Supporting Information

The Mechanism and Origins of *Z* Selectivity of the Catalytic Hydroalkoxylation of Alkynes via Rhodium Vinylidene Complexes to Produce Enol Ethers

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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.

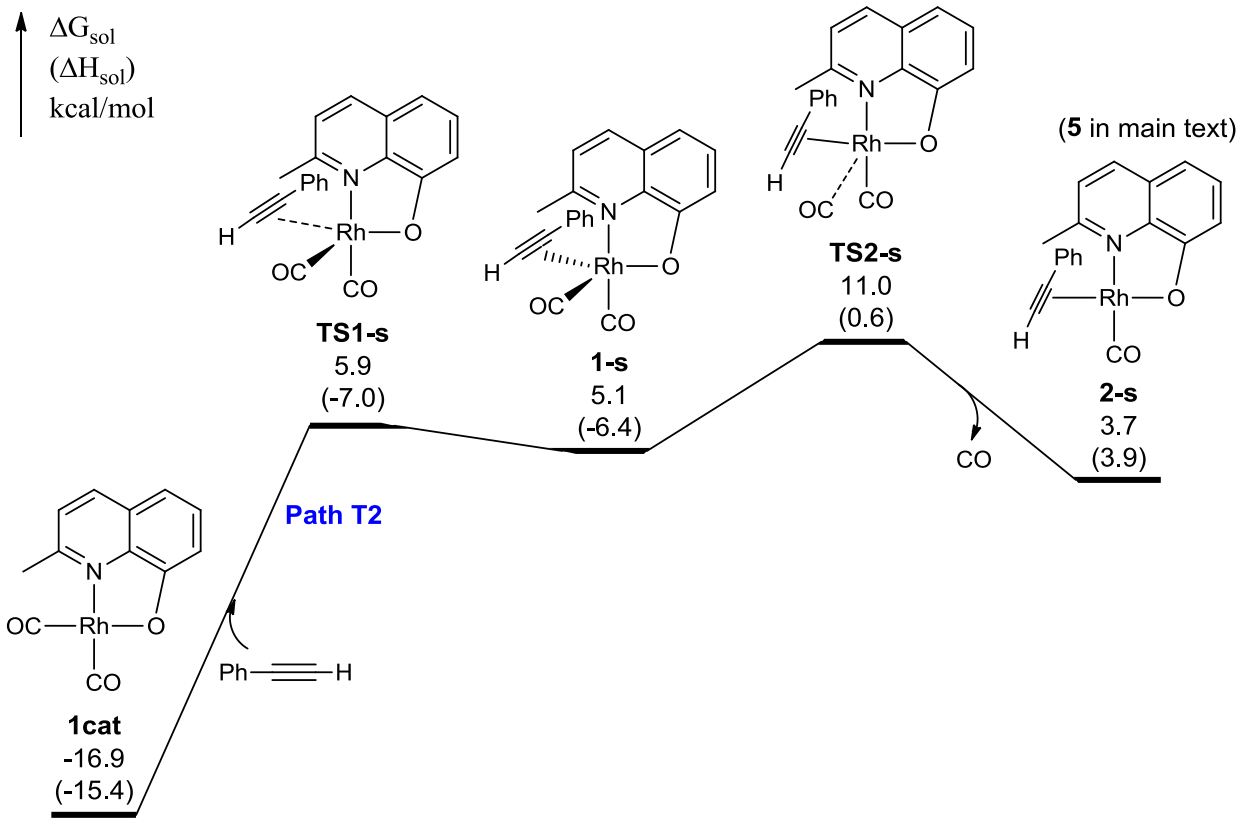


Figure S1 (part 1). Free energy profile for path T2. Energies are mass balanced and relative to **3** (similarly hereinafter except for Figures S2 and S3).

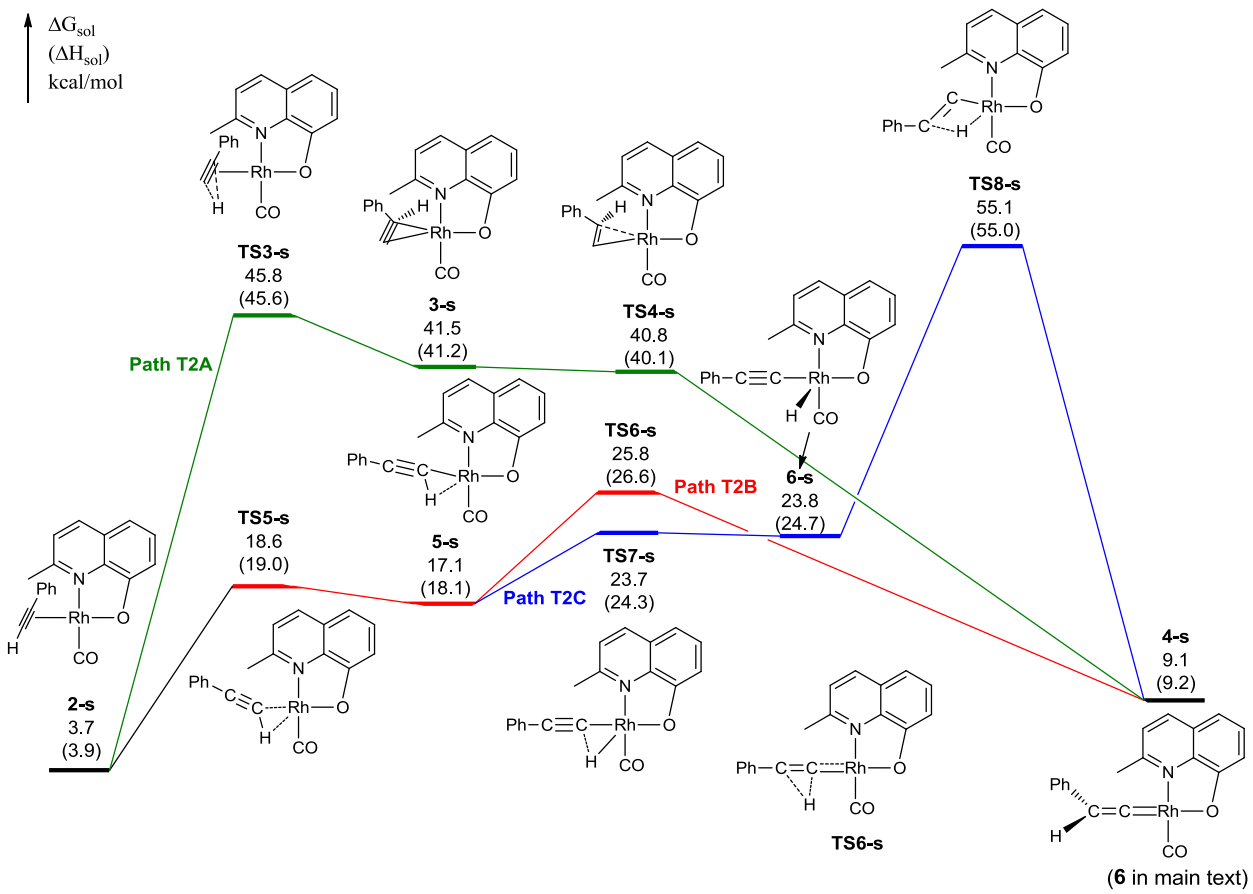


Figure S1 (part 2). Free energy profiles for path T2. Note: the highest barrier (**TS6-s**, 25.8 kcal/mol) of the most favorable pathway is 3.8 kcal/mol higher than the corresponding **TS5** in path T1B (Figure 1). In addition, **TS6-s** is respectively 2.7 and 1.5 kcal /mol higher than **TS24** and **TS25**, the turnover-limiting TSs of the (*Z*)- and (*E*)-product forming paths L1B and L2B (Figure 7). Thus, the reaction of **4-s** with methanol was not pursued.

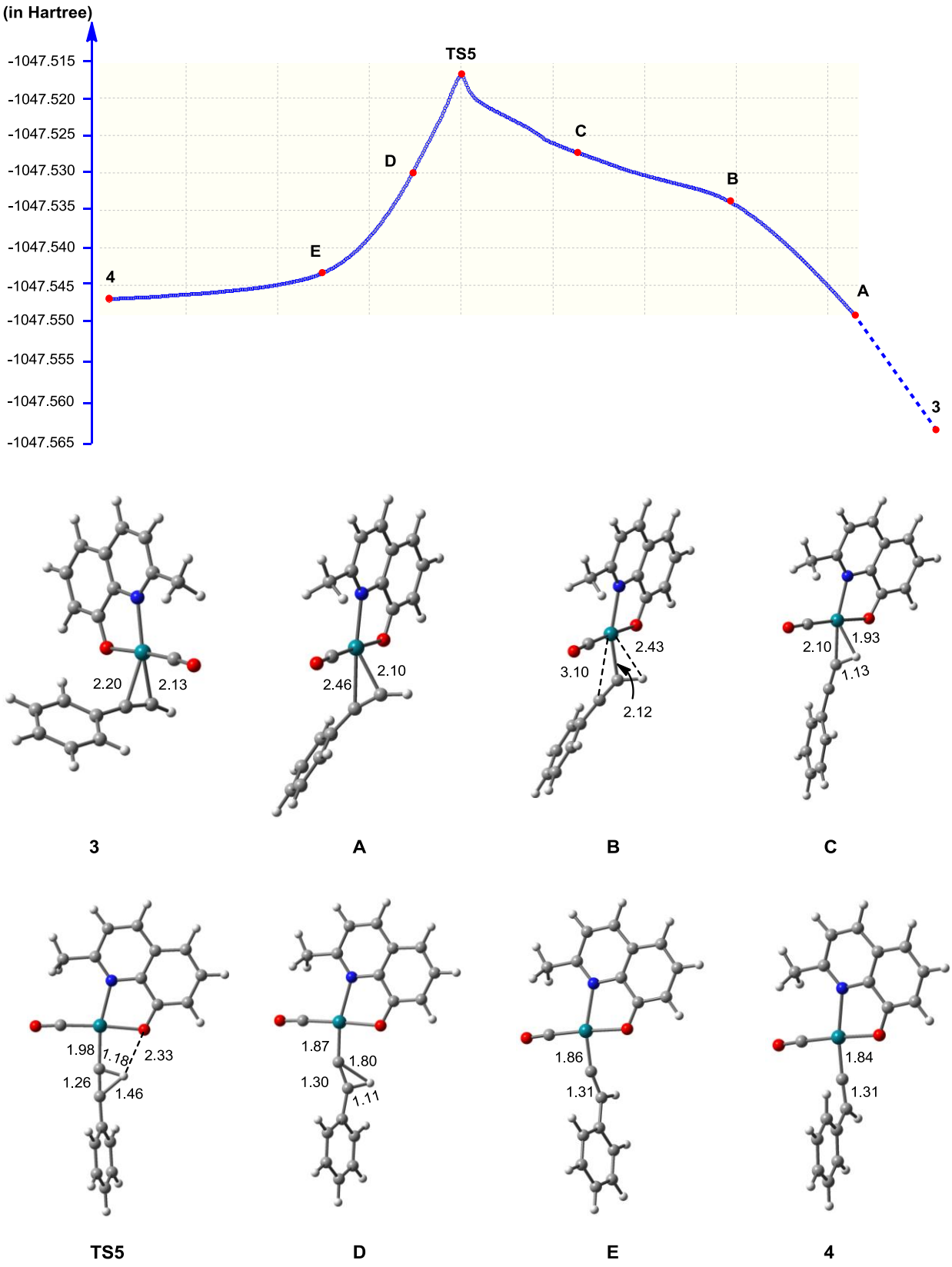
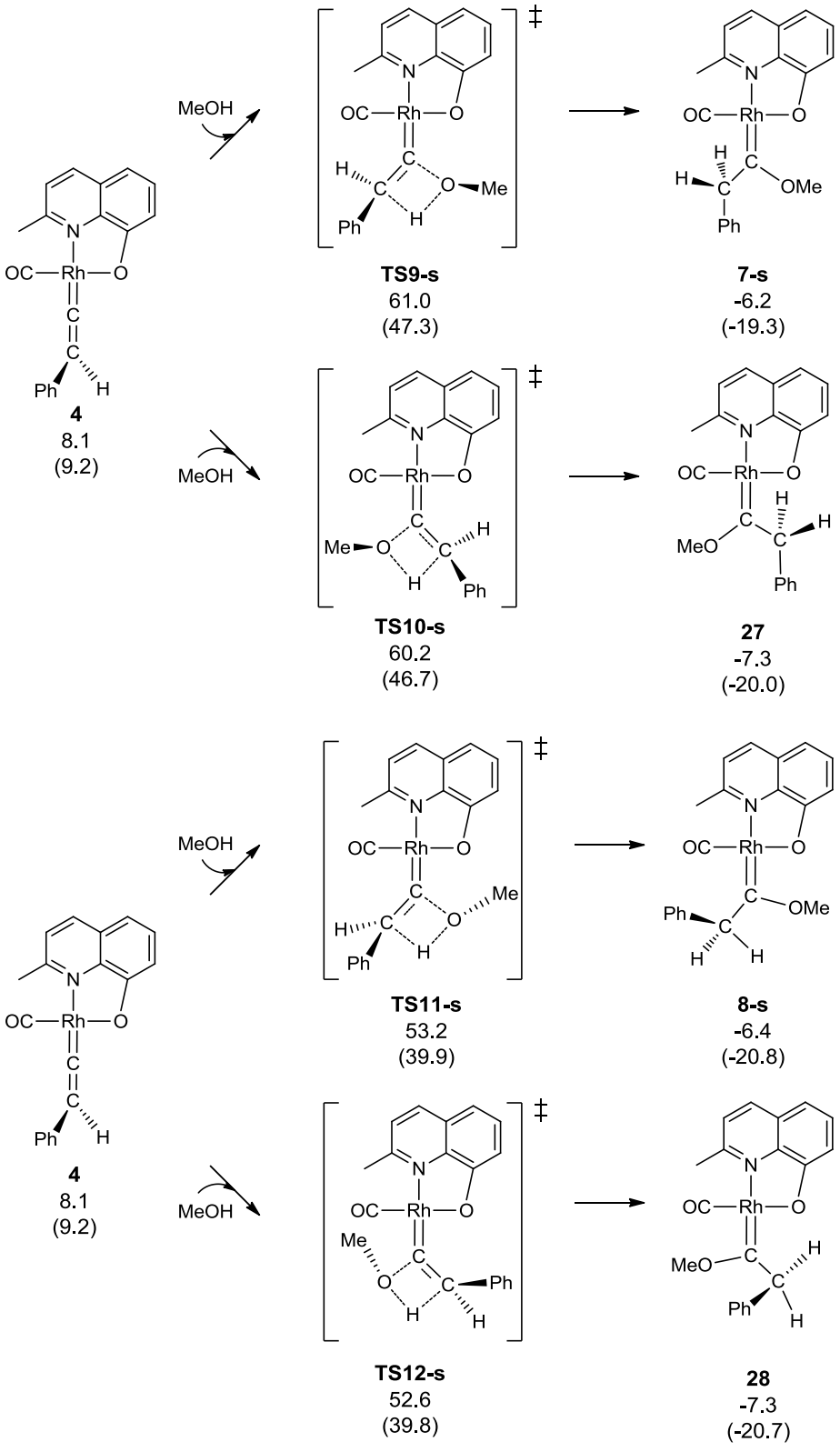
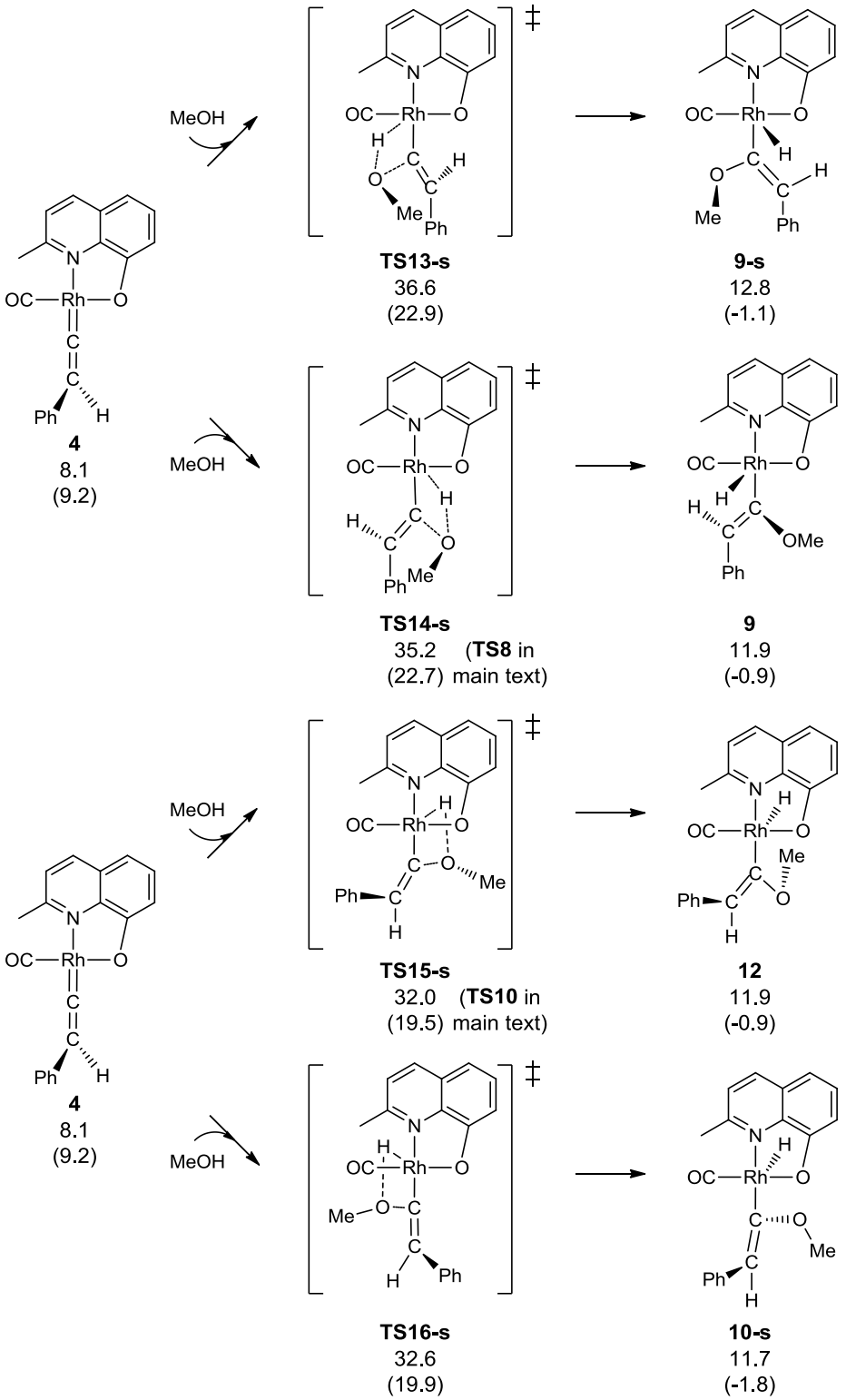


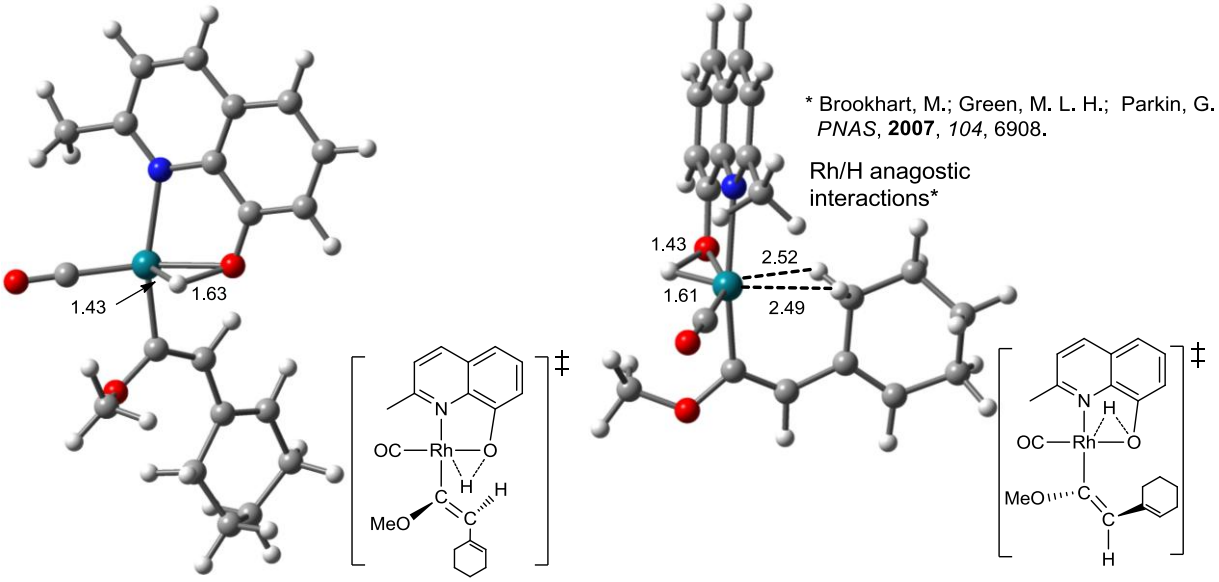
Figure S2. Confirming the **3** → **TS5** → **4** step in Figure 1 by IRC calculation at M06/BS1 level.

