.18318900
H	-4.87084800	-0.91716800	4.81724600
H	-3.44080400	-2.39176300	6.22261300
N	0.90238300	-1.71138000	-1.85090000
O	1.23750300	-2.59862900	-2.61924300

TSB5

B3LYP SCF energy: -1999.15473 a.u.
B3LYP enthalpy: -1998.320697 a.u.
B3LYP free energy: -1998.440798 a.u.
M06 SCF energy in solution: -1998.292617 a.u.
M06 enthalpy in solution: -1997.458584 a.u.
M06 free energy in solution: -1997.578685 a.u.

Cartesian coordinates

Ru	-0.25742800	0.25031500	-0.30416200
O	-1.40007000	-0.02462300	-2.30871300
O	-0.42405300	-1.73774000	-1.39371700
N	-2.72192100	1.61536500	0.57720500
N	-3.22633100	-0.51546800	0.57666600
C	-2.24599600	0.38564200	0.34263200
C	-4.17272900	1.62663700	0.80848400
H	-4.43956400	2.27503400	1.64653700
H	-4.70038600	1.98196300	-0.08644800
C	-4.45026100	0.13952400	1.09171300
H	-5.33760400	-0.23782100	0.57794600
H	-4.55981600	-0.06504100	2.16480300
C	-1.88417500	2.77712800	0.25239800
C	-2.18517300	3.27365100	-1.18402500
H	-2.03417400	2.45304900	-1.89422600
H	-3.23764400	3.58526100	-1.25885200
C	-1.26073600	4.45699900	-1.52714300
H	-1.47893000	4.80357800	-2.54591300
C	-1.48595900	5.60709500	-0.52675900
H	-2.52200300	5.96971700	-0.58838500
H	-0.83450400	6.45606400	-0.77514200
C	-1.18047200	5.10604800	0.89908200
H	-1.33814800	5.91961900	1.61965400
C	-2.13793400	3.94152800	1.23826300
H	-1.97462400	3.59357900	2.26731100
H	-3.17748500	4.29751200	1.17269000
C	0.28669600	4.62910900	0.96634400
H	0.53425800	4.31334000	1.98928100
H	0.95571200	5.46662100	0.71951700
C	0.50287900	3.45132600	-0.02072500
H	1.55677900	3.14123800	0.03269800
C	-0.41785000	2.27973900	0.41093500
H	-0.28735400	2.18313700	1.49841700
C	0.19726700	3.96903900	-1.44631300
H	0.34838300	3.18474900	-2.19442100
H	0.88328900	4.79119800	-1.69594300
C	-3.12774900	-1.94781700	0.53492700
C	-3.67809900	-2.63795800	-0.55988900
C	-3.59118500	-4.03419500	-0.56987200
H	-3.99790900	-4.57491800	-1.42149800
C	-2.98790100	-4.74783500	0.46838200
C	-2.48109700	-4.02993700	1.55696100
H	-2.02712900	-4.56929600	2.38598800
C	-2.54480600	-2.63548200	1.61554700
C	-4.36490900	-1.91670300	-1.69720500
H	-4.42067400	-2.55892400	-2.57984500
H	-5.39385400	-1.63768000	-1.42864700
H	-3.83692800	-1.00323600	-1.98227800
C	-2.86537600	-6.25245500	0.40726300
H	-3.68065400	-6.69842000	-0.17227000
H	-1.92403500	-6.54980100	-0.07341900
H	-2.87503100	-6.69818300	1.40793100
C	-2.01416800	-1.90010300	2.82461600
H	-2.79859500	-1.31822300	3.32547400
H	-1.61052100	-2.60569600	3.55730900
H	-1.21972500	-1.19818800	2.55209900
C	1.35463900	0.69348600	-1.56227800
H	1.57102200	1.74456700	-1.70675400
H	1.27225700	0.12970600	-2.49112200
C	0.93610800	-0.23272000	1.11007900
C	2.03564100	0.02486800	-0.44930000
H	2.68630400	0.71155900	0.09191500
C	2.68398200	-1.34674900	-0.71809800
H	3.01657800	-1.78218900	0.23011600
H	1.92707300	-2.01390600	-1.14108100
H	1.03549800	-1.32227700	1.23664600
C	1.54064200	0.49453100	2.30876600
H	0.78575300	0.41253000	3.10732500
H	1.64878700	1.56268300	2.10170600
C	2.85738600	-0.07141400	2.80931300
C	4.04982300	0.65120400	2.66605300
C	2.91678500	-1.33712000	3.41275300
C	5.26837900	0.12385700	3.10190300
H	4.02299900	1.64190300	2.21647200
C	4.13109100	-1.86857200	3.84797300
H	2.00113700	-1.90926100	3.54893200
C	5.31322100	-1.14030600	3.69176100
H	6.17977600	0.70462400	2.98517800
H	4.15412500	-2.85024000	4.31404700
H	6.25897100	-1.55265000	4.03248500
C	3.87080100	-1.23340600	-1.65766400
C	3.74568300	-1.53913300	-3.01981000
C	5.11850500	-0.80573700	-1.18026400
C	4.83438700	-1.41263600	-3.88479400
H	2.78955700	-1.88809700	-3.40354700
C	6.20815000	-0.67624800	-2.04267600
H	5.23712400	-0.58051700	-0.12225700
C	6.06896900	-0.97755700	-3.39940600
H	4.71784300	-1.65883300	-4.93711900
H	7.16820800	-0.34577200	-1.65391500
H	6.91759900	-0.88005800	-4.07140800
N	-1.10824600	-1.27752700	-2.37843600