Scheme S1. Four Possible Pathways for Concerted Methanol Addition Across C_α=C_β of **4**



Scheme S2. Four Possible Pathways for Concerted Methanol Addition Across Rh=C_α of **4**

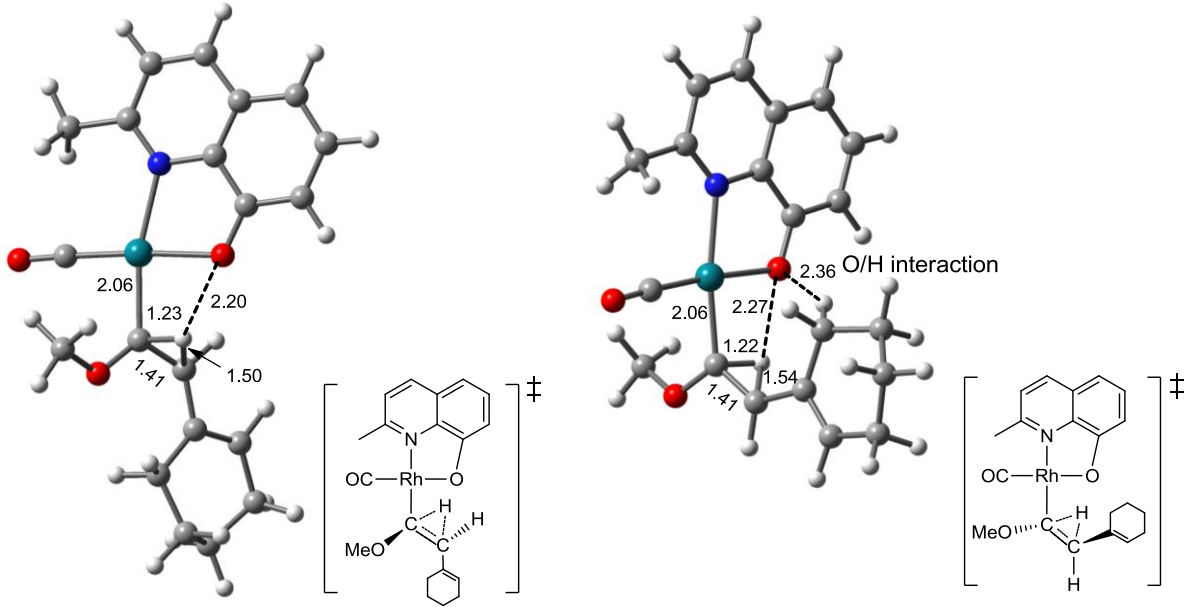




TS17-s (*Z* leading)
$\Delta\Delta G^{\ddagger}$ = 9.5 kcal/mol

TS18-s (*E* leading)
$\Delta\Delta G^{\ddagger}$ = 8.0 kcal/mol

TS17-s minus **TS18-s** = 1.5 kca/ml; selectivity = 93% *E*

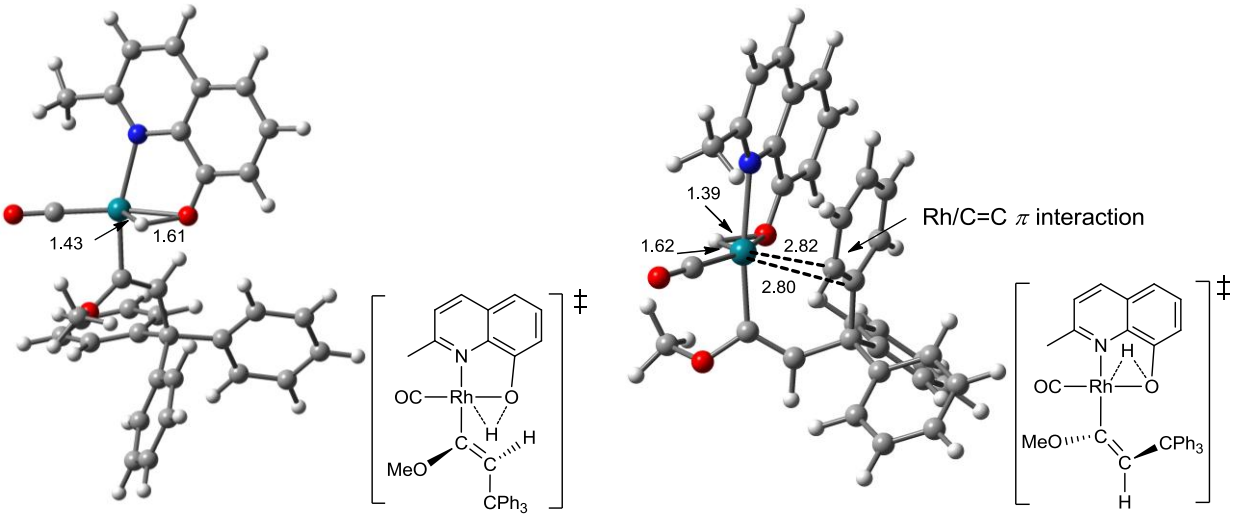


TS19-s (*Z* leading)
$\Delta\Delta G^{\ddagger}$ = 0.0 kcal/mol

TS20-s (*E* leading)
$\Delta\Delta G^{\ddagger}$ = -0.5 kcal/mol

TS19-s minus **TS20-s** = 0.5 kca/ml; selectivity = 67% *E*/33% *Z*

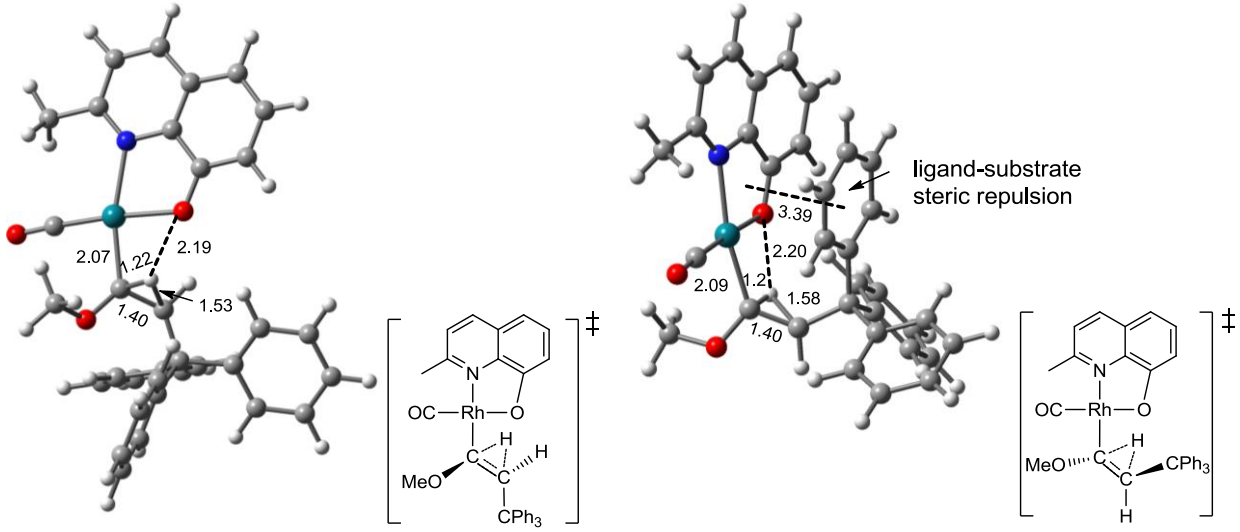
Figure S3. Turnover-limiting TSs involving **sub2** of two different mechanisms: the Rh-bound proton transfer/reductive elimination (top) and the C_{β}-bound proton transfer/1,2 β-hydrogen shift of Fischer carbene (bottom). Energies are relative to **TS19-s**.



TS21-s (*Z* leading)
$\Delta\Delta G^{\ddagger}$ = 8.5 kcal/mol

TS22-s (*E* leading)
$\Delta\Delta G^{\ddagger}$ = 5.2 kcal/mol

TS21-s minus **TS22-s** = 3.3 kca/ml; selectivity = 99.6% *E*



TS23-s (*Z* leading)
$\Delta\Delta G^{\ddagger}$ = 0.0 kcal/mol

TS24-s (*E* leading)
$\Delta\Delta G^{\ddagger}$ = 3.5 kcal/mol

TS24-s minus **TS23-s** = 3.5 kca/ml; selectivity = 99.7% *Z*

Figure S4. Turnover-limiting TSs involving **sub3** of two different mechanisms: the Rh-bound proton transfer/reductive elimination (top) and the C_{β}-bound proton transfer/1,2 β-hydrogen shift of Fischer carbene (bottom). Energies are relative to **TS23-s**.

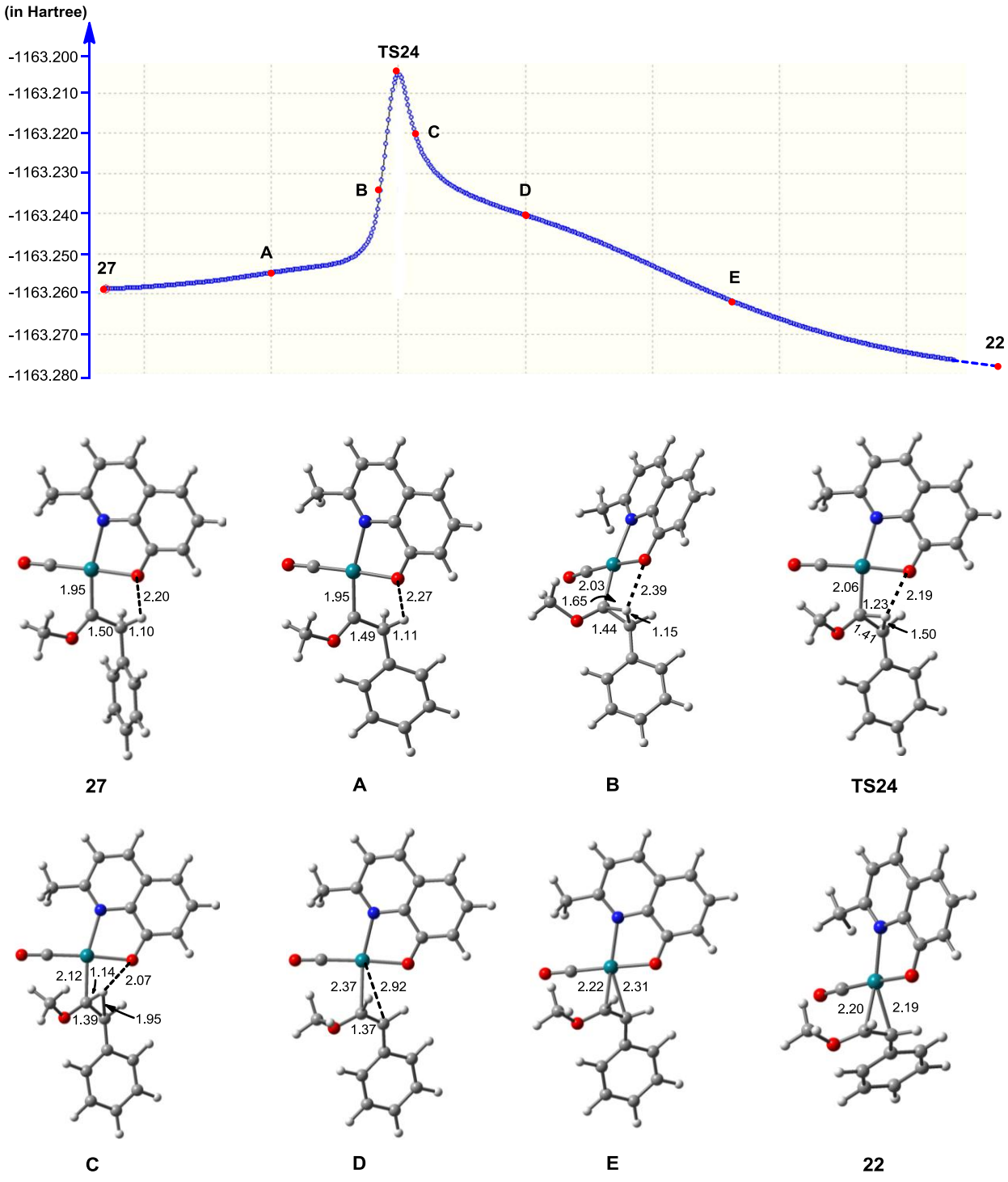


Figure S5. Confirming the **27** → **TS24** → **22** step in Figure 7 by IRC calculation at M06/BS1 level.

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

1cat = 1
SCF energy in gas phase: -852.6933048 a.u.
Enthalpy in gas phase: -852.5021158 a.u.
Free energy in gas phase: -852.5608478 a.u.
SCF energy in solution: -852.9241822 a.u.
Enthalpy in solution: -852.7329932 a.u.
Free energy in solution: -852.7917252 a.u.

Rh	-1.33190200	-0.27185100	0.00407000
C	2.14476100	2.55188400	0.00370700
C	3.18770300	1.66391800	-0.01471600
C	2.93305500	0.27847500	-0.01330200
C	1.57100100	-0.11861800	0.00087000
C	0.80909500	2.09316200	0.01958200
H	4.99056900	-0.39069700	-0.03469800
H	2.32519400	3.62450800	0.00732400
H	4.21935100	2.01612400	-0.02717600
C	3.94766600	-0.70278600	-0.02304600
C	1.21705500	-1.49952200	0.00763800
C	2.24769800	-2.43512900	-0.00015000
C	3.59194600	-2.03325600	-0.01607600
H	1.97770800	-3.48924500	0.00642400
H	4.36698600	-2.79840100	-0.02277000
N	0.53394100	0.78905200	0.01293200
O	-0.04653200	-1.84567400	0.02271800
C	-0.29803100	3.09582400	0.04710800
H	-0.91385700	3.03860000	-0.85929600
H	-0.95426800	2.94122300	0.91203400
H	0.10420600	4.11241300	0.11061500
C	-2.56558200	1.12434700	-0.03408100
O	-3.37428300	1.94606500	-0.06541900
C	-2.75611100	-1.49829200	0.00556700
O	-3.59161100	-2.28347000	0.00960500

TS1
SCF energy in gas phase: -1160.825811 a.u.
Enthalpy in gas phase: -1160.518187 a.u.
Free energy in gas phase: -1160.595988 a.u.
SCF energy in solution: -1161.151078 a.u.
Enthalpy in solution: -1160.843454 a.u.
Free energy in solution: -1160.921255 a.u.

Rh	-0.23012200	-0.76783900	0.49448900
C	4.19737500	-1.06980400	-0.93047300
C	4.57025100	0.24486600	-0.83615900
C	3.64884600	1.21687800	-0.38573900
C	2.34832900	0.74943300	-0.04718500
C	2.88266900	-1.45705600	-0.57756800
H	4.95416700	2.93796000	-0.52245100
H	4.89775700	-1.82881100	-1.27464600
H	5.57998900	0.55743400	-1.10428000
C	3.95703800	2.58721600	-0.26032200
C	1.34773900	1.65847600	0.42883600
C	1.70036200	3.00270800	0.53655400
C	2.98406000	3.45076100	0.19363400
H	0.94740000	3.69828300	0.90262200
H	3.21089700	4.51153500	0.29561400
N	2.00099800	-0.56698800	-0.15211600
O	0.14830200	1.23885500	0.75372900
C	2.45695100	-2.88805300	-0.67719900
H	2.10375500	-3.25906300	0.29409000
H	1.63027700	-3.00827100	-1.39179600
H	3.28254000	-3.52826100	-1.00765300
C	-0.69920300	-2.54805900	0.24806200
O	-0.98505400	-3.65029600	0.06608700
C	-0.87973700	-0.79199300	2.27028900
O	-1.27295800	-0.76346100	3.35122800
C	-1.58945300	0.02741600	-1.42071500
C	-0.49364300	-0.35000600	-1.83145500
H	0.36774700	-0.52887400	-2.44617900
C	-2.88627700	0.50646700	-1.05224500
C	-4.03271400	-0.07099400	-1.61373700
C	-3.00918300	1.57319400	-0.14822200
C	-5.28887300	0.41075900	-1.26923500
H	-3.92550800	-0.89576700	-2.31634100
C	-4.26916800	2.04650200	0.18502400
H	-2.10316800	1.99490200	0.28690900
C	-5.40879100	1.46782000	-0.37146500
H	-6.17865500	-0.04164500	-1.70327600
H	-4.36543600	2.87035300	0.88976500
H	-6.39502800	1.84192200	-0.10203700

2
SCF energy in gas phase: -1160.82636 a.u.
Enthalpy in gas phase: -1160.518193 a.u.
Free energy in gas phase: -1160.599109 a.u.
SCF energy in solution: -1161.150711 a.u.
Enthalpy in solution: -1160.842544 a.u.
Free energy in solution: -1160.92346 a.u.

Rh	-0.26411800	-0.72502800	0.38658700
C	4.24005200	-1.15399000	-0.84132500
C	4.63262700	0.15785400	-0.78618500
C	3.71617300	1.16341500	-0.40217500
C	2.39836300	0.73017100	-0.08576700
C	2.90925600	-1.50329100	-0.51039200
H	5.05285700	2.85819000	-0.56772400
H	4.93647800	-1.93728500	-1.13576500
H	5.65504800	0.44287000	-1.03683200
C	4.04261000	2.53299800	-0.32327500
C	1.39337900	1.67416700	0.31373600
C	1.76620500	3.01624000	0.37734100
C	3.06890600	3.42874300	0.06208700
H	1.01226500	3.73920100	0.68337100
H	3.30965000	4.48946900	0.12634300
N	2.03601700	-0.58165600	-0.14500400
O	0.17706300	1.28804500	0.61109300
C	2.44818600	-2.92590800	-0.56686400
H	2.06025800	-3.24857900	0.40864200
H	1.63269900	-3.04336000	-1.29484700
H	3.26114800	-3.60199900	-0.85438600
C	-0.84989100	-2.47737000	0.18932300
O	-1.20085300	-3.56499100	0.03872600
C	-0.52890900	-0.75479900	2.29186500
O	-0.69097700	-0.71544000	3.42761900
C	-1.69697900	0.01568500	-1.27055100
C	-0.60391900	-0.31983900	-1.75809900
H	0.15879000	-0.40171600	-2.51327300
C	-3.00328900	0.48006900	-0.91269100
C	-4.14310800	-0.10123700	-1.48357300
C	-3.13829600	1.53829900	-0.00020600
C	-5.40405100	0.37022900	-1.14174900
H	-4.02696000	-0.92025200	-2.19157900
C	-4.40231800	2.00304200	0.32867700
H	-2.23620900	1.96629500	0.43719600
C	-5.53546700	1.42048600	-0.23761200
H	-6.28874000	-0.08484700	-1.58346300
H	-4.50763600	2.82264500	1.03709500
H	-6.52550700	1.78650600	0.02892000

TS2
SCF energy in gas phase: -1160.818447 a.u.
Enthalpy in gas phase: -1160.51122 a.u.
Free energy in gas phase: -1160.59009 a.u.
SCF energy in solution: -1161.143484a.u.
Enthalpy in solution: -1160.836257 a.u.
Free energy in solution: -1160.915127 a.u.

Rh	0.15769300	0.63282100	-0.48605300
C	-4.13178500	1.35142500	0.82331200
C	-4.62755400	0.07726800	0.75003000
C	-3.80065100	-0.98170200	0.31715900
C	-2.46414700	-0.64582900	-0.02609400
C	-2.78968600	1.61538200	0.46472500
H	-5.26126400	-2.56962800	0.48240300
H	-4.75655100	2.17832200	1.15526500
H	-5.66195700	-0.13493700	1.02204500
C	-4.23563700	-2.31999900	0.21485000
C	-1.55155100	-1.65203500	-0.47649000
C	-2.02608100	-2.96040300	-0.56145200

C	-3.34784500	-3.28002100	-0.21970300
H	-1.33692800	-3.72818200	-0.90837300
H	-3.67382400	-4.31624400	-0.30241600
N	-1.99049400	0.64091100	0.05039700
O	-0.32374500	-1.33317900	-0.79932500
C	-2.25232000	3.00600600	0.56275400
H	-1.42673400	3.05623100	1.28577800
H	-1.86563600	3.35088900	-0.40468900
H	-3.02814100	3.70711800	0.88921500
C	0.64475300	2.41150900	-0.35083600
O	0.99564800	3.51142200	-0.30844900
C	0.67373800	0.19058600	1.75070100
O	1.62022300	0.20201100	2.39299300
C	2.09530300	0.09905500	-1.32692700
C	1.33693900	0.49547200	-2.24038500
H	1.04189300	0.71536500	-3.25280900
C	3.17322200	-0.42448300	-0.53458900
C	4.25928700	0.38822000	-0.18788700
C	3.10151900	-1.73869200	-0.05251800
C	5.26471000	-0.11286500	0.62856700
H	4.29720000	1.41249200	-0.55708800
C	4.11487500	-2.23102500	0.75744800
H	2.23201700	-2.34243900	-0.31095300
C	5.19482100	-1.42039200	1.10135800
H	6.10706400	0.52111800	0.89970500
H	4.05861400	-3.25178400	1.13148600
H	5.98307300	-1.80857200	1.74412300

3

SCF energy in gas phase: -1047.56272 a.u.
Enthalpy in gas phase: -1047.263992 a.u.
Free energy in gas phase: -1047.335683 a.u.
SCF energy in solution: -1047.85459 a.u.
Enthalpy in solution: -1047.555862 a.u.
Free energy in solution: -1047.627553 a.u.

Rh	0.23428300	0.75942600	-0.67012900
C	-3.67041000	1.29123600	1.43809100
C	-4.23979800	0.06282800	1.23165700
C	-3.54037600	-0.92661100	0.51226100
C	-2.25291300	-0.57262800	0.03080400
C	-2.38151800	1.58104300	0.93662200
H	-5.04365200	-2.47857500	0.63066600
H	-4.19793500	2.06537600	1.99125400
H	-5.23383200	-0.16225600	1.61903700
C	-4.05497100	-2.21614500	0.25766100
C	-1.46917000	-1.50940800	-0.71169900
C	-2.01706600	-2.77056700	-0.93919400
C	-3.29044100	-3.11052600	-0.45853700
H	-1.42508600	-3.48547500	-1.50778100
H	-3.67844900	-4.10804700	-0.66158600
N	-1.69558700	0.66842700	0.25024700
O	-0.28606000	-1.16213600	-1.14643100
C	-1.79211300	2.93039200	1.18916300
H	-0.84571800	2.85386700	1.73798900
H	-1.59085400	3.46050200	0.25020700
H	-2.47650400	3.54614400	1.78266100
C	0.80261800	2.45781700	-0.26505400
O	1.23304900	3.51009500	-0.04454700
H	1.66219700	0.95493900	-3.17510500
C	1.76341700	0.64037800	-2.15103800
C	2.28515200	0.11462900	-1.15003800
C	3.08441200	-0.52229800	-0.14442500
C	2.64551200	-1.71790800	0.44366500
C	4.30330600	0.04462000	0.25052200
C	3.42694300	-2.33568900	1.40951100
H	1.69135300	-2.13497300	0.12337400
C	5.07522300	-0.58134300	1.22028400
H	4.63194700	0.97511900	-0.20969600
C	4.63915600	-1.77005200	1.79977800
H	3.08751300	-3.26508400	1.86338700
H	6.02158600	-0.13919100	1.52655800
H	5.24611300	-2.25778600	2.56074600

4

SCF energy in gas phase: -1047.547015 a.u.
Enthalpy in gas phase: -1047.248123 a.u.
Free energy in gas phase: -1047.32148 a.u.
SCF energy in solution: -1047.840166 a.u.
Enthalpy in solution: -1047.541274 a.u.
Free energy in solution: -1047.614631 a.u.

Rh	0.07328700	0.66863900	-0.42114000
C	4.36194900	1.19363800	0.83503000
C	4.80955300	-0.09960200	0.74710900
C	3.93488800	-1.12483900	0.33756100
C	2.60270600	-0.73923400	0.03592700
C	3.02367900	1.51047000	0.51977000
H	5.34014700	-2.76708800	0.44947200
H	5.02814400	1.99495900	1.14737200
H	5.84337400	-0.34720300	0.99011600
C	4.31659500	-2.47847700	0.21593500
C	1.63965100	-1.70511800	-0.39116300
C	2.06167300	-3.02944200	-0.49888400
C	3.38080500	-3.40085600	-0.19825500
H	1.33301100	-3.76836800	-0.82653800
H	3.66474100	-4.44793400	-0.29613300
N	2.17053600	0.56274500	0.13212900
O	0.41806500	-1.33201600	-0.66599800
C	2.56355900	2.92855500	0.62121300
H	1.75545200	3.03349400	1.35598800
H	2.18646400	3.29449600	-0.34180900
H	3.38597500	3.58222700	0.93074200
C	-0.33302800	2.46908400	-0.21477400
O	-0.63634100	3.57585500	-0.09922900
C	-1.68618200	0.38812700	-0.89810700
C	-2.92293600	0.10328400	-1.22254600
H	-3.15370100	0.19351500	-2.29005600
C	-3.99934600	-0.30968000	-0.31376100
C	-5.31795900	-0.33967400	-0.77616800
C	-3.73443300	-0.66935700	1.01416400
C	-6.35423500	-0.71051600	0.07263100
H	-5.52854300	-0.06605500	-1.81021800
C	-4.77239800	-1.03430400	1.85864000
H	-2.70394400	-0.67279500	1.37056600
C	-6.08593000	-1.05531400	1.39295400
H	-7.37655500	-0.73021000	-0.30140000
H	-4.55438600	-1.31187300	2.88870000
H	-6.89731400	-1.34629300	2.05774200

TS3

SCF energy in gas phase: -1047.491755 a.u.
Enthalpy in gas phase: -1047.196919 a.u.
Free energy in gas phase: -1047.267752 a.u.
SCF energy in solution: -1047.785326 a.u.
Enthalpy in solution: -1047.49049 a.u.
Free energy in solution: -1047.561323 a.u.

Rh	-0.20362500	0.65646100	0.66522300
C	-1.72522000	0.47310600	2.23585700
C	-2.18253600	-0.09729200	1.14848600
H	-1.72483400	-0.88156400	1.97248400
C	-3.13487300	-0.56650800	0.15659200
C	-2.79512900	-1.62514900	-0.69232900
C	-3.70885600	-2.06181800	-1.64135100
C	-4.94824900	-1.43554600	-1.75777300
C	-5.28029400	-0.37411300	-0.92024700
C	-4.37957100	0.06035000	0.04389400
H	-1.81288300	-2.08678600	-0.59176700
H	-3.45151900	-2.89043200	-2.29821800
H	-5.65981700	-1.77777700	-2.50725100
H	-6.24851500	0.11383800	-1.01448400
H	-4.62665000	0.88298800	0.71270700
C	3.72101300	1.45401800	-1.30264600
C	4.31688900	0.22732500	-1.18061800
C	3.63463300	-0.82780100	-0.54177500
C	2.33205800	-0.54306400	-0.05676200
C	2.41861500	1.67486200	-0.79988000
H	5.18245600	-2.32594100	-0.74154700
H	4.23659800	2.27960800	-1.78853100
H	5.32065100	0.05482300	-1.56976500
C	4.18202800	-2.11692100	-0.36607700
C	1.57103900	-1.54904300	0.61336100
C	2.15015100	-2.80537100	0.76828000
C	3.43766400	-3.07779900	0.28093900
H	1.57499000	-3.57187800	1.28433800
H	3.85302600	-4.07453300	0.42454700
O	0.37110700	-1.26103200	1.05498200
C	1.80045700	3.02658000	-0.94961200
H	0.90331500	2.98743900	-1.58040200
H	2.50579000	3.72643500	-1.41049700
H	1.50269900	3.43620700	0.02313000

N	1.74397000	0.69591200	-0.19995400
C	-0.86444000	2.33008500	0.27093800
O	-1.35513800	3.35103800	0.03179600

7

SCF energy in gas phase: -1047.506 a.u.
Enthalpy in gas phase: -1047.20815 a.u.
Free energy in gas phase: -1047.279367 a.u.
SCF energy in solution: -1047.7984 a.u.
Enthalpy in solution: -1047.50055 a.u.
Free energy in solution: -1047.571767 a.u.

Rh	-0.20664800	0.17997100	0.69007700
C	-1.57334100	-0.51883300	2.00373700
C	-1.98698100	-1.13948400	0.85508700
H	-1.48307300	-2.10880000	0.70258600
C	-3.17974200	-0.87637000	0.03454100
C	-3.32038500	-1.52500100	-1.19621700
C	-4.42391800	-1.27202500	-2.00062300
C	-5.39996400	-0.37203500	-1.58183600
C	-5.26995500	0.27218600	-0.35335500
C	-4.16831600	0.02297400	0.45299200
H	-2.54764600	-2.22180400	-1.52122500
H	-4.52340100	-1.77971100	-2.95842900
H	-6.26546100	-0.17357800	-2.21146700
H	-6.03472700	0.97097800	-0.01918100
H	-4.07111600	0.51678000	1.42016200
C	3.49733400	2.13496700	-0.94634600
C	4.33490300	1.05506100	-1.03641700
C	3.88890100	-0.21863100	-0.62883600
C	2.55760500	-0.30091700	-0.14513200
C	2.18075000	1.98491300	-0.45526300
H	5.70909500	-1.31068700	-1.04716200
H	3.82894100	3.12528900	-1.25104800
H	5.35029300	1.16758200	-1.41723000
C	4.68844800	-1.38064300	-0.67446600
C	2.02102600	-1.54597400	0.29905800
C	2.84527600	-2.66640900	0.24434400
C	4.15897900	-2.57556100	-0.23976100
H	2.44059900	-3.61546200	0.59066900
H	4.77041200	-3.47667200	-0.26607900
O	0.78830000	-1.59795300	0.73995600
C	1.29387900	3.18454800	-0.37378200
H	0.43955700	3.09467700	-1.05701200
H	1.84344400	4.09200000	-0.64615900
H	0.89922500	3.32049800	0.64024400
N	1.72525400	0.79333200	-0.07460700
C	-1.20981500	1.74832000	0.55265400
O	-1.88103100	2.68300300	0.46602300

TS4

SCF energy in gas phase: -1047.504933 a.u.
Enthalpy in gas phase: -1047.208263 a.u.
Free energy in gas phase: -1047.279006 a.u.
SCF energy in solution: -1047.796968 a.u.
Enthalpy in solution: -1047.500298 a.u.
Free energy in solution: -1047.571041 a.u.

Rh	-0.14372500	0.38210300	0.72408400
C	-1.64196000	-0.23492900	1.87820600
C	-2.12248200	-1.03426700	0.90045700
H	-1.57953400	-1.99207800	0.84318600
C	-3.30646300	-0.86786500	0.05963400
C	-3.55911200	-1.78967800	-0.96185800
C	-4.66864100	-1.63949000	-1.78345400
C	-5.53886500	-0.57127700	-1.58817900
C	-5.29820300	0.34776600	-0.56745300
C	-4.19102900	0.20295100	0.25386700
H	-2.87025600	-2.62083400	-1.11019000
H	-4.85571100	-2.36066600	-2.57682300
H	-6.41066600	-0.45550600	-2.22954500
H	-5.98294000	1.17874200	-0.40918000
H	-4.00972300	0.91223700	1.06151600
C	3.64900500	1.85176000	-1.19589200
C	4.40195200	0.70839400	-1.18323100
C	3.86446400	-0.48146100	-0.65042600
C	2.54006000	-0.41143800	-0.14639200
C	2.33382400	1.85351700	-0.67712600
H	5.58516500	-1.74986200	-0.98611900
H	4.04752600	2.77907600	-1.60238700
H	5.41722700	0.70404000	-1.58037200
C	4.56919700	-1.70352800	-0.59717900
C	1.91491500	-1.56365500	0.41674500
C	2.64422100	-2.74873300	0.44943400
C	3.95315600	-2.80865300	-0.05326600
H	2.17104700	-3.62827700	0.88212100
H	4.48905100	-3.75590000	-0.00676900
O	0.69282700	-1.47414100	0.88236900
C	1.53773300	3.11725400	-0.70672200
H	0.60969200	2.98758100	-1.27759300
H	2.10885200	3.92751500	-1.17264600
H	1.26398100	3.43737800	0.30657200
N	1.79757000	0.74665900	-0.16924400
C	-0.97482500	2.04080800	0.61271100
O	-1.53542400	3.05044500	0.58011900

TS5

SCF energy in gas phase: -1047.517109 a.u.
Enthalpy in gas phase: -1047.222159 a.u.
Free energy in gas phase: -1047.295085 a.u.
SCF energy in solution: -1047.814466 a.u.
Enthalpy in solution: -1047.519516 a.u.
Free energy in solution: -1047.592442 a.u.

Rh	-0.24417000	-0.68155400	-0.01643700
C	-4.69710700	-1.10208100	0.00555100
C	-5.07691400	0.21294000	0.01585100
C	-4.09859500	1.22881400	0.02186500
C	-2.74313700	0.80821300	0.01543700
C	-3.32818500	-1.45511600	-0.00145100
H	-5.45034300	2.91854200	0.03812100
H	-5.43909900	-1.89790200	0.00218800
H	-6.13169300	0.48931100	0.02038500
C	-4.40703500	2.60646100	0.03423400
C	-1.68294700	1.77007700	0.02397900
C	-2.03489000	3.11863100	0.03689900
C	-3.37806000	3.52203500	0.04128500
H	-1.23136400	3.85304500	0.04329500
H	-3.60592300	4.58753100	0.05067300
N	-2.38078000	-0.52083000	0.00181600
O	-0.44081800	1.36513100	0.01952600
C	-2.94972400	-2.90061600	-0.01158800
H	-2.36181800	-3.15267500	-0.90270600
H	-2.34468900	-3.15977800	0.86595600
H	-3.84299400	-3.53510300	-0.00581900
C	0.06001300	-2.48723000	-0.05210700
O	0.31650100	-3.61857900	-0.07653600
H	1.82550000	0.80550400	0.05881700
C	1.70717200	-0.37021600	-0.02278700
C	2.94192300	-0.12849300	-0.03050700
C	4.32572900	0.21320300	-0.01039500
C	4.98811200	0.55045800	-1.20160300
C	5.03139600	0.19961400	1.20349800
C	6.33625000	0.87325300	-1.17338200
H	4.42870500	0.55179000	-2.13514400
C	6.38088700	0.51769200	1.22158100
H	4.50342800	-0.06557300	2.11746900
C	7.02964100	0.85550900	0.03547600
H	6.85188300	1.13658900	-2.09447400
H	6.93034600	0.50544800	2.16045000
H	8.08853900	1.10768500	0.05280400

TS6

SCF energy in gas phase: -1047.511467 a.u.
Enthalpy in gas phase: -1047.216691 a.u.
Free energy in gas phase: -1047.28933 a.u.
SCF energy in solution: -1047.816506 a.u.
Enthalpy in solution: -1047.52173 a.u.
Free energy in solution: -1047.594369 a.u.

Rh	-0.20140300	-0.56552000	0.03828100
C	-4.63418300	-1.31331000	-0.07205100
C	-5.10329600	-0.02523300	-0.06842700
C	-4.19945500	1.05480900	-0.03659100
C	-2.81935700	0.72720100	-0.00881400
C	-3.24670500	-1.57183800	-0.04381900
H	-5.65407900	2.65730300	-0.04653700
H	-5.32054600	-2.15694800	-0.09481100
H	-6.17445000	0.17680200	-0.08795700
C	-4.59399300	2.41001900	-0.02669800
C	-1.82585100	1.74977100	0.02618900
C	-2.25792600	3.07290100	0.04054700

C	-3.62531600	3.38841100	0.01198100
H	-1.50219300	3.85512900	0.06924200
H	-3.91995800	4.43686900	0.02149600
N	-2.36633400	-0.57137200	-0.01287700
O	-0.55548500	1.42476400	0.02965900
C	-2.76669800	-2.98684800	-0.04096800
H	-2.15384400	-3.20630600	-0.92423300
H	-2.16250300	-3.20047700	0.84972900
H	-3.61264400	-3.68228300	-0.04453100
C	0.23825700	-2.37548300	0.00048100
O	0.56909300	-3.47686000	-0.02101100
H	0.62189700	-0.43803500	1.35148500
C	1.73074800	-0.20920100	-0.02556900
C	2.93583400	0.00703900	0.00729600
C	4.33065300	0.29095700	-0.01647600
C	4.78855100	1.61713800	-0.06447200
C	5.27038500	-0.75163200	0.01429600
C	6.14932300	1.88863900	-0.07988500
H	4.05753000	2.42333800	-0.08918300
C	6.62951000	-0.47260400	-0.00208000
H	4.91420400	-1.77989200	0.05056600
C	7.07335500	0.84664900	-0.04858600
H	6.49293100	2.92116600	-0.11647000
H	7.34893300	-1.28958800	0.02209400
H	8.14031500	1.06338000	-0.06069100

8

SCF energy in gas phase: -1047.515234 a.u.
Enthalpy in gas phase: -1047.218561 a.u.
Free energy in gas phase: -1047.291041 a.u.
SCF energy in solution: -1047.822496 a.u.
Enthalpy in solution: -1047.525823 a.u.
Free energy in solution: -1047.598303 a.u.

Rh	-0.19856600	-0.55538000	-0.02479500
C	-4.63137600	-1.33450100	0.06394600
C	-5.10964700	-0.04975900	0.05723500
C	-4.21272800	1.03661700	0.02205400
C	-2.83122200	0.71755400	-0.00556600
C	-3.24142300	-1.58252600	0.03493300
H	-5.67428300	2.63306000	0.03251400
H	-5.31121300	-2.18332800	0.09200200
H	-6.18203500	0.14487400	0.08064500
C	-4.61307000	2.39045100	0.01380300
C	-1.84328900	1.74577200	-0.03553000
C	-2.27972700	3.06636200	-0.03783700
C	-3.64964900	3.37416800	-0.01700400
H	-1.52795600	3.85245900	-0.06170400
H	-3.95004700	4.42093400	-0.02289000
N	-2.37108800	-0.57540000	-0.00424400
O	-0.57064600	1.42325100	-0.07111400
C	-2.74268700	-2.99103800	0.05462100
H	-2.13743400	-3.21585400	-0.83248400
H	-2.12322600	-3.18096900	0.94095800
H	-3.57814400	-3.69873800	0.07519200
C	0.29591100	-2.35009200	-0.11479200
O	0.65243800	-3.44100300	-0.16462300
H	-0.07136000	-0.69363800	1.49135600
C	1.73194600	-0.19991600	-0.01600500
C	2.93761100	0.00958700	0.01177800
C	4.33356100	0.29496000	0.01677900
C	4.79238900	1.62116200	-0.01750400
C	5.27480000	-0.74570100	0.05910000
C	6.15305400	1.89439800	-0.00880100
H	4.06118100	2.42696700	-0.05091400
C	6.63402800	-0.46564500	0.06746600
H	4.91952800	-1.77466500	0.08522800
C	7.07811900	0.85381300	0.03383800
H	6.49569400	2.92770100	-0.03515500
H	7.35347800	-1.28246300	0.10093800
H	8.14497000	1.07160600	0.04060600

TS8

SCF energy in gas phase: -1163.176017 a.u.
Enthalpy in gas phase: -1162.824202 a.u.
Free energy in gas phase: -1162.902948 a.u.
SCF energy in solution: -1163.514171 a.u.
Enthalpy in solution: -1163.162356 a.u.
Free energy in solution: -1163.241102 a.u.

Rh	-0.38011100	-0.64967900	-0.15956700
C	-4.86623100	-1.07642100	-0.01634400
C	-5.24413500	0.24077400	0.00726400
C	-4.26746400	1.25765800	-0.01541000
C	-2.91306500	0.83509900	-0.06210200
C	-3.49829100	-1.42676900	-0.06220200
H	-5.61086200	2.95417100	0.03860400
H	-5.60892500	-1.87147600	0.00011400
H	-6.29852800	0.51640600	0.04276300
C	-4.56989800	2.63641300	0.00429300
C	-1.84787900	1.79024900	-0.09201200
C	-2.19428900	3.13962700	-0.06877200
C	-3.53626700	3.54691000	-0.02248200
H	-1.38850100	3.87074400	-0.09341200
H	-3.75933200	4.61320900	-0.00817200
N	-2.55458700	-0.48994600	-0.08470900
O	-0.60625100	1.38370600	-0.14844300
C	-3.10642700	-2.86961800	-0.08054100
H	-2.49432100	-3.12508300	0.79392100
H	-2.51993400	-3.11354200	-0.97502900
H	-3.99197800	-3.51452700	-0.07229300
C	-0.02844700	-2.45928000	-0.17341500
O	0.23396700	-3.58704800	-0.18683500
C	1.60004800	-0.31683900	-0.04224400
C	2.65175500	-0.09766200	-0.83153600
H	2.44824100	-0.28793200	-1.88798800
C	4.01095200	0.35354400	-0.51347400
C	5.05490200	0.00205000	-1.38006800
C	4.31353000	1.15173400	0.59948600
C	6.36026800	0.40517900	-1.13137900
H	4.82846600	-0.60185000	-2.25943100
C	5.61985400	1.55650300	0.84524100
H	3.51067200	1.47651100	1.25846900
C	6.64988100	1.18152700	-0.01308600
H	7.15540200	0.11474400	-1.81643000
H	5.83378200	2.18148900	1.71120200
H	7.67165100	1.50209600	0.18302700
H	0.44420000	-0.45870100	1.35950800
O	1.71800700	-0.17185000	1.43262900
C	2.47878100	-1.21623900	2.05915400
H	3.53154100	-1.10279500	1.78268600
H	2.10844000	-2.19900400	1.73672700
H	2.35584400	-1.09439400	3.13816400

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SCF energy in gas phase: -1163.214131 a.u.
Enthalpy in gas phase: -1162.859244 a.u.
Free energy in gas phase: -1162.93766 a.u.
SCF energy in solution: -1163.554782 a.u.
Enthalpy in solution: -1163.199895 a.u.
Free energy in solution: -1163.278311 a.u.

Rh	0.25918700	0.55104000	0.41394300
C	4.56663700	1.48828400	-0.73871700
C	5.06901900	0.21971200	-0.86964900
C	4.23105300	-0.89672500	-0.66968100
C	2.88109700	-0.62366100	-0.32916800
C	3.20907300	1.68518900	-0.39949800
H	5.70215000	-2.43968800	-1.04870500
H	5.19956100	2.35964700	-0.89333500
H	6.11575800	0.05899400	-1.12888900
C	4.66442700	-2.23532800	-0.78978700
C	1.95645800	-1.68878800	-0.10514500
C	2.42443100	-2.99202200	-0.23454200
C	3.76209200	-3.25263100	-0.57435000
H	1.72030400	-3.80559300	-0.07123600
H	4.08618900	-4.28842400	-0.66539800
N	2.39810700	0.65122800	-0.20118200
O	0.70687900	-1.41821300	0.19918700
C	2.66871600	3.07206400	-0.25971900
H	1.86010100	3.25668800	-0.97886500
H	2.26274000	3.23794400	0.74650400
H	3.45031600	3.81924300	-0.43437900
C	-0.28133600	2.31610600	0.62011300
O	-0.63020100	3.40109500	0.77976200
C	-1.68396500	0.04935400	0.73092600
C	-2.53667300	0.43908800	-0.24876100
H	-2.15322100	1.18227800	-0.95286400
C	-3.89987200	-0.00568600	-0.53242700
C	-4.58389200	0.61054700	-1.59343000
C	-4.57293500	-1.01087500	0.18195100
C	-5.88204500	0.25078800	-1.92548800

H	-4.07758800	1.39218700	-2.16216400
C	-5.87085600	-1.37111100	-0.15523900
H	-4.06905000	-1.50605500	1.00725900
C	-6.53596200	-0.74523200	-1.20616800
H	-6.38610900	0.75146300	-2.75139700
H	-6.37119500	-2.15436700	0.41335200
H	-7.55500400	-1.03092700	-1.46219200
O	-2.11259600	-0.70194900	1.75424200
C	-1.19285400	-1.37850200	2.58823000
H	-0.54861700	-2.04747500	2.00850800
H	-0.56508300	-0.65682800	3.13506600
H	-1.79599700	-1.94236100	3.30481600
H	0.60626000	0.62698900	1.91252700

TS9

SCF energy in gas phase: -1163.21247 a.u.
Enthalpy in gas phase: -1162.858707 a.u.
Free energy in gas phase: -1162.936277 a.u.
SCF energy in solution: -1163.545771 a.u.
Enthalpy in solution: -1163.192008 a.u.
Free energy in solution: -1163.269578 a.u.

Rh	-0.30295500	0.44629900	-0.54569900
C	-4.31759200	1.80839400	1.04059900
C	-5.03972800	0.64913500	0.92306700
C	-4.42701300	-0.52144300	0.43305500
C	-3.05755400	-0.41826000	0.07317000
C	-2.95817300	1.84355000	0.66189300
H	-6.14860600	-1.82665400	0.56690300
H	-4.77635600	2.71639400	1.42636800
H	-6.09073600	0.61782100	1.21168600
C	-5.09744400	-1.75559300	0.29229000
C	-2.34191900	-1.55393200	-0.41998700
C	-3.04497800	-2.75153600	-0.54070400
C	-4.40035000	-2.84149100	-0.18911300
H	-2.50876500	-3.62036700	-0.91783100
H	-4.90656000	-3.79943400	-0.30246000
N	-2.35499900	0.75688900	0.18447100
O	-1.07738900	-1.44613300	-0.73286100
C	-2.19114600	3.11908100	0.79796900
H	-1.25972500	2.96615100	1.35602100
H	-1.92759900	3.53031900	-0.18526800
H	-2.78277500	3.87486400	1.32564000
C	0.35917800	2.16786300	-0.61417400
O	0.79741200	3.23053700	-0.71766100
C	1.59212400	-0.21726100	-0.14148000
C	2.76896300	0.36642100	-0.45075700
H	2.72970200	1.21929300	-1.12860500
C	4.11044600	0.02424200	0.02270400
C	5.19889700	0.64682100	-0.60774300
C	4.38100900	-0.86480200	1.07562000
C	6.50540700	0.38037300	-0.22238400
H	5.00642300	1.35068000	-1.41839800
C	5.68893300	-1.12559100	1.46251300
H	3.55442800	-1.33811700	1.59973100
C	6.75786900	-0.51131500	0.81553700
H	7.33034400	0.87484700	-0.73328900
H	5.87478300	-1.81647000	2.28378800
H	7.78097200	-0.72268500	1.12197200
O	1.48643900	-1.31682800	0.62772400
C	1.65812100	-2.55293200	-0.06831500
H	0.85957700	-2.66889000	-0.80977600
H	2.64727100	-2.58658900	-0.54621700
H	1.58083200	-3.34119600	0.68510000
H	0.63274900	0.09741800	-1.75040000

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SCF energy in gas phase: -1163.272532 a.u.
Enthalpy in gas phase: -1162.912877 a.u.
Free energy in gas phase: -1162.98903 a.u.
SCF energy in solution: -1163.603881 a.u.
Enthalpy in solution: -1163.244226 a.u.
Free energy in solution: -1163.320379 a.u.