O	-1.46415100	-1.97744300	-3.31288100

TSB6

B3LYP SCF energy: -1999.142974 a.u.
B3LYP enthalpy: -1998.310096 a.u.
B3LYP free energy: -1998.43369 a.u.
M06 SCF energy in solution: -1998.277599 a.u.
M06 enthalpy in solution: -1997.444721 a.u.
M06 free energy in solution: -1997.568315 a.u.

Cartesian coordinates

Ru	0.09523900	0.10375000	-0.10707700
O	0.89019000	-0.62762100	-2.16816800
O	1.06042700	-1.95229400	-0.45034200
N	1.72927100	2.53848200	-0.38196600
N	3.19029300	0.90981300	-0.27372900
C	1.87510900	1.21219500	-0.24904200
C	3.00896700	3.26281600	-0.40535400
H	3.06787500	3.92568500	-1.27306300
H	3.12379000	3.87390100	0.49811800
C	4.03215700	2.11194800	-0.46903800
H	4.79507000	2.16919500	0.31365000
H	4.54024200	2.06258900	-1.43765500
C	0.42437900	3.16075300	-0.11706800
C	0.36757300	3.60620200	1.36769400
H	0.54290500	2.73420200	2.00855400
H	1.16819300	4.33143500	1.57340000
C	-0.99916200	4.24038000	1.68312900
H	-1.01915200	4.56038500	2.73364700
C	-1.23053000	5.45691800	0.76425300
H	-0.46264800	6.22272500	0.94476000
H	-2.20153800	5.91860100	0.98925000
C	-1.18966700	4.99897400	-0.70806100
H	-1.36140300	5.85994800	-1.36750800
C	0.20336200	4.40360000	-1.01126800
H	0.27944500	4.11225600	-2.06701000
H	0.97256000	5.16870000	-0.82511500
C	-2.28495900	3.93650500	-0.94326200
H	-2.29526800	3.63068900	-1.99785900
H	-3.27121300	4.37235000	-0.72566800
C	-2.02412600	2.70559200	-0.03329600
H	-2.83004900	1.97969800	-0.19281400
C	-0.65280000	2.08892900	-0.43954900
H	-0.67786000	2.03514100	-1.54224700
C	-2.09418200	3.19011100	1.43121700
H	-1.98281100	2.35731000	2.13253300
H	-3.08369200	3.63004700	1.62334000
C	3.81493200	-0.37152300	-0.09301000
C	3.95210800	-0.87995500	1.21295800
C	4.61032500	-2.09946100	1.38381800
H	4.71554000	-2.50146300	2.38953200
C	5.13828400	-2.81247300	0.30216300
C	5.00916500	-2.26406400	-0.97525500
H	5.41371700	-2.80266300	-1.82925400
C	4.35737100	-1.04654900	-1.20101100
C	3.41516400	-0.13253500	2.41089000
H	3.70546600	-0.63379500	3.33932200