Rh	0.07878900	0.99712100	-0.16652600
C	-4.20378600	0.56012900	1.09618100
C	-4.41701100	-0.76622700	0.82944800
C	-3.38120700	-1.55015600	0.28236700
C	-2.14743800	-0.89133500	0.03967100
C	-2.95140500	1.15701000	0.82792500
H	-4.46325700	-3.42041100	0.16676800
H	-4.99371900	1.17764300	1.51852900
H	-5.38353000	-1.22783900	1.03390900
C	-3.51403400	-2.92170100	-0.02281700
C	-1.03574500	-1.60094500	-0.51076800
C	-1.21236700	-2.95440800	-0.79689200
C	-2.43570800	-3.59543200	-0.55347400
H	-0.36846600	-3.50071700	-1.21419900
H	-2.52797800	-4.65466500	-0.79131800
N	-1.95145000	0.44363200	0.31310800
O	0.08673800	-0.97268800	-0.72960900
C	-2.76167700	2.60781500	1.13061000
H	-1.96758200	2.75916600	1.87206000
H	-2.48896100	3.17145300	0.22995800
H	-3.68363000	3.04180800	1.53270100
C	0.10955400	2.78044500	0.25312000
O	0.21732900	3.91295600	0.48211200
C	1.88487400	1.25097000	-1.44615300
C	2.29496400	1.06779600	-0.12138400
H	2.51809900	1.99753200	0.40692300
C	2.89827000	-0.11253300	0.51099500
C	3.43182300	0.05756300	1.79663200
C	2.98886000	-1.37755800	-0.08911700
C	4.04310400	-0.99327700	2.46628400
H	3.36184000	1.03664000	2.27315300
C	3.60334200	-2.42523000	0.58312000
H	2.55547200	-1.52979700	-1.07197300
C	4.13301900	-2.24155300	1.85806000
H	4.45278800	-0.83668200	3.46293000
H	3.66802700	-3.40138400	0.10450300
H	4.61498000	-3.06961300	2.37561400
O	2.04607500	0.29793200	-2.38278300
C	1.20961800	0.43528300	-3.51390900
H	0.16951100	0.20833500	-3.24571000
H	1.27210900	1.45560100	-3.92455400
H	1.56582200	-0.27848200	-4.26048600
H	1.78967800	2.27000600	-1.84405200

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SCF energy in gas phase: -1471.419728 a.u.
Enthalpy in gas phase: -1470.942896 a.u.
Free energy in gas phase: -1471.036116 a.u.
SCF energy in solution: -1471.84562 a.u.
Enthalpy in solution: -1471.368788 a.u.
Free energy in solution: -1471.462008 a.u.

Rh	0.56037100	0.91963700	0.11769700
C	-3.79581800	1.91228300	-1.25643600
C	-4.17565000	0.69690300	-1.76362900
C	-3.26865600	-0.38662400	-1.77911700
C	-1.98008700	-0.13908600	-1.23048600
C	-2.48914400	2.08103500	-0.74225400
H	-4.56653500	-1.84427900	-2.71762600
H	-4.48389400	2.75618300	-1.24462900
H	-5.17874700	0.55152300	-2.16663900
C	-3.57904000	-1.66241600	-2.29544300
C	-0.99439600	-1.18270000	-1.17120500
C	-1.34291400	-2.41947000	-1.71629100
C	-2.61395200	-2.64579700	-2.26337200
H	-0.60327700	-3.21815700	-1.67599800
H	-2.83980700	-3.63293100	-2.66680500
N	-1.62771200	1.07891600	-0.73376600
O	0.16250000	-0.98101300	-0.60065800
C	-2.04050800	3.40156400	-0.19716700
H	-1.79392100	3.32689100	0.87145900
H	-1.13218200	3.74705400	-0.70997300
H	-2.81439400	4.16888800	-0.31445300
C	1.10035900	2.54648100	0.77478600
O	1.43639700	3.57394400	1.19218900
C	1.07541800	-0.06647900	2.14642700
C	-0.27314200	0.30846800	2.12271600
H	-0.45738500	1.28027500	2.58840100
C	-1.47232400	-0.53691500	2.03732500
C	-2.71546300	0.08598700	2.22429800
C	-1.45398200	-1.90767500	1.74836600
C	-3.90177900	-0.62362200	2.11081900
H	-2.74339300	1.15402300	2.44890200
C	-2.64444900	-2.61619400	1.63353500
H	-0.50443600	-2.40399200	1.57333700
C	-3.87013000	-1.98275100	1.80885500
H	-4.85415800	-0.11443300	2.25236000
H	-2.61033700	-3.67626200	1.38558200

H	-4.79777200	-2.54406800	1.70872500
O	1.48316600	-1.34390700	2.05707500
C	2.88772000	-1.50411900	2.09095900
H	3.36559300	-0.88461200	1.31978000
H	3.28396000	-1.23496800	3.08200100
H	3.09543800	-2.55747200	1.88804700
H	1.80302800	0.61722900	2.59714100
C	2.28761400	0.79399300	-1.37626700
C	1.31056100	1.39611600	-1.85823000
H	0.74460000	1.89457100	-2.62721900
C	3.48157600	0.05169000	-1.11146300
C	4.63407100	0.68398600	-0.62329400
C	3.49485200	-1.33138300	-1.35038200
C	5.78416700	-0.05730300	-0.38661200
H	4.61084600	1.75674400	-0.43360200
C	4.65305500	-2.06086900	-1.11563300
H	2.57908500	-1.80901900	-1.69535800
C	5.79806300	-1.42868300	-0.63499400
H	6.67766300	0.43790200	-0.01007900
H	4.66142800	-3.13291700	-1.30563900
H	6.70327800	-2.00497900	-0.45142000

TS10

SCF energy in gas phase: -1163.182101 a.u.
Enthalpy in gas phase: -1162.830642 a.u.
Free energy in gas phase: -1162.909548 a.u.
SCF energy in solution: -1163.518764 a.u.
Enthalpy in solution: -1163.167305 a.u.
Free energy in solution: -1163.246211 a.u.

Rh	-0.02678400	0.46174700	-0.50614100
C	4.03201600	1.84766300	0.87990900
C	4.66160500	0.64537100	1.06794300
C	3.97292400	-0.55961600	0.81831900
C	2.62983200	-0.44331700	0.37436200
C	2.69128100	1.89091000	0.43578800
H	5.57851600	-1.91867300	1.32752300
H	4.55008700	2.78597000	1.06749600
H	5.69641300	0.60597900	1.40925400
C	4.54762300	-1.83804500	0.98627300
C	1.85029900	-1.60991900	0.09227400
C	2.45886800	-2.84951100	0.27290500
C	3.78754400	-2.95340000	0.71350100
H	1.86943300	-3.74045900	0.06377700
H	4.22134800	-3.94462700	0.84085600
N	2.01591300	0.77122700	0.19343900
O	0.61029500	-1.48677700	-0.31364300
C	2.02430200	3.21275900	0.23051300
H	1.15081500	3.32466200	0.88516500
H	1.67565400	3.32204000	-0.80404200
H	2.71422700	4.03600100	0.44538100
C	-0.73458800	2.15649700	-0.70527000
O	-1.21271000	3.19984700	-0.83578200
C	-1.72144200	-0.23626900	-1.33352900
C	-2.98210300	-0.58076800	-1.07617100
H	-3.60801200	-0.92063100	-1.90824500
C	-3.61986300	-0.49109800	0.23701000
C	-5.01403400	-0.38995000	0.31573100
C	-2.88303400	-0.50674500	1.43038000
C	-5.65399500	-0.27643000	1.54354700
H	-5.59796600	-0.38969400	-0.60557400
C	-3.52382700	-0.38862600	2.65691600
H	-1.80131500	-0.64114800	1.38272600
C	-4.91034000	-0.26918300	2.71962300
H	-6.73913800	-0.19330000	1.58254300
H	-2.93604900	-0.40476800	3.57377100
H	-5.40910500	-0.18214200	3.68362500
O	-1.24466800	-0.39160400	-2.72705800
C	-1.01675800	-1.76286200	-3.10681100
H	-1.98466800	-2.26397700	-3.20622400
H	-0.40441900	-2.25493800	-2.34192600
H	-0.50802500	-1.73951600	-4.07399500
H	-0.17510100	0.18551800	-2.20727200

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SCF energy in gas phase: -1163.225717 a.u.
Enthalpy in gas phase: -1162.871294 a.u.
Free energy in gas phase: -1162.947023 a.u.
SCF energy in solution: -1163.554652 a.u.
Enthalpy in solution: -1163.200229 a.u.
Free energy in solution: -1163.275958 a.u.

Rh	-0.46311700	0.51559300	0.52751100
C	2.93895700	-2.44244000	1.05163700
C	3.94598900	-1.78507400	0.39526200
C	3.69881500	-0.53756000	-0.21768300
C	2.37983800	-0.02439900	-0.09903500
C	1.64941900	-1.86853300	1.13491900
H	5.68199000	-0.20398700	-1.01743000
H	3.11225900	-3.41003300	1.51870900
H	4.94436500	-2.21888600	0.33139400
C	4.67203800	0.19374800	-0.93079600
C	2.02038100	1.22036400	-0.70891000
C	3.01444500	1.90627400	-1.40366200
C	4.31638400	1.39402600	-1.50656100
H	2.74773400	2.85173700	-1.87226300
H	5.06022100	1.96529000	-2.06072100
N	1.39504200	-0.68952100	0.58151700
O	0.79284600	1.67013400	-0.61849700
C	0.54884300	-2.59104600	1.84288700
H	-0.29894300	-2.77253300	1.16715700
H	0.17553500	-2.00679900	2.69427700
H	0.89459900	-3.55795700	2.22466500
C	-1.66682800	-0.38379500	1.62025800
O	-2.42156900	-0.91088700	2.31063600
C	-2.01642600	1.76471700	0.04954200
C	-2.93183500	1.23673300	-0.79599000
H	-3.81664300	1.80860100	-1.08459600
C	-2.75964800	-0.14339100	-1.23642800
C	-3.81348700	-1.07060300	-1.21109400
C	-1.47316000	-0.61753000	-1.58075800
C	-3.57551900	-2.41943300	-1.42698000
H	-4.81655400	-0.72258200	-0.96496200
C	-1.23671700	-1.98327800	-1.77431200
H	-0.69155600	0.10628800	-1.83047900
C	-2.28234100	-2.88960400	-1.68142700
H	-4.40397100	-3.12490400	-1.37663800
H	-0.22999300	-2.32064500	-2.02216700
H	-2.10775200	-3.95281500	-1.83611000
C	-1.09206700	3.72253300	1.01135600
H	-0.28899300	3.73116900	0.26502800
H	-0.70429000	3.29256500	1.94824700
H	-1.44951100	4.73797500	1.20280400
O	-2.21164800	2.99248700	0.54964800
H	-0.03302100	1.31837500	1.77683400

TS11

SCF energy in gas phase: -1163.208265 a.u.
Enthalpy in gas phase: -1162.855032 a.u.
Free energy in gas phase: -1162.929987 a.u.
SCF energy in solution: -1163.543554 a.u.
Enthalpy in solution: -1163.190321 a.u.
Free energy in solution: -1163.265276 a.u.

Rh	-0.09530400	0.57906400	0.60463200
C	2.50300200	-3.09034500	0.23408100
C	3.68319300	-2.52091900	-0.16739400
C	3.76721000	-1.12763700	-0.36112100
C	2.58614000	-0.38059900	-0.11042000
C	1.36454400	-2.28905700	0.47352400
H	5.83920000	-1.04396900	-0.98161000
H	2.42228000	-4.16588000	0.37660100
H	4.56388600	-3.13712100	-0.35054400
C	4.93630200	-0.46550500	-0.79295500
C	2.56022300	1.03355400	-0.30777600
C	3.73512300	1.64491600	-0.74159900
C	4.90081500	0.89976500	-0.97392400
H	3.71929300	2.72157400	-0.89910500
H	5.79620900	1.42122900	-1.31013200
N	1.41666300	-0.96738000	0.31278700
O	1.45909500	1.70298500	-0.08882000
C	0.09391100	-2.94081300	0.91421200
H	-0.75225800	-2.65728900	0.27388900
H	-0.16092600	-2.66037300	1.94423200
H	0.18985900	-4.03160100	0.88380900
C	-1.46057700	-0.38105500	1.43061200
O	-2.27028300	-0.92423500	2.04607000
C	-1.38651500	1.99023800	-0.22652300
C	-2.56164200	1.63499500	-0.78142400
H	-3.10112100	2.45110600	-1.27122700
C	-3.14855700	0.29324800	-0.87451600
C	-4.46387900	0.06756700	-0.45147100

C	-2.42882000	-0.78635000	-1.40861500
C	-5.02337600	-1.20296700	-0.50682900
H	-5.03882500	0.90198300	-0.04936600
C	-2.99151400	-2.05745800	-1.47202200
H	-1.42135100	-0.61167100	-1.78871500
C	-4.28634100	-2.27253100	-1.00968900
H	-6.04058700	-1.36132700	-0.15183800
H	-2.41862800	-2.88102300	-1.89795500
H	-4.72728300	-3.26692100	-1.05638500
C	-0.49395700	4.02364100	0.62149700
H	0.35505100	3.55183100	1.13452900
H	-1.31811900	4.19920500	1.32991700
H	-0.16984200	4.97832800	0.19950700
O	-0.92423100	3.23229900	-0.46496200
H	-0.79314800	1.78117400	1.35227800

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SCF energy in gas phase: -1163.2743 a.u.
Enthalpy in gas phase: -1162.91568 a.u.
Free energy in gas phase: -1162.993528 a.u.
SCF energy in solution: -1163.606396 a.u.
Enthalpy in solution: -1163.247776 a.u.
Free energy in solution: -1163.325624 a.u.

Rh	-0.19974800	-0.08885500	-0.34439700
C	3.39144100	2.60405700	-0.41561900
C	4.33267300	1.78649800	0.15097400
C	3.97962100	0.48640100	0.56523500
C	2.62993600	0.09811600	0.35803200
C	2.06341800	2.15562800	-0.59704000
H	5.91879000	-0.11182100	1.31612800
H	3.64794400	3.61158300	-0.73623400
H	5.35796200	2.13051300	0.29005200
C	4.88494300	-0.41692900	1.16210300
C	2.17415900	-1.19661900	0.75705100
C	3.10262000	-2.05587500	1.34270600
C	4.43540800	-1.66411400	1.53686200
H	2.75883900	-3.04239800	1.64797600
H	5.12683400	-2.36894900	1.99734600
N	1.69911400	0.93074400	-0.22223500
O	0.92572500	-1.52953100	0.56622500
C	1.06628800	3.07994400	-1.21675400
H	0.21869700	3.25911100	-0.54435200
H	0.66730600	2.67050000	-2.15293700
H	1.52648600	4.04787700	-1.44316200
C	-1.26249000	1.16450800	-1.17439100
O	-1.97402000	1.90026800	-1.71746800
C	-1.62872500	-1.64554200	-1.01421900
C	-1.90547900	-1.27827800	0.30471300
H	-1.44466600	-1.90950300	1.06983100
C	-3.03600500	-0.43818400	0.73743700
C	-4.15690000	-0.20562900	-0.06632800
C	-2.98659600	0.15378300	2.00668400
C	-5.18417000	0.62096400	0.37463900
H	-4.23342300	-0.68414400	-1.04261000
C	-4.01580600	0.97229800	2.44952900
H	-2.11371000	-0.02809100	2.63490600
C	-5.11688100	1.21470600	1.63103000
H	-6.04815200	0.79353000	-0.26502900
H	-3.95811500	1.42670900	3.43736700
H	-5.92494600	1.85741200	1.97612500
C	-0.31222000	-2.87219800	-2.48355400
H	0.59361800	-2.25274500	-2.42177000
H	-0.93857500	-2.51931600	-3.31904700
H	-0.03615900	-3.91574800	-2.65283000
O	-1.02272600	-2.82493000	-1.26484300
H	-2.18714200	-1.22891900	-1.86410500

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SCF energy in gas phase: -1471.421619 a.u.
Enthalpy in gas phase: -1470.945119 a.u.
Free energy in gas phase: -1471.037866 a.u.
SCF energy in solution: -1471.846114 a.u.
Enthalpy in solution: -1471.369614 a.u.
Free energy in solution: -1471.462361 a.u.

Rh	-0.37200600	-0.26555000	0.43452000
C	3.95604200	1.14615800	1.43598400
C	3.99244700	2.33613500	0.75879300
C	2.84547100	2.80822100	0.07868300
C	1.69262800	1.97720700	0.13399600
C	2.76193700	0.38477000	1.45997800
H	3.68606400	4.65656300	-0.67369800
H	4.83280800	0.77135800	1.96185000
H	4.90333900	2.93577000	0.73546000
C	2.80150900	4.02196900	-0.63811200
C	0.48863900	2.34008900	-0.56301800
C	0.49699600	3.55319800	-1.25500300
C	1.63437400	4.37226800	-1.28272900
H	-0.40846500	3.84062400	-1.78678500
H	1.59006400	5.30715600	-1.84113700
N	1.68060600	0.80240500	0.82549500
O	-0.55477400	1.55465800	-0.55619400
C	2.70809200	-0.92557700	2.18046500
H	2.65048700	-1.75683000	1.46070700
H	1.82336200	-0.98207800	2.82843400
H	3.60006300	-1.07682400	2.79934300
C	-0.38884700	-1.88873600	1.29673900
O	-0.41757600	-2.90406300	1.85143100
C	-0.86234300	-1.43385100	-1.48366800
C	0.46069000	-0.98216600	-1.49088600
H	0.62558300	-0.05681700	-2.04846000
C	1.65846000	-1.81170100	-1.26867700
C	2.91648100	-1.20300200	-1.37498500
C	1.61199700	-3.17188100	-0.93179200
C	4.08299300	-1.91615400	-1.12840300
H	2.97160400	-0.14631600	-1.64223100
C	2.77791000	-3.88452300	-0.68212500
H	0.65222500	-3.68298100	-0.85353700
C	4.02035900	-3.26052100	-0.77360300
H	5.04626000	-1.41382500	-1.20934600
H	2.71498400	-4.93897100	-0.41746800
H	4.93210600	-3.82168000	-0.57642300
O	-1.79522700	-0.83481300	-2.25220600
C	-3.09051100	-1.38123700	-2.10697100
H	-3.43153100	-1.31286900	-1.06272100
H	-3.10592000	-2.43316700	-2.43270800
H	-3.75780200	-0.79317300	-2.74139300
H	-1.10826500	-2.46315000	-1.19639800
C	-2.24268500	0.46502400	1.51283000
C	-1.22102500	0.69786300	2.18562700
H	-0.65060800	1.11553900	2.99792400
C	-3.53909300	0.42066800	0.90579900
C	-4.52807100	-0.45452900	1.37575800
C	-3.81800400	1.27802900	-0.17019100
C	-5.78235300	-0.46662700	0.77812800
H	-4.29996900	-1.11782300	2.20893800
C	-5.07908800	1.26509900	-0.75006000
H	-3.01780000	1.91755700	-0.54119300
C	-6.06155400	0.39459400	-0.28061100
H	-6.54841800	-1.14744100	1.14547900
H	-5.29619800	1.93439500	-1.58104300
H	-7.04803500	0.38694000	-0.74137000

TS12

SCF energy in gas phase: -1163.204711 a.u.
Enthalpy in gas phase: -1162.848709 a.u.
Free energy in gas phase: -1162.928114 a.u.
SCF energy in solution: -1163.541658 a.u.
Enthalpy in solution: -1163.185656 a.u.
Free energy in solution: -1163.265061 a.u.

Rh	0.28363500	0.64099600	-0.09943900
C	4.69928700	1.49169500	0.16713400
C	5.21534300	0.23522800	-0.00879800
C	4.35040800	-0.86191900	-0.19373500
C	2.95887800	-0.58436800	-0.18923700
C	3.30179700	1.69873300	0.16891400
H	5.87171600	-2.38949100	-0.38068800
H	5.35321200	2.34908200	0.31069200
H	6.29294400	0.06972900	-0.00789200
C	4.80188900	-2.18698100	-0.37892600
C	2.01256000	-1.63668400	-0.37468700
C	2.49827300	-2.92717800	-0.55249600
C	3.87725500	-3.19160400	-0.55192200
H	1.77615100	-3.72858000	-0.69760000
H	4.21481900	-4.21709600	-0.69525900
N	2.45760100	0.68356600	-0.00518700
O	0.72928600	-1.35550700	-0.37460700
C	2.76984800	3.08000400	0.37239700
H	2.16099500	3.40083300	-0.48196500
H	2.13954700	3.13218000	1.26883000

H	3.58701400	3.79908000	0.49336200
C	-0.18271100	2.38042000	0.30399000
O	-0.54210900	3.44197800	0.58344100
C	-1.55449000	0.38319500	-0.39799600
C	-2.79066800	0.55295000	-0.80304500
H	-2.72931700	1.34726300	-1.56762200
C	-4.14125100	0.06605000	-0.52011800
C	-5.21702300	0.83313400	-0.98715600
C	-4.40425300	-1.11060100	0.19170100
C	-6.52650700	0.45032900	-0.73055100
H	-5.01745700	1.74608300	-1.54933400
C	-5.71728600	-1.48879600	0.44096100
H	-3.56928600	-1.72559800	0.51881300
C	-6.78154500	-0.71290900	-0.01091300
H	-7.34969800	1.06219500	-1.09575600
H	-5.91101200	-2.40754600	0.99273700
H	-7.80717000	-1.01716500	0.19150100
O	-1.57135600	-1.88926700	0.95024600
H	-0.70187500	-1.95620400	0.49953300
C	-1.36955400	-1.53421900	2.29444300
H	-0.66821000	-0.68956500	2.39951700
H	-2.33939800	-1.22253500	2.70410400
H	-0.99780100	-2.37893800	2.89568400

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SCF energy in gas phase: -1163.217543 a.u.
Enthalpy in gas phase: -1162.859382 a.u.
Free energy in gas phase: -1162.93723 a.u.
SCF energy in solution: -1163.551667 a.u.
Enthalpy in solution: -1163.193506 a.u.
Free energy in solution: -1163.271354 a.u.