H	3.79400800	0.89658900	2.45450600
H	2.32211600	-0.06940500	2.38529300
C	5.80620700	-4.15176100	0.50884300
H	5.07347700	-4.96760500	0.45319600
H	6.56553100	-4.34453800	-0.25650100
H	6.28857400	-4.21352200	1.49057700
C	4.25661400	-0.49801600	-2.60623900
H	5.03692500	0.25044800	-2.80389800
H	4.38297700	-1.30118700	-3.33698900
H	3.28431400	-0.03359500	-2.78994800
C	-0.44426100	0.00962500	1.68440900
H	-1.06171000	0.69211100	2.27911800
C	-1.63096000	-0.92722200	-0.91047300
C	-1.97562900	-0.88264400	0.47777600
H	-2.69887700	-0.12354300	0.76984600
C	-2.09821900	-2.22552800	1.21357400
H	-2.90630500	-2.76650000	0.69786700
H	-1.18658800	-2.80820100	1.04410800
H	-0.09964400	-0.83405900	2.29990000
H	-1.26119600	-1.90220300	-1.23357100
C	-2.41230300	-0.23217100	-2.02024400
H	-1.71588600	0.01548200	-2.82908300
H	-2.85175000	0.70141800	-1.66504200
C	-2.42875200	-2.17026400	2.69179500
C	-3.60643800	-1.55462000	3.14180600
C	-1.58621800	-2.76431000	3.64081400
C	-3.92189400	-1.51525800	4.50036100
H	-4.29036800	-1.11081500	2.42107900
C	-1.89982600	-2.73184400	5.00144700
H	-0.67683100	-3.26037400	3.30827800
C	-3.06710900	-2.10259400	5.43635100
H	-4.83919000	-1.03255600	4.82767900
H	-1.23176400	-3.19968700	5.71995000
H	-3.31335500	-2.07543000	6.49443400
C	-3.50565300	-1.14293400	-2.55743300
C	-3.21558600	-2.10169900	-3.53872800
C	-4.81558600	-1.06829400	-2.06442900
C	-4.20626100	-2.96262200	-4.01331000
H	-2.20482100	-2.16874500	-3.93594800
C	-5.81026900	-1.92617800	-2.53786400
H	-5.06132100	-0.32376300	-1.30941900
C	-5.50781100	-2.87789200	-3.51381700
H	-3.96194000	-3.69686300	-4.77667700
H	-6.82200600	-1.84783900	-2.14775900
H	-6.28085300	-3.54567200	-3.88470900
N	1.24058300	-1.78166300	-1.70746600
O	1.70996300	-2.64772900	-2.42948600

CH_2=CH_2

B3LYP SCF energy: -78.58745746 a.u.
B3LYP enthalpy: -78.53223246 a.u.
B3LYP free energy: -78.55840246 a.u.
M06 SCF energy in solution: -78.53974354 a.u.
M06 enthalpy in solution: -78.48451854 a.u.
M06 free energy in solution: -78.51068854 a.u.

Cartesian coordinates

C	0.66535500	0.00000000	0.00000300
C	-0.66535500	0.00000000	-0.00000400
H	1.24030000	0.92285100	-0.00000900
H	1.24029900	-0.92285100	0.00002400
H	-1.24030000	-0.92285100	0.00001100
H	-1.24029900	0.92285100	-0.00002200

PhCH_2CH=CH_2

B3LYP SCF energy: -348.956969 a.u.
B3LYP enthalpy: -348.785764 a.u.
B3LYP free energy: -348.828799 a.u.
M06 SCF energy in solution: -348.7649546 a.u.
M06 enthalpy in solution: -348.5937496 a.u.
M06 free energy in solution: -348.6367846 a.u.

Cartesian coordinates

C	-2.41784000	-0.17005200	0.49954800
C	-3.47439800	0.54667400	0.11429900
H	-2.22389000	-0.30916700	1.56378100
H	-3.69947200	0.71292400	-0.93762400
H	-4.15843800	0.99011100	0.83299700
C	-1.42736100	-0.82014400	-0.43414300
H	-1.72945300	-0.62016400	-1.47159000
H	-1.46743700	-1.91099500	-0.30534100
C	0.00646300	-0.35846300	-0.21447200
C	1.03567000	-1.28169300	0.00189200
C	0.32740000	1.00638300	-0.23650000
C	2.35389300	-0.85793300	0.18532100
H	0.80377000	-2.34450900	0.02467900
C	1.64198600	1.43400400	-0.05474800
H	-0.46415100	1.73556400	-0.39118900
C	2.66136100	0.50226400	0.15689900
H	3.13836700	-1.59181400	0.35198800
H	1.87173800	2.49639400	-0.07635500
H	3.68592200	0.83541300	0.30007000

***i*-PrOC_6H_4CH=CH_2 (R'CH=CH_2)**

B3LYP SCF energy: -502.8053055 a.u.
B3LYP enthalpy: -502.5692465 a.u.
B3LYP free energy: -502.6205655 a.u.
M06 SCF energy in solution: -502.5627434 a.u.
M06 enthalpy in solution: -502.3266844 a.u.
M06 free energy in solution: -502.3780034 a.u.

Cartesian coordinates

C	2.23866000	2.74723200	0.37058600
C	1.25036600	1.93541100	-0.02765700
H	2.11876900	3.82620400	0.34192700

H	3.18957600	2.37899400	0.74729600
H	0.31226500	2.37901300	-0.34911400
C	1.28996400	0.46421600	-0.06229900
C	0.07853500	-0.27220500	-0.12030000
C	2.49404000	-0.25428500	-0.06073700
C	0.10327500	-1.67181900	-0.15481000
C	2.52307000	-1.64662600	-0.09420900
H	3.42863300	0.29926500	-0.05326100
C	1.32215300	-2.35220000	-0.14019300
H	-0.81829600	-2.24051800	-0.18762200
H	3.47307200	-2.17305500	-0.09404300
H	1.32350100	-3.43862600	-0.16916700
O	-1.06440500	0.47737300	-0.14414500
C	-2.36329500	-0.13968300	-0.18840400
H	-2.32924800	-0.99212900	-0.87987100
C	-3.30165700	0.91867600	-0.75855900
H	-4.31969200	0.52241500	-0.83797900
H	-3.32246600	1.79986100	-0.10816400
H	-2.97026700	1.23182800	-1.75335100
C	-2.78350300	-0.60523500	1.20637200
H	-3.76968400	-1.08193800	1.16900800
H	-2.07153500	-1.32361000	1.62316200
H	-2.83903600	0.25242700	1.88559500

***Z*-PhCH$_2$CH=CHCH$_2$Ph**
B3LYP SCF energy: -619.3230803 a.u.
B3LYP enthalpy: -619.0357503 a.u.
B3LYP free energy: -619.0944873 a.u.
M06 SCF energy in solution: -618.9876924 a.u.
M06 enthalpy in solution: -618.7003624 a.u.
M06 free energy in solution: -618.7590994 a.u.