Rh	0.34902100	0.67081000	0.05595700
C	4.77942600	1.45223400	-0.13306100
C	5.27123100	0.17839500	-0.21659600
C	4.38543400	-0.91947700	-0.17927200
C	3.00427700	-0.62332700	-0.06095400
C	3.38735300	1.67696200	-0.01904400
H	5.87877700	-2.47638600	-0.34792600
H	5.44581100	2.31212200	-0.15350600
H	6.34216000	-0.00409200	-0.30808500
C	4.81480400	-2.26417400	-0.25333900
C	2.05305100	-1.68861200	-0.00579200
C	2.51058000	-2.99434900	-0.08230100
C	3.88307500	-3.27338200	-0.20653000
H	1.78153400	-3.80205000	-0.04127100
H	4.20512900	-4.31211100	-0.26388300
N	2.52536800	0.66515500	0.00867600
O	0.77990100	-1.37229800	0.13570800
C	2.87292300	3.07603000	0.07286600
H	2.25689700	3.32758700	-0.79997700
H	2.24437100	3.20430500	0.96255300
H	3.69802200	3.79497900	0.12536200
C	-0.16336900	2.41355100	-0.00907900
O	-0.54222500	3.51156600	-0.05090500
C	-1.57737600	0.13774200	0.01124200
C	-2.79393200	0.68438300	-0.14977600
H	-2.75301600	1.77390900	-0.21713600
C	-4.14709600	0.12762600	-0.22018600
C	-5.21910600	0.98015000	0.08881200
C	-4.44926000	-1.18774800	-0.60827800
C	-6.53305400	0.53565900	0.04165900
H	-5.00397100	2.01050000	0.37384600
C	-5.76531200	-1.62990300	-0.65931000
H	-3.64525400	-1.86017100	-0.89642700
C	-6.81385300	-0.77611200	-0.32935200
H	-7.34306900	1.21904800	0.29217000
H	-5.97396000	-2.65270100	-0.97052600
H	-7.84333000	-1.12758000	-0.37085100
O	-1.64361400	-1.39163500	0.20813500
C	-1.94926800	-1.74685500	1.57919400
H	-1.28839000	-1.18502300	2.24801000
H	-2.99759200	-1.49824100	1.75538700
H	-1.78714500	-2.82364800	1.67371900
H	-0.65614700	-1.67681400	0.05080900

TS13

SCF energy in gas phase: -1163.208362 a.u.
Enthalpy in gas phase: -1162.852071 a.u.
Free energy in gas phase: -1162.931486 a.u.
SCF energy in solution: -1163.545445 a.u.
Enthalpy in solution: -1163.189154 a.u.
Free energy in solution: -1163.268569 a.u.

Rh	0.03782100	-0.16620800	0.41458600
C	3.92956200	-2.39191900	-0.04992300
C	4.72146600	-1.41506000	-0.59294600
C	4.19663900	-0.12678000	-0.81903100
C	2.83795500	0.07965500	-0.46406400
C	2.58533800	-2.11833300	0.28735300
H	5.98858700	0.76542600	-1.64071400
H	4.32056000	-3.39065300	0.13211800
H	5.76020200	-1.62014900	-0.85325100
C	4.94746500	0.93439900	-1.37036200
C	2.22482800	1.35419900	-0.66075400
C	3.00079000	2.37298500	-1.20320300
C	4.34406600	2.15805900	-1.55091400
H	2.53413400	3.34451000	-1.35599400
H	4.91353600	2.98354600	-1.97576700
N	2.05757900	-0.91374900	0.08096100
O	0.96529500	1.52113500	-0.33079500
C	1.74936100	-3.20120200	0.88882000
H	0.88325200	-3.43578100	0.25720900
H	1.37186400	-2.90666700	1.87580400
H	2.33225900	-4.12016200	1.01255300
C	-0.81655800	-1.58280700	1.24682600
O	-1.38734000	-2.41777700	1.80283100
C	-1.61568600	0.69121900	0.43117700
C	-2.84548400	1.13751600	0.30638800
H	-3.05589700	2.10756600	0.76000900
C	-3.92598700	0.42043000	-0.38171400
C	-5.24681600	0.84214300	-0.19564300
C	-3.67750800	-0.67979100	-1.21432800
C	-6.29592200	0.17516500	-0.81612900
H	-5.44653200	1.70023300	0.44602900
C	-4.72858900	-1.34567600	-1.82789400
H	-2.64878600	-0.99527600	-1.39173600
C	-6.04178900	-0.92301400	-1.63132700
H	-7.31793400	0.51788500	-0.66247100
H	-4.52041500	-2.19708200	-2.47399200
H	-6.86316500	-1.44405500	-2.12012200
C	-0.15144100	2.81754100	2.53780700
H	0.30060000	1.82242300	2.68903400
H	-0.92984800	2.95953800	3.29583600
H	0.62474600	3.58278900	2.69696000
O	-0.75615500	2.93371400	1.27325600
H	-0.07672400	2.71256500	0.60223400

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SCF energy in gas phase: -1163.216179 a.u.
Enthalpy in gas phase: -1162.858765 a.u.
Free energy in gas phase: -1162.936975 a.u.
SCF energy in solution: -1163.552189 a.u.
Enthalpy in solution: -1163.194775 a.u.
Free energy in solution: -1163.272985 a.u.

Rh	0.02106400	-0.00632000	0.22117400
C	-3.59262200	2.67743100	0.20139100
C	-4.58251500	1.78663200	-0.11139800
C	-4.25992000	0.43385400	-0.35354300
C	-2.89227200	0.07374900	-0.24894300
C	-2.24757400	2.24909900	0.29599600
H	-6.27029600	-0.25391800	-0.76303100
H	-3.81977600	3.72551200	0.38584600
H	-5.62232000	2.10668500	-0.18147400
C	-5.22325500	-0.54426500	-0.68967300
C	-2.49189900	-1.27623600	-0.49899400
C	-3.46626900	-2.20705500	-0.82663600
C	-4.81979200	-1.83869700	-0.91592400
H	-3.15547600	-3.23129800	-1.02657400
H	-5.55560400	-2.59829100	-1.17601000
N	-1.91171700	0.98100600	0.08402500
O	-1.20803000	-1.57112800	-0.42858200
C	-1.18297800	3.23635300	0.64578300
H	-0.35940100	3.19690600	-0.07709900
H	-0.75625300	3.02124700	1.63412900
H	-1.58358400	4.25595600	0.66382400
C	1.14505300	1.21944600	0.97065400
O	1.85002500	1.96832000	1.50838500
C	1.47570800	-1.37386900	0.16741300
C	2.77829100	-1.59713000	-0.05271400
H	3.15632300	-2.62150400	0.02345100

C	3.75989300	-0.56706800	-0.39768600
C	5.09045200	-0.71774800	0.01332000
C	3.42221100	0.55517300	-1.16601700
C	6.04614000	0.24114900	-0.29611700
H	5.36912500	-1.59757400	0.59507400
C	4.37819900	1.51508400	-1.47253400
H	2.40014600	0.65575700	-1.53071200
C	5.69153700	1.36583500	-1.03594400
H	7.07331800	0.10970200	0.04112900
H	4.09753800	2.38175300	-2.06949600
H	6.43986100	2.11769000	-1.28141600
C	0.63334800	-3.06759300	1.79054900
H	0.13448100	-2.23499100	2.30135600
H	1.63727500	-3.21684200	2.19331100
H	0.04918800	-3.98908000	1.85671800
O	0.78209500	-2.75199300	0.38895800
H	-0.16353800	-2.55681900	0.00597400

TS14

SCF energy in gas phase: -1163.216813 a.u.
Enthalpy in gas phase: -1162.862422 a.u.
Free energy in gas phase: -1162.938768 a.u.
SCF energy in solution: -1163.551161 a.u.
Enthalpy in solution: -1163.19677 a.u.
Free energy in solution: -1163.273116 a.u.

Rh	0.34443000	0.72752600	-0.09832800
C	4.80264700	1.37681300	0.03485100
C	5.25785700	0.08777300	0.08357900
C	4.34018300	-0.98313500	0.01726900
C	2.96856900	-0.64466900	-0.09378700
C	3.41636700	1.64335600	-0.06413400
H	5.78593300	-2.58812400	0.14367300
H	5.49372800	2.21622800	0.07516700
H	6.32307600	-0.12814500	0.16746900
C	4.72884500	-2.34221800	0.05340300
C	1.99377600	-1.68444800	-0.19213800
C	2.40689100	-3.00308100	-0.15470700
C	3.77134300	-3.32375900	-0.02645800
H	1.65771700	-3.78815100	-0.24370900
H	4.06461300	-4.37199800	-0.00092500
N	2.52621400	0.65840100	-0.11654500
O	0.73066900	-1.31259000	-0.35693800
C	2.93618700	3.05666100	-0.10899700
H	2.31032000	3.22928900	-0.99341500
H	2.32494100	3.29237600	0.77171800
H	3.77810600	3.75718200	-0.13745100
C	-0.16180400	2.45171100	0.16365000
O	-0.53097200	3.54055100	0.33380100
C	-1.56784300	0.14757100	-0.05324000
C	-2.79408700	0.68366900	-0.17341000
H	-2.76744900	1.77142500	-0.27027700
C	-4.14160500	0.11056600	-0.17517600
C	-5.21535900	0.97025200	0.10750500
C	-4.43962600	-1.22914700	-0.47291900
C	-6.52535200	0.51229000	0.11900700
H	-5.00461200	2.01800600	0.32459900
C	-5.75176900	-1.68546200	-0.46438700
H	-3.63587800	-1.91038100	-0.73899800
C	-6.80142300	-0.82238800	-0.16352400
H	-7.33615400	1.20302800	0.34603400
H	-5.95684100	-2.72779300	-0.70571100
H	-7.82796300	-1.18483800	-0.15862000
O	-1.56413700	-1.35100100	0.16950200
H	-0.50546300	-1.61401800	-0.07072200
C	-1.79309300	-1.68995300	1.55200800
H	-1.10216600	-1.11993600	2.18521100
H	-2.83059800	-1.44603300	1.79333300
H	-1.62284600	-2.76568700	1.65190000

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SCF energy in gas phase: -1163.22745 a.u.
Enthalpy in gas phase: -1162.868903 a.u.
Free energy in gas phase: -1162.94675 a.u.
SCF energy in solution: -1163.563978 a.u.
Enthalpy in solution: -1163.205431 a.u.
Free energy in solution: -1163.283278 a.u.

Rh	-0.29074800	-0.71044300	-0.11394200
C	-4.76477900	-1.45231600	0.04706600
C	-5.25125900	-0.17837800	0.14295100
C	-4.36624300	0.91664600	0.01945800
C	-2.99953700	0.61312400	-0.19608300
C	-3.37798100	-1.67760200	-0.13965300
H	-5.83592000	2.48020900	0.28234600
H	-5.42665600	-2.31243700	0.12451300
H	-6.31241000	0.00903900	0.30584100
C	-4.78278800	2.26552500	0.10562700
C	-2.09110900	1.69017400	-0.36357700
C	-2.51070300	2.99432900	-0.28127400
C	-3.86797900	3.27968500	-0.02783400
H	-1.79211600	3.79827300	-0.43238700
H	-4.18592500	4.31784300	0.04000700
N	-2.51829100	-0.67134700	-0.24112700
O	-0.81137700	1.33612900	-0.68799800
C	-2.85424000	-3.07294400	-0.20356600
H	-2.08411600	-3.16274500	-0.97841900
H	-2.38788500	-3.35559900	0.75065400
H	-3.65817700	-3.78880200	-0.40909600
C	0.25508500	-2.35125500	0.40308400
O	0.62960900	-3.40044100	0.73406600
C	1.59135600	-0.05816400	0.03639000
C	2.78789800	-0.62315200	-0.22654300
H	2.74399500	-1.68189800	-0.48942800
C	4.13975400	-0.06159700	-0.21645000
C	5.21736500	-0.95827300	-0.30714400
C	4.44079200	1.30955100	-0.14038300
C	6.53282000	-0.51632600	-0.30435600
H	5.00541100	-2.02603200	-0.37660900
C	5.75778100	1.75034900	-0.14247800
H	3.62654500	2.02835000	-0.09421500
C	6.81235900	0.84451400	-0.21979200
H	7.34472300	-1.23953700	-0.37182200
H	5.96321200	2.81908100	-0.08709900
H	7.84286400	1.19628600	-0.21926700
O	1.55628400	1.31243400	0.41224700
C	1.65078900	1.48007200	1.81861500
H	0.83071200	0.94940800	2.32740300
H	2.61111400	1.09489000	2.18937400
H	1.58782000	2.55433000	2.02552700
H	-0.07390500	1.83996800	-0.26292700

TS15

SCF energy in gas phase: -1163.221441 a.u.
Enthalpy in gas phase: -1162.86404 a.u.
Free energy in gas phase: -1162.942703 a.u.
SCF energy in solution: -1163.563185 a.u.
Enthalpy in solution: -1163.205784 a.u.
Free energy in solution: -1163.284447 a.u.

Rh	-0.31044500	-0.85262200	0.20546700
C	-4.74195100	-0.88099000	-0.80109600
C	-5.04860400	0.45079400	-0.80166300
C	-4.06783200	1.39156500	-0.41380200
C	-2.79951600	0.87614700	-0.04424200
C	-3.44260700	-1.31806800	-0.44067600
H	-5.27637200	3.16124300	-0.69341000
H	-5.48179500	-1.62615300	-1.08597300
H	-6.03855500	0.80114100	-1.09259300
C	-4.29857300	2.78662300	-0.39391900
C	-1.80838800	1.79914100	0.37395200
C	-2.04325100	3.14977200	0.38839700
C	-3.30019000	3.64626700	-0.01249800
H	-1.26138800	3.83127500	0.72177300
H	-3.47236700	4.72014100	-0.00233600
N	-2.49411400	-0.45944900	-0.08411000
O	-0.63026200	1.24586300	0.80679200
C	-3.11361700	-2.77244100	-0.47190500
H	-2.49105200	-3.00937100	-1.34569900
H	-2.53760300	-3.05627800	0.41681500
H	-4.02136900	-3.38386200	-0.52521600
C	0.09279500	-2.54410800	-0.27495900
O	0.37091600	-3.62794600	-0.58784000
C	1.65703100	-0.51460400	0.47615600
C	2.51367600	-0.30257400	-0.55260900
H	2.12431300	-0.58454500	-1.53280200
C	3.86619400	0.25347000	-0.57118300
C	4.50924400	0.36689600	-1.81656900
C	4.57591100	0.68909600	0.56252400
C	5.79192800	0.88332600	-1.93169700
H	3.97853600	0.03581600	-2.71071400
C	5.86136800	1.20210500	0.44478100

H	4.10810100	0.61716400	1.53970100
C	6.48041500	1.30547800	-0.79785900
H	6.25786000	0.95594900	-2.91411700
H	6.38850800	1.52706900	1.34182900
H	7.48741400	1.71151200	-0.88244200
O	2.03508600	-0.13451800	1.74305600
C	1.51095400	-0.89341900	2.81245000
H	0.41460500	-0.81396300	2.86863200
H	1.77961200	-1.95491000	2.71129800
H	1.95532100	-0.49170200	3.72908400
H	0.13922900	1.82956300	0.70137200

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SCF energy in gas phase: -1163.225881 a.u.
Enthalpy in gas phase: -1162.867841 a.u.
Free energy in gas phase: -1162.946902 a.u.
SCF energy in solution: -1163.565112 a.u.
Enthalpy in solution: -1163.207072 a.u.
Free energy in solution: -1163.286133 a.u.

Rh	-0.38822400	-1.03528700	0.06103000
C	-4.80599400	-0.18310400	-0.57980500
C	-4.85080800	1.17560800	-0.44066700
C	-3.68904300	1.87453600	-0.04151500
C	-2.52644500	1.09929800	0.19456700
C	-3.59579000	-0.88699900	-0.35513500
H	-4.54637600	3.85796700	-0.07848600
H	-5.68883900	-0.74619800	-0.87542700
H	-5.76984500	1.73058600	-0.62773600
C	-3.64555100	3.27873300	0.11964100
C	-1.35571900	1.77002700	0.63117800
C	-1.32779300	3.13256000	0.78591200
C	-2.48273100	3.89292800	0.51128700
H	-0.41560100	3.61462400	1.13388200
H	-2.44512500	4.97338200	0.63081600
N	-2.48497700	-0.25971200	0.01072100
O	-0.29526500	0.96180800	0.94932200
C	-3.55244000	-2.36492700	-0.55240500
H	-3.08174800	-2.61177900	-1.51423900
H	-2.95580200	-2.84431800	0.23204900
H	-4.56079200	-2.79393000	-0.55229900
C	-0.34004600	-2.67254200	-0.70108500
O	-0.30547400	-3.72519700	-1.19347900
C	1.61962000	-0.98587900	0.17251100
C	2.20014400	0.08126100	-0.45965700
H	1.55945200	0.57765900	-1.19626100
C	3.57484500	0.58184700	-0.42881700
C	3.91228200	1.62902800	-1.30477100
C	4.58203400	0.11285200	0.43271900
C	5.18469400	2.18188200	-1.32653500
H	3.14927900	2.00777500	-1.98772100
C	5.85423600	0.67084300	0.41142600
H	4.35855300	-0.69630700	1.12018100
C	6.16854200	1.70625000	-0.46397800
H	5.40989500	2.98907700	-2.02307400
H	6.61349100	0.28645200	1.09232400
H	7.16901800	2.13596100	-0.47622200
O	2.39686800	-1.78708500	0.93253800
C	1.77741600	-2.75200500	1.75500600
H	0.97434600	-2.30618600	2.35802300
H	1.36105700	-3.57561200	1.15888000
H	2.55984400	-3.14579900	2.41147000
H	0.59635900	1.30312800	0.70610900

TS16

SCF energy in gas phase: -1163.21584 a.u.
Enthalpy in gas phase: -1162.861691 a.u.
Free energy in gas phase: -1162.938262 a.u.
SCF energy in solution: -1163.551607 a.u.
Enthalpy in solution: -1163.197458 a.u.
Free energy in solution: -1163.274029 a.u.

Rh	0.03160700	0.06181200	0.09384900
C	-3.64812800	2.65390300	0.20975700
C	-4.63066600	1.71830300	0.03371600
C	-4.28299600	0.37021900	-0.20505800
C	-2.89946900	0.06420100	-0.24252500
C	-2.28488100	2.27438600	0.17829600
H	-6.29592700	-0.40669900	-0.36548400
H	-3.89384800	3.69933100	0.38536600
H	-5.68368000	1.99841600	0.06700000
C	-5.23614000	-0.65482700	-0.40309900
C	-2.47993300	-1.27423200	-0.51374700
C	-3.43997700	-2.25244200	-0.70261300
C	-4.81005300	-1.93980200	-0.63846700
H	-3.11189800	-3.26728700	-0.92181500
H	-5.53970300	-2.73341900	-0.79153900
N	-1.92563100	1.01319500	-0.02944900
O	-1.17709200	-1.50673100	-0.61637500
C	-1.22245400	3.30176900	0.39209700
H	-0.43392300	3.20885300	-0.36414500
H	-0.74545200	3.17365400	1.37314100
H	-1.63870100	4.31434300	0.34713400
C	1.13304100	1.27726400	0.88677500
O	1.81647600	2.03131200	1.44484100
C	1.44392100	-1.35634100	0.11975100
C	2.75202200	-1.61165400	-0.01900000
H	3.09216400	-2.64795100	0.07858900
C	3.78895100	-0.61691000	-0.29639100
C	5.08675300	-0.82506500	0.18830800
C	3.54237900	0.52497300	-1.07079300
C	6.09762900	0.09519900	-0.05614100
H	5.29563600	-1.72086800	0.77491200
C	4.55316500	1.44647400	-1.31230200
H	2.54787000	0.67067700	-1.49241700
C	5.83231100	1.23949400	-0.80326500
H	7.09748700	-0.08118600	0.33805600
H	4.34218600	2.32908100	-1.91458100
H	6.62306600	1.96237800	-0.99772900
C	0.49125300	-3.01232500	1.68224700
H	0.00864800	-2.17398300	2.20123700
H	1.47364400	-3.21006200	2.11794100
H	-0.13035300	-3.91149600	1.71402600
O	0.68752700	-2.67603200	0.29640400
H	-0.28578800	-2.40159500	-0.13100900

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SCF energy in gas phase: -1163.226624 a.u.
Enthalpy in gas phase: -1162.868766 a.u.
Free energy in gas phase: -1162.946931 a.u.
SCF energy in solution: -1163.56388 a.u.
Enthalpy in solution: -1163.206022 a.u.
Free energy in solution: -1163.284187 a.u.

Rh	0.09373000	-0.00230100	0.16339600
C	-3.54697800	2.68740300	0.26251600
C	-4.55667400	1.78739500	0.06297900
C	-4.24343000	0.44287600	-0.24176800
C	-2.86808000	0.10924500	-0.32060600
C	-2.19376600	2.27065400	0.20065200
H	-6.27428000	-0.28426700	-0.38395000
H	-3.76173900	3.73047500	0.48587600
H	-5.60164700	2.08994800	0.12681800
C	-5.22185400	-0.55489900	-0.45859700
C	-2.51786300	-1.22150000	-0.66697000
C	-3.47990000	-2.17708600	-0.87843500
C	-4.84323800	-1.84027900	-0.75470400
H	-3.18014600	-3.18530500	-1.15968600
H	-5.59523600	-2.60942400	-0.91753200
N	-1.86726300	1.01300000	-0.06745700
O	-1.18279400	-1.46091800	-0.85244400
C	-1.09735400	3.24886500	0.45791200
H	-0.29232800	3.12647000	-0.27675000
H	-0.65251700	3.08140000	1.44858500
H	-1.46709000	4.27964700	0.42042100
C	1.17032500	1.06204600	1.15753600
O	1.82952700	1.73629800	1.83502900
C	1.43636000	-1.48501700	0.23488100
C	2.75185000	-1.63438700	-0.00235300
H	3.16096100	-2.64636500	0.09733200
C	3.70599300	-0.58982300	-0.37145600
C	5.04705900	-0.71803900	0.01735000
C	3.34767300	0.53130400	-1.13499000
C	5.98538700	0.25391600	-0.30312400
H	5.34531400	-1.59369500	0.59582700
C	4.28575800	1.50583000	-1.45291500
H	2.31897100	0.61987400	-1.48584300
C	5.60745300	1.37609300	-1.03562900
H	7.01875800	0.13541500	0.02078100
H	3.98463200	2.36847000	-2.04662200
H	6.34216500	2.13836800	-1.29072700
C	0.53700100	-2.95991100	1.84717800

H	-0.00907200	-2.13412300	2.33184200
H	1.50669300	-3.08362500	2.35111100
H	-0.03636400	-3.88979600	1.93033700
O	0.73232300	-2.70098600	0.46895300
H	-0.82088800	-2.29416900	-0.45745700

TS17

SCF energy in gas phase: -1163.221248 a.u.
Enthalpy in gas phase: -1162.864194 a.u.
Free energy in gas phase: -1162.940716 a.u.
SCF energy in solution: -1163.564549 a.u.
Enthalpy in solution: -1163.207495 a.u.
Free energy in solution: -1163.284017 a.u.