Cartesian coordinates

C	0.35788400	0.56601500	1.06146900
C	-0.35788400	-0.56601500	1.06146900
H	0.61933800	0.99662600	2.02848300
H	-0.61933800	-0.99662600	2.02848300
C	0.85245800	1.35717500	-0.12537700
H	0.56242700	0.86686500	-1.06265900
H	1.95153900	1.36795400	-0.11550600
C	0.35788400	2.79744600	-0.13321800
C	1.25608100	3.86521000	-0.24312400
C	-1.01149500	3.08453900	-0.04285100
C	0.80251500	5.18583900	-0.26952100
H	2.32266200	3.66104900	-0.31040300
C	-1.46923000	4.40140200	-0.07004400
H	-1.72067200	2.26638000	0.05667800
C	-0.56282600	5.45835400	-0.18379700
H	1.51749300	6.00025900	-0.35473800
H	-2.53512700	4.60349300	-0.00007900
H	-0.91881100	6.48501500	-0.20299600
C	-0.85245800	-1.35717500	-0.12537700
H	-0.56242700	-0.86686500	-1.06265900
H	-1.95153900	-1.36795400	-0.11550600
C	-0.35788400	-2.79744600	-0.13321800
C	1.01149500	-3.08453900	-0.04285100
C	-1.25608100	-3.86521000	-0.24312400
C	1.46923000	-4.40140200	-0.07004400
H	1.72067200	-2.26638000	0.05667800
C	-0.80251500	-5.18583900	-0.26952100
H	-2.32266200	-3.66104900	-0.31040300
C	0.56282600	-5.45835400	-0.18379700
H	2.53512700	-4.60349300	-0.00007900
H	-1.51749300	-6.00025900	-0.35473800
H	0.91881100	-6.48501500	-0.20299600

***E*-PhCH$_2$CH=CHCH$_2$Ph**
B3LYP SCF energy: -619.3258451 a.u.
B3LYP enthalpy: -619.0387071 a.u.
B3LYP free energy: -619.0981421 a.u.
M06 SCF energy in solution: -618.9893438 a.u.
M06 enthalpy in solution: -618.7022058 a.u.
M06 free energy in solution: -618.7616408 a.u.

Cartesian coordinates

C	4.54101100	-1.43883100	0.08994100
C	3.26287000	-0.94435600	0.34686200
C	3.00100300	0.43209800	0.29609600
C	4.05194000	1.29841400	-0.02603400
C	5.33371600	0.80783900	-0.28533200
C	5.58256000	-0.56341700	-0.22750900
H	4.72475500	-2.50936400	0.13576500
H	2.45334200	-1.63034600	0.58415600
H	3.86573800	2.36943600	-0.07243900
H	6.13570500	1.49829800	-0.53399900
H	6.57863600	-0.94837500	-0.42951100
C	1.60781400	0.96805800	0.59648800
H	1.37272700	0.81755900	1.65925900
H	1.61019300	2.05492000	0.43273700
C	0.52528200	0.33491400	-0.24165100
C	-0.52528200	-0.33491400	0.24165100
H	0.64096400	0.43590800	-1.32238100
H	-0.64096400	-0.43590800	1.32238100
C	-1.60781400	-0.96805800	-0.59648800
H	-1.61019300	-2.05492000	-0.43273700
H	-1.37272700	-0.81755900	-1.65925900
C	-3.00100300	-0.43209800	-0.29609600
C	-4.05194000	-1.29841400	0.02603400
C	-3.26287000	0.94435600	-0.34686200
C	-5.33371600	-0.80783900	0.28533200
H	-3.86573800	-2.36943600	0.07243900
C	-4.54101100	1.43883100	-0.08994100
H	-2.45334200	1.63034600	-0.58415600
C	-5.58256000	0.56341700	0.22750900
H	-6.13570500	-1.49829800	0.53399900
H	-4.72475500	2.50936400	-0.13576500
H	-6.57863600	0.94837500	0.42951100