Rh	0.15094400	0.74953600	0.19229900
C	-3.83444100	0.74616600	-1.99526000
C	-4.54851400	-0.19027400	-1.30165200
C	-3.91687600	-0.92800200	-0.27515700
C	-2.55312100	-0.63432800	-0.02533800
C	-2.47731700	0.99790200	-1.67269200
H	-5.63111700	-2.11959900	0.28579800
H	-4.29442800	1.31886500	-2.79782600
H	-5.59602200	-0.38443400	-1.53091500
C	-4.58083400	-1.91559700	0.48934700
C	-1.88828000	-1.38360600	0.97868700
C	-2.54204200	-2.33913100	1.71303100
C	-3.90631600	-2.59757800	1.46975600
H	-2.00135900	-2.90186900	2.47330400
H	-4.41423600	-3.35577200	2.06147200
N	-1.85903300	0.33421800	-0.70306100
O	-0.55319700	-1.11643700	1.11906700
C	-1.71944100	2.04085400	-2.42308200
H	-0.72571100	1.67174500	-2.70311300
H	-1.56613600	2.93222800	-1.79954700
H	-2.25712000	2.34699400	-3.32732000
C	0.80752500	2.29853300	-0.46505900
O	1.23619900	3.30107800	-0.86714100
C	1.75399200	0.64015900	1.41477900
C	2.88107700	-0.08698200	1.24249000
H	3.54708300	-0.12829700	2.11177300
C	3.36291200	-0.80071300	0.06389400
C	4.70130100	-1.22766200	0.05102400
C	2.58031800	-1.11093300	-1.06108000
C	5.24003300	-1.90643500	-1.03364200
H	5.32802500	-1.00609200	0.91623300
C	3.11932300	-1.78513500	-2.14891500
H	1.52920600	-0.81050900	-1.07537200
C	4.45228800	-2.18791700	-2.14610800
H	6.28411300	-2.21721400	-1.01008400
H	2.48581000	-2.00816900	-3.00743400
H	4.87036600	-2.72131700	-2.99853800
C	1.08034600	2.40906200	2.84760200
H	0.09606000	2.53873400	2.37061800
H	1.78399900	3.13221200	2.40585000
H	0.99828800	2.60118300	3.92246100
O	1.55329800	1.08930400	2.70552200
H	-0.17805900	-1.37921300	1.97528700

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SCF energy in gas phase: -1163.232075 a.u.
Enthalpy in gas phase: -1162.873804 a.u.
Free energy in gas phase: -1162.950779 a.u.
SCF energy in solution: -1163.568685 a.u.
Enthalpy in solution: -1163.210414 a.u.
Free energy in solution: -1163.287389 a.u.

Rh	-1.03379700	-0.76859800	0.12564400
C	2.86486700	-2.99206700	-0.54846900
C	3.78497300	-2.01850500	-0.27412600
C	3.35565000	-0.78223500	0.25864600
C	1.96416600	-0.63420000	0.48163100
C	1.48344300	-2.75080400	-0.34083000
H	5.29795400	0.16023900	0.36628900
H	3.17220100	-3.95691000	-0.94665100
H	4.84733600	-2.18178400	-0.45466500
C	4.23277400	0.28616900	0.55602000
C	1.50545800	0.57368700	1.06173000
C	2.36335100	1.60851300	1.33241900
C	3.73912100	1.46314100	1.06127100
H	1.97057400	2.53892300	1.74197100
H	4.40982400	2.29261600	1.27426000
N	1.04692000	-1.59570200	0.14494800
O	0.16924000	0.61748800	1.36529000
C	0.48479800	-3.80224500	-0.69145700
H	-0.02455700	-3.55630900	-1.63320200
H	-0.28866200	-3.87491900	0.08218400
H	0.96520300	-4.77962700	-0.81358400
C	-2.03084900	-1.83858500	-0.92869400
O	-2.66615500	-2.52219700	-1.62342100
C	-2.59388200	0.48771300	0.33940700
C	-2.41742400	1.82958100	0.17059500
O	-3.82084100	0.14030900	0.80605700
C	-3.97052400	-1.08377900	1.48578200
H	-3.19105800	-1.21801500	2.24975400
H	-3.94088500	-1.94000000	0.79685400
H	-4.95398900	-1.05015200	1.96633300
H	-0.20311200	1.52028100	1.27589700
H	-3.20164700	2.48217000	0.56847500
C	-1.27046400	2.49881900	-0.44184600
C	-0.55392300	1.96905400	-1.53400000
C	-0.83078700	3.73183000	0.07751500
C	0.56060500	2.62178100	-2.04725400
H	-0.89775300	1.03743000	-1.98251600
C	0.27798700	4.38945000	-0.44665500
H	-1.38278900	4.17497800	0.90859700
C	0.98764900	3.83386700	-1.50769100
H	1.09066100	2.18603500	-2.89371300
H	0.58769600	5.34420100	-0.02224200
H	1.85556400	4.34574700	-1.92003700

TS18

SCF energy in gas phase: -1163.183656 a.u.
Enthalpy in gas phase: -1162.8314 a.u.
Free energy in gas phase: -1162.911228 a.u.
SCF energy in solution: -1163.524016 a.u.
Enthalpy in solution: -1163.17176 a.u.
Free energy in solution: -1163.251588 a.u.

Rh	-0.27740100	0.58338600	-0.21006500
C	-4.71395600	1.44070000	0.18816500
C	-5.20636600	0.18173400	0.40460600
C	-4.33067800	-0.92512800	0.41998100
C	-2.95417600	-0.65379000	0.20998300
C	-3.32728000	1.63780500	-0.01001000
H	-5.81981300	-2.45125800	0.78314700
H	-5.37391400	2.30539100	0.16625600
H	-6.27269700	0.01813200	0.56131300
C	-4.76054000	-2.25527500	0.62295200
C	-2.01696000	-1.72600300	0.20137300
C	-2.47124900	-3.01578700	0.41063500
C	-3.83809200	-3.27475300	0.61541400
H	-1.74111300	-3.82242000	0.40654200
H	-4.16208000	-4.30193900	0.77276000
N	-2.47914000	0.61639800	0.00695700
O	-0.71814900	-1.48833000	-0.02928700
C	-2.79591600	3.01781600	-0.22797400
H	-2.08897400	3.04367000	-1.06530700
H	-2.26353000	3.37544300	0.66420200
H	-3.60696500	3.72412000	-0.43635700
C	0.33854400	2.25410400	0.24768400
O	0.74491700	3.27658900	0.59667800
C	1.68017200	0.10666400	-0.48541100
C	2.64389500	0.24349400	0.46002100
H	2.32279600	0.72415500	1.38486600
C	4.05141800	-0.14288400	0.43551600
C	4.82832500	0.15694500	1.56854300
C	4.69218100	-0.78705000	-0.63771000
C	6.17655200	-0.16260400	1.63224400
H	4.35116400	0.65655000	2.41320300
C	6.04240700	-1.10552100	-0.57074300
H	4.12037200	-1.03522600	-1.52683700
C	6.79527000	-0.79740300	0.55902700
H	6.74875300	0.08754300	2.52511000
H	6.51456100	-1.60369700	-1.41727300
H	7.85365900	-1.04991500	0.60263900
O	1.99897000	-0.45628900	-1.68013800
C	0.99235600	-0.59524000	-2.65530300
H	0.48693300	0.36688900	-2.84967100
H	0.24653100	-1.34668600	-2.36114400
H	1.49181500	-0.91987600	-3.57348600
H	-0.13181800	-0.58075200	0.92227700

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SCF energy in gas phase: -1163.213109 a.u.
Enthalpy in gas phase: -1162.858284 a.u.
Free energy in gas phase: -1162.936624 a.u.
SCF energy in solution: -1163.555034 a.u.
Enthalpy in solution: -1163.200209 a.u.
Free energy in solution: -1163.278549 a.u.

Rh	0.26642100	0.49701400	0.20694300
C	4.65408500	1.59715600	-0.34267400
C	5.19860300	0.35255300	-0.52767600
C	4.37735500	-0.79276300	-0.48242200
C	2.99669800	-0.57293700	-0.24108300
C	3.26826100	1.74056800	-0.10622700
H	5.91510600	-2.27266100	-0.84636400
H	5.27515300	2.49005100	-0.37314500
H	6.26694600	0.23424900	-0.71054200
C	4.85436600	-2.10982900	-0.66183300
C	2.08452700	-1.67071500	-0.17904000
C	2.59533200	-2.95056900	-0.36728700
C	3.96424900	-3.15869700	-0.60181200
H	1.90093200	-3.78744900	-0.32669400
H	4.32299900	-4.17746300	-0.74172100
N	2.47088100	0.67833700	-0.05600900
O	0.81228800	-1.45344500	0.06435600
C	2.68276100	3.10321700	0.08386600
H	2.13031000	3.17202400	1.02916900
H	1.98540600	3.35015200	-0.72786500
H	3.46569900	3.86912400	0.09476300
C	-0.35389000	2.23023100	0.42728300
O	-0.77252900	3.29645900	0.54274900
C	-1.67395100	-0.08453200	0.39807400
C	-2.67685700	0.35595600	-0.40435600
H	-2.40414500	1.13685600	-1.11491000
C	-4.07942700	-0.04347800	-0.45723200
C	-4.94113600	0.71705500	-1.26667100
C	-4.62936600	-1.13962100	0.22943800
C	-6.28960900	0.41220500	-1.37901100
H	-4.53204000	1.56717000	-1.81476700
C	-5.97962000	-1.44329900	0.11372400
H	-3.98676700	-1.75611400	0.85013400
C	-6.81923000	-0.67248200	-0.68556400
H	-6.93061000	1.02417700	-2.01253500
H	-6.38118800	-2.29962800	0.65460900
H	-7.87685200	-0.91732100	-0.77037600
O	-1.92473500	-1.04274300	1.31629300
C	-1.03454900	-1.21063200	2.40006600
H	-0.66699700	-0.23444700	2.76471200
H	-0.18311600	-1.83764500	2.11262500
H	-1.60196400	-1.69091600	3.20337200
H	-0.09580000	0.65737200	-1.27538800

TS19

SCF energy in gas phase: -1163.210498 a.u.
Enthalpy in gas phase: -1162.856387 a.u.
Free energy in gas phase: -1162.934393 a.u.
SCF energy in solution: -1163.546886 a.u.
Enthalpy in solution: -1163.192775 a.u.
Free energy in solution: -1163.270781 a.u.

Rh	0.26362100	0.43471700	-0.20222700
C	4.55117000	1.76804000	0.43727800
C	5.21070600	0.58032300	0.25283000
C	4.48688200	-0.59324300	-0.03874600
C	3.07548700	-0.46347100	-0.12098300
C	3.14418400	1.82721000	0.33636700
H	6.17042500	-1.94532600	-0.18852000
H	5.09805000	2.68151100	0.66125100
H	6.29730600	0.53028300	0.32734300
C	5.08736600	-1.85294500	-0.25087400
C	2.25429500	-1.59655900	-0.40819200
C	2.88927200	-2.81816900	-0.61738200
C	4.28559900	-2.93563300	-0.53634200
H	2.26793300	-3.68183900	-0.84631100
H	4.73921300	-3.91160400	-0.70450400
N	2.43164700	0.73521100	0.06581800
O	0.95132400	-1.46794000	-0.45245900
C	2.44884000	3.13666200	0.52856600
H	1.74555100	3.09929700	1.37015000
H	1.88153900	3.41854200	-0.36745800
H	3.17104600	3.93457200	0.73174400
C	-0.41861200	2.14800200	-0.05262000
O	-0.87832600	3.20355600	0.01353400
C	-1.66098100	-0.26531200	0.04837700
C	-2.78608100	0.32136100	-0.43916000
H	-2.63634200	1.21393300	-1.04636800
C	-4.18689900	-0.03890000	-0.24325300
C	-5.15320000	0.83827400	-0.76552000
C	-4.64249600	-1.19155500	0.41986100
C	-6.51059700	0.58667500	-0.63035000
H	-4.82070900	1.73606500	-1.28843100
C	-6.00185100	-1.43985900	0.55487800
H	-3.92054000	-1.89543600	0.82149900
C	-6.94386200	-0.55657900	0.03458100
H	-7.23387600	1.28694800	-1.04599100
H	-6.32967800	-2.34054100	1.07261900
H	-8.00804700	-0.75918400	0.14453700
O	-1.75560900	-1.44033600	0.68977300
C	-0.95215900	-1.68567000	1.83450900
H	-0.75730300	-0.75187800	2.38161700
H	-0.00654600	-2.15060200	1.53912300
H	-1.52482500	-2.36643400	2.47273700
H	-0.61916100	0.21882100	-1.46530000

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SCF energy in gas phase: -1163.278836 a.u.
Enthalpy in gas phase: -1162.919518 a.u.
Free energy in gas phase: -1162.996298 a.u.
SCF energy in solution: -1163.609503 a.u.
Enthalpy in solution: -1163.250185 a.u.
Free energy in solution: -1163.326965 a.u.

Rh	-0.08552600	0.00140800	0.30445900
C	3.60976500	2.38773700	-0.59273900
C	4.53384100	1.38397400	-0.70977100
C	4.13968000	0.04009400	-0.54877700
C	2.76893600	-0.19157300	-0.26368300
C	2.25810200	2.09057700	-0.30570800
H	6.07861000	-0.86201800	-0.87767100
H	3.89733500	3.42935700	-0.71947900
H	5.57745500	1.60997800	-0.93067100
C	5.02849000	-1.05097300	-0.66032500
C	2.27758700	-1.52319500	-0.09576400
C	3.18888400	-2.56992000	-0.21585600
C	4.54271600	-2.32890100	-0.49302900
H	2.81562300	-3.58450700	-0.08906400
H	5.22009200	-3.17787400	-0.57726900
N	1.85504600	0.83217100	-0.14184700
O	1.00906200	-1.71766900	0.15811200
C	1.27446700	3.20926700	-0.19113200
H	0.82288200	3.24299400	0.80795900
H	0.46108200	3.09718200	-0.91844000
H	1.76090300	4.17370300	-0.37347800
C	-1.13431400	1.50139700	0.50294300
O	-1.82851600	2.41210400	0.67494100
C	-1.50420700	-1.18985900	1.48299400
C	-1.83394100	-1.30485000	0.12873000
H	-1.31587200	-2.12142600	-0.38060800
C	-3.00083700	-0.78159900	-0.59725100
C	-3.04270700	-0.99781700	-1.98226800
C	-4.06479200	-0.09550100	0.00434400
C	-4.10675400	-0.54135000	-2.74707000
H	-2.21517100	-1.52785800	-2.45599100
C	-5.13009600	0.35832500	-0.76423500
H	-4.05002600	0.08380600	1.07589300
C	-5.15711400	0.14055400	-2.13850800
H	-4.11788800	-0.72022400	-3.82107300
H	-5.94991000	0.88755300	-0.28074800
H	-5.99594800	0.49787600	-2.73362500
O	-2.29415400	-0.53929200	2.37095700
C	-1.64224600	-0.19367900	3.57594700
H	-0.87638200	0.57522800	3.39546500
H	-1.16450400	-1.07530500	4.03001100
H	-2.40546600	0.19617500	4.25380600
H	-0.80336700	-1.91059800	1.92212700

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SCF energy in gas phase: -1471.428632 a.u.
Enthalpy in gas phase: -1470.951579 a.u.
Free energy in gas phase: -1471.043865 a.u.
SCF energy in solution: -1471.850658 a.u.
Enthalpy in solution: -1471.373605 a.u.

Free energy in solution: -1471.465891 a.u.

Rh	-0.40922600	-0.02260700	0.48183800
C	4.07306200	-0.80332100	1.39577400
C	4.27367700	-1.95371100	0.68103700
C	3.20105800	-2.55947200	-0.01379300
C	1.94355700	-1.90082100	0.06597600
C	2.78402800	-0.21753400	1.44511700
H	4.29313900	-4.24665000	-0.81866500
H	4.88993800	-0.32538300	1.93401000
H	5.25960600	-2.41805400	0.63754200
C	3.32704100	-3.74651600	-0.76540300
C	0.80229700	-2.41415500	-0.64028200
C	0.97690900	-3.59483800	-1.36267800
C	2.21904100	-4.24373600	-1.41677500
H	0.11596800	-3.99706200	-1.89396000
H	2.30306100	-5.16209800	-1.99720800
N	1.76823800	-0.75977100	0.79535500
O	-0.34369100	-1.78095500	-0.61475800
C	2.54490200	1.03094600	2.23260400
H	2.25270400	1.85729100	1.57010800
H	1.73437400	0.88524200	2.95948000
H	3.44491200	1.33590200	2.77856900
C	-0.62046100	1.54954600	1.41539100
O	-0.78098200	2.52408700	2.01559900
C	-0.99819800	1.05693100	-1.47590100
C	0.38772300	0.92399300	-1.42485300
H	0.75236800	0.00130200	-1.87827600
C	1.42321400	1.94849400	-1.22525300
C	2.76021700	1.53575800	-1.33916600
C	1.17155300	3.29171400	-0.90546400
C	3.80871800	2.41986300	-1.12445700
H	2.97468600	0.49638600	-1.59451200
C	2.22427400	4.17472800	-0.69283900
H	0.14623600	3.64432900	-0.83163500
C	3.54537400	3.74635000	-0.79462900
H	4.83564100	2.06767600	-1.21361500
H	2.00663300	5.21330800	-0.44727600
H	4.36308000	4.44489100	-0.62488100
O	-1.60816600	2.25984600	-1.37845500
C	-2.98921300	2.20503700	-1.08854100
H	-3.50393100	1.47755500	-1.73509500
H	-3.15073000	1.91535400	-0.03949900
H	-3.39432000	3.20480500	-1.26338100
H	-1.59759000	0.26105200	-1.93347800
C	-2.29054500	-0.87200000	1.31124300
C	-1.32586400	-1.14674200	2.06097100
H	-0.85691400	-1.64987000	2.89080000
C	-3.56360800	-0.80049900	0.65317500
C	-4.63086800	-0.08875400	1.21701700
C	-3.73156600	-1.43395900	-0.58831600
C	-5.84306300	-0.00383300	0.54280900
H	-4.49333000	0.39992400	2.18105400
C	-4.94923900	-1.34924100	-1.24949300
H	-2.88542200	-1.97734200	-1.00997200
C	-6.00526700	-0.63087200	-0.68996800
H	-6.66815600	0.55212100	0.98503900
H	-5.07694400	-1.84526300	-2.21045000
H	-6.95732800	-0.56366100	-1.21378600

TS20

SCF energy in gas phase: -1163.182507 a.u.
Enthalpy in gas phase: -1162.830487 a.u.
Free energy in gas phase: -1162.908582 a.u.
SCF energy in solution: -1163.522508 a.u.
Enthalpy in solution: -1163.170488 a.u.
Free energy in solution: -1163.248583 a.u.

Rh	-0.11231600	-1.01934500	0.14163900
C	4.25133600	-0.50031500	-0.99857700
C	4.49005600	0.77604400	-0.56278300
C	3.46073800	1.51242900	0.06200500
C	2.20538700	0.86453300	0.19510400
C	2.97177600	-1.08042700	-0.83495600
H	4.59366200	3.31243400	0.45556700
H	5.03537800	-1.08534300	-1.47500800
H	5.47217200	1.23327400	-0.68549300
C	3.62597800	2.82358300	0.55973100
C	1.12324900	1.53584800	0.83161000
C	1.31850800	2.82233400	1.30272600
C	2.56669600	3.45570400	1.16810300
H	0.48224800	3.32388900	1.78510200
H	2.68837400	4.46571700	1.55584600
N	1.98295300	-0.40831600	-0.25905200
O	-0.05106300	0.91840600	0.99509100
C	2.71317200	-2.46884500	-1.32539700
H	2.10190400	-2.45323000	-2.23862900
H	2.16907700	-3.05710300	-0.57688300
H	3.65043200	-2.98515800	-1.56050000
C	-0.53839800	-2.33242200	-1.07628200
O	-0.84500600	-3.09403000	-1.88970800
C	-1.97326300	-1.32974100	0.89995200
C	-3.05363700	-0.53479800	0.77412800
O	-2.12579900	-2.45234200	1.66739400
C	-1.01568200	-2.83279700	2.44515500
H	-0.68479900	-2.01043000	3.09849400
H	-0.16613200	-3.15715300	1.81829100
H	-1.33250800	-3.67993300	3.06170600
H	-3.89530600	-0.75658900	1.43750700
C	-3.19017600	0.63865900	-0.08911200
C	-2.76186200	0.65838000	-1.42708200
C	-3.79135600	1.79946300	0.42008600
C	-2.88399900	1.80863900	-2.20311100
H	-2.37323800	-0.25581200	-1.87296900
C	-3.91888000	2.94322200	-0.35488200
H	-4.14321700	1.79616900	1.45206900
C	-3.45494300	2.95838700	-1.66959100
H	-2.54905800	1.79468400	-3.23962900
H	-4.38032100	3.83418000	0.06957400
H	-3.55477000	3.85608900	-2.27754600
H	-0.63363300	0.46950600	-0.25106300

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SCF energy in gas phase: -1163.211455 a.u.
Enthalpy in gas phase: -1162.8572 a.u.
Free energy in gas phase: -1162.935167 a.u.
SCF energy in solution: -1163.552043 a.u.
Enthalpy in solution: -1163.197788 a.u.
Free energy in solution: -1163.275755 a.u.

Rh	-0.19942800	-0.89116800	0.27199000
C	3.83205000	-0.63583000	-1.84391900
C	4.36197700	0.47005200	-1.23060000
C	3.63674800	1.13585300	-0.22109700
C	2.36314900	0.59930300	0.10159300
C	2.55659000	-1.11488200	-1.46948300
H	5.08238300	2.68997400	0.20607300
H	4.37892800	-1.15862700	-2.62603300
H	5.34439900	0.84665100	-1.51671400
C	4.10515400	2.28153600	0.45885900
C	1.54735000	1.20821600	1.10516600
C	2.04613300	2.33678600	1.74687400
C	3.30979300	2.85811400	1.42364700
H	1.42587400	2.80557200	2.50827600
H	3.66039000	3.74387100	1.95173900
N	1.85263000	-0.50828100	-0.51972900
O	0.37599800	0.69305200	1.39988600
C	1.97758600	-2.31296900	-2.15199700
H	1.06651700	-2.04722700	-2.70481800
H	1.71097000	-3.09427600	-1.42937300
H	2.68924300	-2.74163400	-2.86600500
C	-0.84612500	-2.36830200	-0.64463600
O	-1.28709300	-3.25879400	-1.22838000
C	-1.96783900	-0.86603500	1.28626000
C	-3.00944800	-0.04722000	1.07294300
O	-2.03462300	-1.73857300	2.33234600
C	-0.82599900	-1.96403100	3.02540100
H	-0.40180500	-1.02472900	3.40585000
H	-0.07542100	-2.46541400	2.38446900
H	-1.05723100	-2.63483400	3.85792100
H	-3.77074700	-0.01941500	1.85814800
C	-3.18558500	0.86271500	-0.06470900
C	-3.13197700	0.41659300	-1.39455400
C	-3.44173600	2.22154000	0.16128000
C	-3.28349900	1.30502000	-2.45694900
H	-3.02177400	-0.64995900	-1.59141400
C	-3.59956900	3.10673700	-0.89683000
H	-3.49647600	2.58006200	1.18918900
C	-3.51187900	2.65397500	-2.21242100
H	-3.24343600	0.93324000	-3.48003200
H	-3.78760300	4.16056100	-0.69531200
H	-3.63603900	3.34985500	-3.04048200

H	-0.89380600	-0.06166700	-0.81269700

TS21

SCF energy in gas phase: -1163.208159 a.u.
Enthalpy in gas phase: -1162.855199 a.u.
Free energy in gas phase: -1162.932886 a.u.
SCF energy in solution: -1163.543981 a.u.
Enthalpy in solution: -1163.191021 a.u.
Free energy in solution: -1163.268708 a.u.

Rh	-0.10715000	-0.11210900	0.02941100
C	3.45679800	2.65441400	-0.45515600
C	4.47042700	1.82238600	-0.05593500
C	4.18826800	0.49726000	0.33188400
C	2.82583200	0.09820800	0.28629700
C	2.12191700	2.19467000	-0.47453800
H	6.21660900	-0.10834100	0.78408400
H	3.66166100	3.67845300	-0.76030600
H	5.50272800	2.17289100	-0.03696500
C	5.17444400	-0.42166300	0.75048900
C	2.44060100	-1.22788600	0.65632500
C	3.44832000	-2.10178500	1.06020500
C	4.79083900	-1.69615600	1.10510500
H	3.15926300	-3.11195000	1.34397400
H	5.54289300	-2.41360700	1.43111500
N	1.82186100	0.95026800	-0.10808200
O	1.18398500	-1.58718300	0.59898700
C	1.03203600	3.12066000	-0.90841800
H	0.36253700	3.36435700	-0.07338300
H	0.42207500	2.67399400	-1.70254800
H	1.44689500	4.06087400	-1.28744000
C	-1.33928100	1.23750700	-0.30715400
O	-2.09850500	2.08697700	-0.47932700
C	-1.40995700	-1.49434400	-0.76120500
C	-2.75981200	-1.53278500	-0.74847700
O	-0.77241100	-2.48552000	-1.41162300
C	0.31609900	-2.17826400	-2.26799300
H	1.25813000	-2.15569300	-1.70736800
H	0.15717600	-1.21569200	-2.77656400
H	0.35496400	-2.97942600	-3.01261400
H	-3.19787400	-2.24156200	-1.45689400
C	-3.69909100	-0.69897600	0.00419900
C	-3.61206800	-0.49588000	1.38833700
C	-4.74454000	-0.07053200	-0.68887800
C	-4.49277600	0.36184400	2.04086800
H	-2.86220100	-1.03802100	1.96425300
C	-5.62698100	0.77954000	-0.03858500
H	-4.83604300	-0.23601100	-1.76285100
C	-5.49555300	1.01054000	1.32972800
H	-4.40198700	0.50861500	3.11612100
H	-6.41917700	1.27155800	-0.60099100
H	-6.18507900	1.68002300	1.84118900
H	-1.13152800	-0.78419700	0.98336300

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SCF energy in gas phase: -1163.275953 a.u.
Enthalpy in gas phase: -1162.916702 a.u.
Free energy in gas phase: -1162.993357 a.u.
SCF energy in solution: -1163.607678 a.u.
Enthalpy in solution: -1163.248427 a.u.
Free energy in solution: -1163.325082 a.u.

Rh	-0.26190300	-0.81232000	0.04607800
C	3.98558700	-0.74549700	-1.38798100
C	4.43458600	0.40913600	-0.80451000
C	3.56202900	1.18652600	-0.01649300
C	2.23521100	0.70313700	0.12842200
C	2.65206800	-1.17473500	-1.20084000
H	4.96234200	2.75466700	0.49735900
H	4.64473300	-1.35292900	-2.00474800
H	5.46358500	0.74117400	-0.94503000
C	3.94225200	2.39171200	0.61241500
C	1.27474400	1.43026100	0.89771800
C	1.69355500	2.61520200	1.49974900
C	3.00879200	3.08081500	1.35498900
H	0.96532000	3.17278200	2.08585400
H	3.29136800	4.01232700	1.84424000
N	1.80539000	-0.46709200	-0.45534700
O	0.05750300	0.97020600	1.01288600
C	2.19646300	-2.43889900	-1.85408600
H	1.32303200	-2.26187900	-2.49309800
H	1.91484500	-3.19382600	-1.10928500
H	2.99236700	-2.86225500	-2.47628900
C	-0.58484800	-2.46655400	-0.68411200
O	-0.85994900	-3.51303000	-1.09879100
C	-1.94665200	-0.93586200	1.44284500
C	-2.45105300	-0.63095700	0.17670900
O	-2.19666100	-2.15985100	1.96643400
C	-1.29163400	-2.54588200	2.98108400
H	-1.23039900	-1.77776900	3.76736800
H	-0.28870300	-2.70521900	2.55801200
H	-1.66900100	-3.47791800	3.40854000
H	-2.93257300	-1.46916500	-0.33513500
C	-2.80745000	0.69144200	-0.36047300
C	-2.81627600	1.86714500	0.39890500
C	-3.17889500	0.76264300	-1.70959400
C	-3.17841800	3.07506600	-0.18247300
H	-2.52841800	1.83733000	1.44753100
C	-3.54044800	1.97053200	-2.28986000
H	-3.17296200	-0.15179700	-2.30499800
C	-3.54019600	3.13383100	-1.52609700
H	-3.18148900	3.98080100	0.42196500
H	-3.82551300	2.00331900	-3.34017600
H	-3.82687500	4.08375500	-1.97427800
H	-1.65740300	-0.16231500	2.16395600

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SCF energy in gas phase: -1471.425558 a.u.
Enthalpy in gas phase: -1470.949129 a.u.
Free energy in gas phase: -1471.04247 a.u.
SCF energy in solution: -1471.850461 a.u.
Enthalpy in solution: -1471.374032 a.u.
Free energy in solution: -1471.467373 a.u.

Rh	-0.51938700	0.76615600	-0.06123200
C	3.74015900	1.74714400	-1.68089900
C	4.21445600	0.48101900	-1.90372400
C	3.39796600	-0.64364100	-1.64919200
C	2.09270100	-0.37800800	-1.15014200
C	2.42029700	1.92893100	-1.20449700
H	4.81091000	-2.17016200	-2.24979600
H	4.35991300	2.62149900	-1.87307800
H	5.22647400	0.32465200	-2.27913300
C	3.81332800	-1.97544400	-1.85826200
C	1.20610100	-1.45546000	-0.81096000
C	1.66060100	-2.75319400	-1.04339200
C	2.94063100	-2.99949100	-1.56119800
H	0.99508100	-3.57722400	-0.78975900
H	3.24943900	-4.03229400	-1.72134100
N	1.63891000	0.89298000	-0.95422500
O	0.03464900	-1.21902200	-0.27859700
C	1.86923800	3.30019200	-0.96702700
H	1.56910400	3.42321200	0.08315300
H	0.97331600	3.47605800	-1.57888900
H	2.60427600	4.07698000	-1.20670700
C	-1.18570900	2.46745800	0.17056900
O	-1.60815000	3.53497100	0.30785200
C	-1.21843900	0.16805900	1.93794600
C	0.09662100	0.66857300	2.04394100
H	0.14949700	1.68424900	2.44880300
C	1.33642300	-0.10932700	2.20326500
C	2.55605700	0.58110000	2.19202900
C	1.36630400	-1.50031200	2.34834700
C	3.76584300	-0.09359400	2.27639100
H	2.54417400	1.66837900	2.09323700
C	2.57692800	-2.17781500	2.42728300
H	0.43476800	-2.06254800	2.37439400
C	3.78083000	-1.48174500	2.38410000
H	4.70018000	0.46571600	2.25226400
H	2.57785400	-3.26301800	2.51896900
H	4.72674400	-2.01766800	2.44235000
O	-2.20664800	0.88950700	2.53391200
C	-3.51054000	0.61079600	2.07928200
H	-3.70124600	-0.47380600	2.04599600
H	-3.66867900	1.02489600	1.07109600
H	-4.20301900	1.08158000	2.78207700
H	-1.43018800	-0.90245600	1.81854200
C	-2.14500800	0.15784600	-1.63710900
C	-1.18088800	0.71175100	-2.18414000
H	-0.54357200	1.05222200	-2.98115700
C	-3.31760700	-0.54908000	-1.22166300
C	-4.58522500	0.03097200	-1.36694500

C	-3.19822100	-1.83513000	-0.67231800
C	-5.71673300	-0.66334600	-0.95805900
H	-4.66823100	1.02872300	-1.79597000
C	-4.33680800	-2.52167800	-0.27382200
H	-2.20017000	-2.25887400	-0.55959500
C	-5.59572400	-1.93844800	-0.41133100
H	-6.69935600	-0.20827300	-1.07033700
H	-4.24261900	-3.52043700	0.14948300
H	-6.48489500	-2.48168200	-0.09578700

TS22

SCF energy in gas phase: -1163.218469 a.u.
Enthalpy in gas phase: -1162.86528 a.u.
Free energy in gas phase: -1162.941782 a.u.
SCF energy in solution: -1163.550224 a.u.
Enthalpy in solution: -1163.197035 a.u.
Free energy in solution: -1163.273537 a.u.

Rh	0.48752000	-1.10371200	-0.06342600
C	4.77941300	0.22827100	0.41970300
C	4.62797600	1.58576900	0.34588100
C	3.36777100	2.13556800	0.02041000
C	2.31288200	1.22038800	-0.21636000
C	3.67043600	-0.62573000	0.20102300
H	3.94327200	4.21847700	0.12097900
H	5.74320300	-0.21757800	0.65701500
H	5.46891000	2.25464700	0.52902500
C	3.12557300	3.52558500	-0.07260100
C	1.03139300	1.72066500	-0.58613200
C	0.82133200	3.07979800	-0.66785700
C	1.87083600	3.97977000	-0.39708600
H	-0.16258300	3.44203700	-0.96023700
H	1.67887300	5.04892300	-0.46431200
N	2.47317900	-0.13923400	-0.09697400
O	0.08230700	0.81228900	-0.89426400
C	3.83253600	-2.10489200	0.32349600
H	3.42813500	-2.46182200	1.28094500
H	3.28741600	-2.62323300	-0.47401700
H	4.88910500	-2.39222600	0.27857700
C	0.67308700	-2.76352000	0.65587100
O	0.78857100	-3.82668700	1.11058800
C	-1.50268900	-1.12703100	-0.03273400
C	-2.01168100	0.10531200	0.42991400
H	-1.45977400	0.47648800	1.30399000
C	-3.41747100	0.55846500	0.38051000
C	-3.90565600	1.35412900	1.42578800
C	-4.27924200	0.28995600	-0.69252400
C	-5.20170900	1.85411500	1.41119200
H	-3.24926900	1.57915300	2.26805900
C	-5.57558700	0.78927400	-0.70746100
H	-3.92520500	-0.31782300	-1.52225300
C	-6.04686200	1.57256900	0.34284200
H	-5.55290700	2.46577600	2.24150200
H	-6.22507400	0.56494200	-1.55302000
H	-7.06396000	1.96096400	0.32691900
O	-2.35111800	-1.95060900	-0.63068900
C	-1.84420100	-3.09417500	-1.30545100
H	-1.03995600	-2.81003200	-1.99432400
H	-1.46676700	-3.82849300	-0.58392500
H	-2.68721200	-3.52054700	-1.85547400
H	-0.98376500	0.81639600	-0.42206800

TS23

SCF energy in gas phase: -1163.219809 a.u.
Enthalpy in gas phase: -1162.866896 a.u.
Free energy in gas phase: -1162.942311 a.u.
SCF energy in solution: -1163.550962 a.u.
Enthalpy in solution: -1163.198049 a.u.
Free energy in solution: -1163.273464 a.u.

Rh	-1.24445000	-0.56480800	0.17640100
C	2.13824300	-3.42683200	-0.67257900
C	3.20031000	-2.65508600	-0.28668100
C	2.97556600	-1.42451000	0.36946900
C	1.62594700	-1.05951600	0.59562600
C	0.81378200	-2.97739200	-0.44953600
H	5.04845700	-0.84865300	0.60234400
H	2.28921800	-4.38485300	-1.16624400
H	4.22452100	-2.97945200	-0.47168200
C	4.01464600	-0.56453700	0.79398200
C	1.33637200	0.14945300	1.29255200
C	2.36907300	0.96838800	1.69466600
C	3.70555600	0.61355000	1.42881000
H	2.13185300	1.89147800	2.22024900
H	4.50098700	1.28376400	1.74933900
N	0.57107000	-1.82139900	0.15283400
O	0.04269800	0.41057300	1.55578100
C	-0.34144400	-3.80264600	-0.91284800
H	-0.72525900	-3.43348400	-1.87421900
H	-1.16500400	-3.75839400	-0.19113200
H	-0.04674900	-4.84893700	-1.05373600
C	-2.47811800	-1.33104300	-0.92502100
O	-3.27454800	-1.82463500	-1.61217400
C	-2.22748400	1.13828600	0.42504300
C	-1.37886300	2.27149600	0.50865900
O	-3.45138300	1.35724400	0.88536700
C	-4.30993300	0.25121200	1.13392000
H	-3.78767500	-0.52216600	1.70879400
H	-4.66822100	-0.17138100	0.18741700
H	-5.15610500	0.64586800	1.70234200
H	-0.48681300	1.48028100	1.33257100
H	-1.83707200	3.13959200	0.99814700
C	-0.28199200	2.62006000	-0.42889100
C	0.06348100	1.86854200	-1.56038700
C	0.50740600	3.73878000	-0.12187200
C	1.18251100	2.19643500	-2.31942400
H	-0.54990700	1.01230100	-1.84207700
C	1.61331800	4.07556200	-0.89065900
H	0.24567000	4.34254500	0.74905400
C	1.96717200	3.29614400	-1.98906700
H	1.43193800	1.59103300	-3.19032300
H	2.20695800	4.94992000	-0.62593300
H	2.83853200	3.55312600	-2.58915000

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SCF energy in gas phase: -1163.259164 a.u.
Enthalpy in gas phase: -1162.900588 a.u.
Free energy in gas phase: -1162.979215 a.u.
SCF energy in solution: -1163.588901 a.u.
Enthalpy in solution: -1163.230325 a.u.
Free energy in solution: -1163.308952 a.u.

Rh	-0.33377900	-0.74884400	0.03846000
C	-4.84038500	-0.81557900	-0.33792800
C	-5.12276300	0.52229000	-0.26455600
C	-4.07899400	1.45388100	-0.09150500
C	-2.76339700	0.92786700	-0.00757700
C	-3.50558700	-1.27133500	-0.24736500
H	-5.30129000	3.24023200	-0.06271200
H	-5.63377800	-1.54909400	-0.46660500
H	-6.15007500	0.88112100	-0.33433000
C	-4.28803100	2.84704500	0.00460300
C	-1.64329800	1.79875700	0.17772100
C	-1.89729200	3.16538800	0.27305500
C	-3.20193900	3.67419600	0.18345200
H	-1.04863100	3.83145200	0.41825300
H	-3.35083500	4.75069900	0.26078300
N	-2.49716800	-0.41759200	-0.09276300
O	-0.43652500	1.29964000	0.25088600
C	-3.22851900	-2.73788700	-0.32561800
H	-2.62979900	-2.98461400	-1.21131900
H	-2.67169500	-3.08104300	0.55478900
H	-4.16214900	-3.30847000	-0.38108000
C	-0.17586800	-2.56744100	-0.16742500
O	-0.04394900	-3.71286400	-0.30841800
C	1.60356700	-0.55945300	0.14439300
C	2.23808000	0.50438300	-0.70418300
H	1.99258000	0.24960000	-1.74810200
C	3.70883300	0.74854600	-0.52356700
C	4.64144000	0.15877500	-1.37617400
C	4.16606200	1.56001700	0.51614200
C	6.00404200	0.37437200	-1.19634100
H	4.29322700	-0.47384400	-2.19413900
C	5.52656900	1.77621100	0.70081500
H	3.44136900	2.02710100	1.18505200
C	6.44990600	1.18353800	-0.15639800
H	6.71987800	-0.08824600	-1.87422100
H	5.86805400	2.41399800	1.51484600
H	7.51584300	1.35536100	-0.01533900
O	2.48109700	-1.16066800	0.89415100
C	2.07499900	-2.13466800	1.86267800
H	1.10469400	-1.85679600	2.28664500

H	2.01441900	-3.11663000	1.38346400
H	2.85626300	-2.13752000	2.62578800
H	1.63260000	1.40552700	-0.50139700

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SCF energy in gas phase: -1163.262185 a.u.
Enthalpy in gas phase: -1162.902908 a.u.
Free energy in gas phase: -1162.980362 a.u.
SCF energy in solution: -1163.590724 a.u.
Enthalpy in solution: -1163.231447 a.u.
Free energy in solution: -1163.308901 a.u.

Rh	0.18277900	0.71093900	0.42351600
C	-3.72906100	1.20930600	-1.79119700
C	-4.45249200	0.17033800	-1.27001900
C	-3.87475500	-0.67416300	-0.30009900
C	-2.53903200	-0.38350200	0.08270100
C	-2.40142400	1.44181900	-1.36483500
H	-5.58123100	-1.97374000	-0.00739600
H	-4.16044100	1.87205900	-2.53862200
H	-5.47707400	-0.01499000	-1.59397300
C	-4.55602500	-1.76034900	0.29142200
C	-1.87248500	-1.18583800	1.06327300
C	-2.58593800	-2.24357700	1.62409300
C	-3.90579700	-2.52109900	1.23723300
H	-2.08609200	-2.85067200	2.37688600
H	-4.42295700	-3.35903400	1.70374200
N	-1.82660800	0.66183500	-0.45341200
O	-0.63880400	-0.91323100	1.39912100
C	-1.63607300	2.58235100	-1.95400900
H	-0.75136900	2.22957600	-2.49860200
H	-1.28986100	3.27247300	-1.17481600
H	-2.25935300	3.14878300	-2.65475200
C	0.97670700	2.12837700	-0.43375900
O	1.51109300	3.00962200	-0.96893400
C	1.83077200	0.32988400	1.38319500
C	2.31864900	-1.08808500	1.40581400
O	2.63954000	1.09190400	2.07085500
C	2.35268500	2.48276800	2.26233500
H	1.27044900	2.63704100	2.31856400
H	2.77987800	3.05664200	1.43451500
H	2.83938400	2.76089700	3.19983500
H	3.11139300	-1.20234200	2.15986700
C	2.81984400	-1.46026000	0.02943600
C	4.05457500	-0.97918900	-0.40849300
C	2.04892300	-2.24281400	-0.83032200
C	4.51923900	-1.28459600	-1.68336900
H	4.65605600	-0.36383800	0.26320100
C	2.51493400	-2.55269100	-2.10369800
H	1.07723200	-2.60408800	-0.49282000
C	3.74948200	-2.07401700	-2.53300600
H	5.48572200	-0.90734000	-2.01413800
H	1.90906100	-3.17129200	-2.76404200
H	4.11282200	-2.31727500	-3.53018000
H	1.45660500	-1.71229900	1.67987500

TS24

SCF energy in gas phase: -1163.205286 a.u.
Enthalpy in gas phase: -1162.850781 a.u.
Free energy in gas phase: -1162.928809 a.u.
SCF energy in solution: -1163.536907 a.u.
Enthalpy in solution: -1163.182402 a.u.
Free energy in solution: -1163.26043 a.u.

Rh	-0.36848500	-0.76539000	0.05004600
C	-4.79639400	-0.70025400	-0.69777500
C	-5.08554000	0.60604000	-0.40994700
C	-4.05224000	1.48660700	-0.02714700
C	-2.74289700	0.94370900	0.04107300
C	-3.46820000	-1.17825700	-0.61011500
H	-5.27676200	3.25218000	0.23250800
H	-5.57991900	-1.39298600	-0.99836200
H	-6.10760100	0.98048000	-0.47408600
C	-4.26714100	2.84725200	0.28452100
C	-1.63457000	1.76914500	0.41536800
C	-1.89353500	3.10472200	0.71420000
C	-3.19339100	3.62873000	0.64751900
H	-1.05244400	3.73307100	1.00260400
H	-3.34924300	4.67943200	0.89041900
N	-2.47259100	-0.37558500	-0.24453600
O	-0.43051400	1.25669200	0.45725100
C	-3.18524600	-2.60876600	-0.93444100
H	-2.45733800	-2.69374000	-1.75034700
H	-2.76798600	-3.13630200	-0.06774200
H	-4.10097700	-3.12745200	-1.23940800
C	-0.19134000	-2.53146600	-0.36498500
O	-0.02985600	-3.65059600	-0.64120700
C	1.66156600	-0.64572300	0.40124900
C	2.36000000	0.37975400	-0.26267200
H	1.69397300	1.07503000	-0.77792400
C	3.77940500	0.68364800	-0.34374300
C	4.13608000	1.91987900	-0.90979000
C	4.79785600	-0.18790400	0.07892700
C	5.46645600	2.28374700	-1.04367400
H	3.34848600	2.59491200	-1.24499400
C	6.12817900	0.18145300	-0.05908300
H	4.53199600	-1.14813000	0.50792300
C	6.46587500	1.41287600	-0.61559300
H	5.72683600	3.24462400	-1.48305100
H	6.91118700	-0.50010000	0.26819300
H	7.51267500	1.69340800	-0.71982500
O	2.44154100	-1.51825400	1.08978700
C	1.80174000	-2.33880500	2.05573600
H	1.05437500	-1.76856800	2.62184600
H	1.31652500	-3.19977600	1.58120100
H	2.59048800	-2.69075700	2.72738800
H	1.52633400	0.43528500	0.97895500

TS25

SCF energy in gas phase: -1163.202237 a.u.
Enthalpy in gas phase: -1162.848158 a.u.
Free energy in gas phase: -1162.924889 a.u.
SCF energy in solution: -1163.535877 a.u.
Enthalpy in solution: -1163.181798 a.u.
Free energy in solution: -1163.258529 a.u.

Rh	-0.09246000	-1.07392700	0.11971200
C	4.14695300	-0.31060900	-1.14676600
C	4.37716800	0.89912100	-0.54908000
C	3.36899600	1.50362200	0.23105800
C	2.14315700	0.79710500	0.34748800
C	2.89945500	-0.95933500	-0.99479000
H	4.47462400	3.27952200	0.78433700
H	4.91546800	-0.79355400	-1.74703000
H	5.33653300	1.40464700	-0.66420500
C	3.53034400	2.74583300	0.88232100
C	1.07030300	1.32972500	1.13312800
C	1.27480100	2.55872800	1.75741000
C	2.48823100	3.25056500	1.62793800
H	0.46104200	2.96562700	2.35513600
H	2.60270100	4.20886100	2.13383600
N	1.92727800	-0.41368900	-0.27027100
O	-0.04704100	0.65969500	1.24447900
C	2.67148300	-2.27771100	-1.66031400
H	1.85947200	-2.21492800	-2.39573200
H	2.38978200	-3.04621600	-0.93003900
H	3.57511400	-2.61409900	-2.18079300
C	-0.25750800	-2.61856500	-0.84089300
O	-0.40995800	-3.60756000	-1.43290200
C	-2.06124500	-1.26397500	0.71611300
C	-3.08412000	-0.33937600	0.42717600
O	-2.58374300	-2.36018000	1.34484500
C	-1.68864100	-3.14976500	2.10510700
H	-1.06476300	-2.52588400	2.76013700
H	-1.03584500	-3.75129200	1.45941600
H	-2.31080700	-3.81426100	2.71236100
H	-1.91020700	-0.32655000	1.46207200
C	-3.03622600	0.89214300	-0.33021100
C	-4.05973400	1.82932300	-0.10798500
C	-2.04666900	1.17864200	-1.28601300
C	-4.07679800	3.03473400	-0.79060100
H	-4.83851900	1.60234100	0.62055800
C	-2.06621800	2.38787800	-1.96425400
H	-1.26909200	0.43773400	-1.48186500
C	-3.07491400	3.31669000	-1.71737100
H	-4.87017200	3.75595100	-0.60494100
H	-1.29471400	2.60316600	-2.70089300
H	-3.08834100	4.26036800	-2.26032600
H	-4.04947600	-0.57317800	0.89470300

TS1-s

SCF energy in gas phase: -1160.822201 a.u.

Enthalpy in gas phase: -1160.514558 a.u.
Free energy in gas phase: -1160.588068 a.u.
SCF energy in solution: -1161.150123 a.u.
Enthalpy in solution: -1160.84248 a.u.
Free energy in solution: -1160.91599 a.u.

Rh	1.61808800	-0.40001600	-0.15224400
C	-0.40836200	3.30228200	1.15440400
C	-1.57775500	3.24725400	0.44458200
C	-1.81037500	2.19928700	-0.47189100
C	-0.78209700	1.22235800	-0.60280100
C	0.58239700	2.31054600	0.97869200
H	-3.77614600	2.82511700	-1.11483500
H	-0.21771000	4.10782000	1.86068500
H	-2.34400200	4.01161000	0.57832900
C	-2.99328900	2.07626400	-1.22491200
C	-0.92952600	0.10444700	-1.49760800
C	-2.12233400	0.04602500	-2.23483300
C	-3.12393900	1.00903600	-2.09254500
H	-2.24715800	-0.79610900	-2.91332000
H	-4.03395900	0.90961900	-2.68409800
N	0.38064400	1.30610000	0.12879400
O	-0.00049600	-0.78656700	-1.60164900
C	1.86972700	2.40776200	1.73209900
H	2.11857900	1.46152100	2.22641600
H	2.70549000	2.65112800	1.06138500
H	1.81262000	3.19553100	2.49146300
C	2.52612900	-1.99285100	-0.49546000
O	3.03838700	-2.99723700	-0.71540000
C	0.25058100	-1.28910100	1.54268400
C	1.38307700	-1.01810100	1.97893600
H	2.17311100	-1.00900300	2.70994800
C	-1.12097700	-1.56831500	1.25646900
C	-1.47755000	-2.69433600	0.50197700
C	-2.11648400	-0.68090700	1.69179300
C	-2.81104100	-2.93593700	0.20871300
H	-0.69591300	-3.35853400	0.13668700
C	-3.44838400	-0.92987700	1.39031600
H	-1.83124600	0.20019000	2.26707300
C	-3.79724300	-2.05596000	0.64994300
H	-3.08347400	-3.81068600	-0.37878400
H	-4.21626000	-0.23681700	1.72897000
H	-4.84191700	-2.24663100	0.41029100
C	3.09510300	0.65376400	-0.74878000
O	3.94630900	1.34272900	-1.10813400

1-s
SCF energy in gas phase: -1160.822261 a.u.
Enthalpy in gas phase: -1160.513647 a.u.
Free energy in gas phase: -1160.589361 a.u.
SCF energy in solution: -1161.150132 a.u.
Enthalpy in solution: -1160.841518 a.u.
Free energy in solution: -1160.917232 a.u.

Rh	-1.61066200	-0.39275400	0.13350900
C	0.43966200	3.28604000	-1.20481000
C	1.61450900	3.22286200	-0.50420700
C	1.83786100	2.18753300	0.42871000
C	0.79638600	1.22773700	0.58156500
C	-0.56223700	2.30946400	-1.00958500
H	3.81465300	2.79739300	1.05351900
H	0.25429700	4.08588000	-1.91894600
H	2.39045000	3.97420900	-0.65484100
C	3.02130900	2.06241500	1.18053500
C	0.92434200	0.13144500	1.50692800
C	2.12029700	0.06969600	2.23895200
C	3.13763900	1.01190900	2.07026200
H	2.23192000	-0.75423700	2.94163300
H	4.04790700	0.91073900	2.66117100
N	-0.36493900	1.31244400	-0.15030700
O	-0.02335700	-0.73469700	1.64125200
C	-1.85775800	2.41538900	-1.74760100
H	-2.10663400	1.47999200	-2.26232700
H	-2.68730000	2.63474700	-1.06107700
H	-1.81483400	3.22180100	-2.48807000
C	-2.54503900	-1.97656500	0.44366600
O	-3.07944100	-2.97423200	0.64009200
C	-0.29250600	-1.27975600	-1.49731600
C	-1.40693300	-0.97918500	-1.97472400
H	-2.15963000	-0.96392900	-2.74551600
C	1.07726400	-1.59425900	-1.22455600
C	1.41299000	-2.71490500	-0.45316100
C	2.08976800	-0.73675900	-1.67894200
C	2.74225400	-2.98121900	-0.16186900
H	0.61903200	-3.35576800	-0.07283400
C	3.41736100	-1.00868200	-1.37722100
H	1.82079000	0.14176200	-2.26599300
C	3.74533100	-2.12947400	-0.61991400
H	2.99831200	-3.85248500	0.43808900
H	4.19855100	-0.33793100	-1.73005100
H	4.78657000	-2.33798200	-0.38014400
C	-3.02837500	0.69032900	0.85525200
O	-3.83026100	1.40374700	1.27088800

TS2-s
SCF energy in gas phase: -1160.813021 a.u.
Enthalpy in gas phase: -1160.505963 a.u.
Free energy in gas phase: -1160.5835 a.u.
SCF energy in solution: -1161.137343 a.u.
Enthalpy in solution: -1160.830285 a.u.
Free energy in solution: -1160.907822 a.u.

Rh	-0.14166400	1.30598100	0.17811400
C	1.65192400	-2.01124600	-2.32960100
C	2.61883800	-2.46441400	-1.47620600
C	2.82157000	-1.82395700	-0.23620800
C	1.96002100	-0.73512100	0.06943000
C	0.82678200	-0.91875900	-1.97111900
H	4.47975400	-3.04405800	0.42177000
H	1.49961800	-2.47726200	-3.30117700
H	3.25294500	-3.30838200	-1.74912100
C	3.83062700	-2.20603100	0.67076300
C	2.12372900	-0.01009100	1.29257800
C	3.14647600	-0.41529500	2.15327400
C	3.97750600	-1.49836200	1.84462000
H	3.27235000	0.14110500	3.08008600
H	4.75782200	-1.78028900	2.55061100
N	0.96398700	-0.31816900	-0.79116700
O	1.34104500	0.99188100	1.58374300
C	-0.18632800	-0.44719500	-2.96619200
H	-1.19906100	-0.78198500	-2.70617000
H	-0.20865100	0.64612500	-3.02962800
H	0.05274400	-0.84551600	-3.95871400
C	-0.96931100	2.51109100	1.32336500
O	-1.47042200	3.23822500	2.05873100
C	-2.01574400	0.52773200	-0.43713600
C	-1.76888700	1.51402800	-1.18087900
H	-1.97232600	2.22813300	-1.96316200
C	-2.65876400	-0.65599800	0.06624300
C	-2.08412600	-1.41799800	1.09188500
C	-3.87303100	-1.07074200	-0.50356200
C	-2.71634100	-2.57124200	1.53914900
H	-1.14051100	-1.08844000	1.52915100
C	-4.49711600	-2.22334800	-0.05004700
H	-4.31656900	-0.47450700	-1.30014500
C	-3.92083600	-2.97628200	0.97149500
H	-2.26407100	-3.15647400	2.33763100
H	-5.43985500	-2.53772600	-0.49464500
H	-4.41312600	-3.88051700	1.32510700
C	1.19897900	2.80614600	-1.11650600
O	0.93814200	3.31243100	-2.11130400

2-s
SCF energy in gas phase: -1047.556131 a.u.
Enthalpy in gas phase: -1047.257744 a.u.
Free energy in gas phase: -1047.329813 a.u.
SCF energy in solution: -1047.847987 a.u.
Enthalpy in solution: -1047.5496 a.u.
Free energy in solution: -1047.621669 a.u.

Rh	-0.07875300	1.22140700	-0.45888000
C	1.74621700	-2.91951200	-0.99232000
C	2.93721300	-2.73920700	-0.34507300
C	3.24229300	-1.48647800	0.22154600
C	2.26098100	-0.46820500	0.08787000
C	0.80996000	-1.86405600	-1.09481900
H	5.19519100	-2.01447100	0.98582800
H	1.49648200	-3.87813900	-1.44222700
H	3.66033900	-3.55127900	-0.26443100
C	4.45522900	-1.22108200	0.89235100
C	2.50697800	0.83070800	0.62779900
C	3.71593700	1.05160100	1.28277200

C	4.67290800	0.03550900	1.41084600
H	3.89268300	2.04443900	1.69198600
H	5.60513800	0.25280400	1.93075300
N	1.05795800	-0.66757000	-0.56000200
O	1.61231300	1.78047700	0.50417800
C	-0.46314200	-2.13836200	-1.82986700
H	-1.33411000	-2.10262900	-1.16294800
H	-0.63618600	-1.40275100	-2.62226700
H	-0.42623700	-3.13509900	-2.28249300
C	-0.78850800	2.90270000	-0.19101800
O	-1.22319600	3.95432100	-0.01580000
C	-2.01639200	0.39333400	-0.82277000
C	-1.58021800	0.84540500	-1.90948000
H	-1.58898700	1.14682400	-2.94413500
C	-2.85387200	-0.30466300	0.11415600
C	-2.54195300	-0.34296500	1.47918200
C	-3.98792400	-0.98863100	-0.35240500
C	-3.35481900	-1.04518400	2.36016900
H	-1.65647200	0.18583600	1.83175000
C	-4.79315600	-1.68901300	0.53403400
H	-4.22283600	-0.96140500	-1.41593600
C	-4.47913100	-1.71858100	1.89157800
H	-3.10732000	-1.06675100	3.41990200
H	-5.67137400	-2.21622000	0.16526000
H	-5.11267000	-2.26978400	2.58426100

TS3-s

SCF energy in gas phase: -1047.481827 a.u.
Enthalpy in gas phase: -1047.187448 a.u.
Free energy in gas phase: -1047.258824 a.u.
SCF energy in solution: -1047.777616 a.u.
Enthalpy in solution: -1047.483237 a.u.
Free energy in solution: -1047.554613 a.u.

Rh	0.04743700	1.29413800	0.40818400
C	-1.54553700	-2.87411900	1.16838000
C	-2.73139900	-2.80423200	0.49075700
C	-3.10999200	-1.60197100	-0.13987900
C	-2.19819900	-0.51729500	-0.04529000
C	-0.67884400	-1.75751100	1.22515900
H	-5.01928400	-2.28281300	-0.89316700
H	-1.24582900	-3.78744100	1.67801700
H	-3.39910600	-3.66486200	0.44299500
C	-4.33182200	-1.44102800	-0.82663700
C	-2.52607000	0.74565100	-0.62363600
C	-3.74446100	0.86432900	-1.28901200
C	-4.62846800	-0.21860300	-1.38820400
H	-3.98934600	1.83059700	-1.72563400
H	-5.57092500	-0.08118700	-1.91686700
N	-0.98971500	-0.61383200	0.61437400
O	-1.69891900	1.75500100	-0.51476800
C	0.59175400	-1.88710100	1.99822600
H	0.73667800	-1.03838000	2.67989300
H	0.58363100	-2.80651900	2.59351400
H	1.46700800	-1.93044900	1.33585500
C	0.66104900	3.00639100	0.06802800
O	1.04351600	4.07137100	-0.14498200
C	1.58770300	0.94768000	1.91512400
C	2.04416200	0.58856700	0.72464200
C	2.83272900	-0.26360300	-0.16477900
C	2.40816900	-0.48715900	-1.47629600
C	3.99595700	-0.88168300	0.31135400
C	3.14150300	-1.32830000	-2.30583700
H	1.49775000	0.00048000	-1.82544600
C	4.72663200	-1.71338100	-0.52530600
H	4.31104300	-0.70769600	1.33997000
C	4.29917400	-1.93781700	-1.83312700
H	2.80759700	-1.50521700	-3.32628800
H	5.63082400	-2.19315600	-0.15544800
H	4.87427300	-2.59285300	-2.48519100
H	2.58799300	1.57626400	1.16490000

3-s

SCF energy in gas phase: -1047.496904 a.u.
Enthalpy in gas phase: -1047.199096 a.u.
Free energy in gas phase: -1047.270316 a.u.
SCF energy in solution: -1047.788054 a.u.
Enthalpy in solution: -1047.490246 a.u.
Free energy in solution: -1047.561466 a.u.

Rh	-0.00580900	1.32357600	-0.34358300
C	1.23625400	-2.99347500	-0.95008700
C	2.50331600	-2.95828600	-0.44034500
C	3.02606600	-1.74612000	0.05435800
C	2.17116300	-0.61362000	0.00160500
C	0.42540900	-1.83256600	-0.96343600
H	4.97596800	-2.49855300	0.60287800
H	0.81992700	-3.91560000	-1.35022500
H	3.12453500	-3.85414300	-0.42268600
C	4.33306200	-1.62044400	0.56767800
C	2.64311500	0.65676500	0.44099200
C	3.94241600	0.74196500	0.93652800
C	4.76905700	-0.38707400	1.00042300
H	4.29454400	1.71571700	1.27102500
H	5.77774500	-0.27861100	1.39694300
N	0.87912400	-0.67260200	-0.48470000
O	1.86263900	1.70641500	0.37344000
C	-0.94999500	-1.95471400	-1.52186500
H	-1.22421700	-1.06496200	-2.11051100
H	-1.02055500	-2.83270100	-2.17399400
H	-1.69728600	-2.06873500	-0.72530100
C	-0.40671700	3.10096400	0.06469100
O	-0.66770000	4.18419400	0.34395300
C	-1.47030600	1.00405300	-1.66178000
C	-2.21909800	1.13339700	-0.51256200
C	-2.91437800	0.01425300	0.19085000
C	-2.43350800	-0.49203200	1.39902400
C	-4.06709500	-0.53339400	-0.37710200
C	-3.09405900	-1.54394000	2.02643800
H	-1.52628000	-0.06690200	1.82970800
C	-4.72321500	-1.58540400	0.25232900
H	-4.43611900	-0.13937800	-1.32385200
C	-4.23660700	-2.09451300	1.45345200
H	-2.70954000	-1.93661100	2.96627800
H	-5.61630700	-2.01286100	-0.20057600
H	-4.74926100	-2.92021200	1.94392900
H	-2.67441200	2.12106800	-0.35577300

TS4-s

SCF energy in gas phase: -1047.496183 a.u.
Enthalpy in gas phase: -1047.199486 a.u.
Free energy in gas phase: -1047.270133 a.u.
SCF energy in solution: -1047.788657 a.u.
Enthalpy in solution: -1047.49196 a.u.
Free energy in solution: -1047.562607 a.u.

Rh	0.10764800	1.14204800	-0.26208800
C	1.49780400	-3.13126600	-0.19340600
C	2.84468500	-2.94992300	-0.02738300
C	3.36751700	-1.64991300	0.13574200
C	2.43442800	-0.58238400	0.09990300
C	0.62154900	-2.02170400	-0.21782400
H	5.45087000	-2.19322300	0.34635200
H	1.07500600	-4.12748200	-0.30596900
H	3.52360000	-3.80286500	-0.00991500
C	4.73676700	-1.37143300	0.32988500
C	2.86139400	0.76419600	0.28568400
C	4.22100100	0.99793000	0.47155400
C	5.13886500	-0.06314800	0.49056600
H	4.54899800	2.02602000	0.61069200
H	6.19427300	0.16081700	0.64055000
N	1.08922300	-0.78145700	-0.09599100
O	1.97512700	1.73243100	0.30402300
C	-0.84146600	-2.23066900	-0.38282400
H	-1.18676500	-1.73238500	-1.30249700
H	-1.09043900	-3.29602600	-0.44188800
H	-1.40578900	-1.78575000	0.44798300
C	-0.43241800	2.88953100	0.02599500
O	-0.75496100	3.96566300	0.28415100
C	-1.27671000	0.61038900	-1.56947200
C	-2.34880900	1.05048300	-0.86550000
C	-3.31677100	0.12948700	-0.22734800
C	-3.65946700	0.29971400	1.11747300
C	-3.87212300	-0.92803100	-0.95212600
C	-4.52719400	-0.59309900	1.73353100
H	-3.21807300	1.12161200	1.68186000
C	-4.74561000	-1.81537700	-0.33235700
H	-3.61670200	-1.04509700	-2.00448400
C	-5.06865100	-1.65425900	1.01120500
H	-4.78025700	-0.46132500	2.78399800
H	-5.17586600	-2.63629200	-0.90330300
H	-5.74852300	-2.35249700	1.49605900

H	-2.60912000	2.11462200	-0.87870000

4-s

SCF energy in gas phase: -1047.550029 a.u.
Enthalpy in gas phase: -1047.251234 a.u.
Free energy in gas phase: -1047.323109 a.u.
SCF energy in solution: -1047.839947 a.u.
Enthalpy in solution: -1047.541152 a.u.
Free energy in solution: -1047.613027 a.u.

Rh	0.31321300	1.17704800	-0.10433300
C	1.63847000	-3.13374300	-0.24723200
C	2.99592300	-2.97528900	-0.16240500
C	3.54335400	-1.68818300	0.00232800
C	2.62660000	-0.60692500	0.04420700
C	0.77619400	-2.01470600	-0.19357700
H	5.62259800	-2.27929400	0.09439400
H	1.19700200	-4.12242500	-0.35317700
H	3.66180800	-3.83764200	-0.20401500
C	4.92772800	-1.44195400	0.13486700
C	3.09346800	0.72692000	0.24320100
C	4.46394400	0.92587600	0.37697300
C	5.36448400	-0.14948700	0.31733600
H	4.81650900	1.94376900	0.53109400
H	6.42990800	0.05054900	0.42300200
N	1.26550400	-0.77995500	-0.07764500
O	2.23172500	1.71289600	0.30807900
C	-0.69808500	-2.24341000	-0.25392900
H	-1.21868300	-1.71184000	0.55157800
H	-1.12061200	-1.88390700	-1.19990400
H	-0.92467200	-3.31122000	-0.16224300
C	-0.28289500	2.94601800	0.00817200
O	-0.65451600	4.02910600	0.08081900
C	-1.37997200	0.72848700	-0.66109200
C	-2.58717000	0.49159600	-1.13062200
C	-3.70761400	-0.09162500	-0.38581300
C	-4.84834400	-0.51934500	-1.07338700
C	-3.66329300	-0.24478000	1.00782400
C	-5.91524500	-1.09013400	-0.38985000
H	-4.89350700	-0.40073800	-2.15625800
C	-4.72870400	-0.81890900	1.68611500
H	-2.78865200	0.10794600	1.55657100
C	-5.85930700	-1.24505500	0.99148700
H	-6.79628300	-1.41441300	-0.94145800
H	-4.68019800	-0.92806200	2.76843400
H	-6.69477800	-1.69239400	1.52689100
H	-2.73843400	0.70406700	-2.19521600

TS5-s

SCF energy in gas phase: -1047.523313 a.u.
Enthalpy in gas phase: -1047.226891 a.u.
Free energy in gas phase: -1047.299238 a.u.
SCF energy in solution: -1047.821965 a.u.
Enthalpy in solution: -1047.525543 a.u.
Free energy in solution: -1047.59789 a.u.

Rh	-0.26799900	-0.96774800	-0.51356800
C	-2.42421500	2.98338000	-0.46495100
C	-3.60880500	2.61183000	0.11163900
C	-3.82401800	1.26775300	0.47848100
C	-2.76207400	0.35925700	0.21978000
C	-1.40872400	2.02797100	-0.69576900
H	-5.82251600	1.51240400	1.26847800
H	-2.24297300	4.01633900	-0.75545000
H	-4.39533800	3.34539300	0.29154900
C	-5.01597600	0.80693300	1.07488300
C	-2.89222100	-1.02391200	0.55907000
C	-4.08891400	-1.43514400	1.14983400
C	-5.12733400	-0.52893500	1.39803200
H	-4.18883600	-2.48741900	1.40884600
H	-6.04398100	-0.89677900	1.85818000
N	-1.57538000	0.75158000	-0.35770700
O	-1.92082000	-1.85692300	0.31452400
C	-0.13504700	2.46623000	-1.34329700
H	0.73632400	2.19320800	-0.73741100
H	-0.00782800	1.99482100	-2.32751600
H	-0.13066300	3.55157000	-1.49288400
C	0.61314200	-2.58229300	-0.48155100
O	1.17509500	-3.59035300	-0.43812400
C	1.57047600	-0.15535800	-1.23499000
C	2.65032700	0.12196500	-0.70079000
C	3.85153500	0.39499800	-0.01090800
C	4.19776600	1.71531200	0.32836000
C	4.71106400	-0.66113700	0.34341800
C	5.37990600	1.97027400	1.00463800
H	3.52595400	2.52600700	0.05096300
C	5.88709200	-0.39668600	1.02679200
H	4.43003100	-1.67938700	0.08001200
C	6.22218600	0.91604200	1.35485200
H	5.64722000	2.99230800	1.26521400
H	6.54735800	-1.21488100	1.30657300
H	7.14811800	1.11983000	1.88986400
H	1.07353200	-0.25848800	-2.20826500

5-s

SCF energy in gas phase: -1047.526978 a.u.
Enthalpy in gas phase: -1047.229328 a.u.
Free energy in gas phase: -1047.30265 a.u.
SCF energy in solution: -1047.824688 a.u.
Enthalpy in solution: -1047.527038 a.u.
Free energy in solution: -1047.60036 a.u.

Rh	-0.41705200	1.11496700	0.43542200
C	-2.09724300	-3.04363900	0.63779500
C	-3.30296200	-2.84823800	0.01814500
C	-3.67828000	-1.55586200	-0.40091000
C	-2.74289700	-0.51507200	-0.16455400
C	-1.21075700	-1.96264900	0.84407000
H	-5.62261100	-2.06542100	-1.20217600
H	-1.80070600	-4.03143400	0.98442100
H	-3.98785400	-3.68062700	-0.14549600
C	-4.91220700	-1.26092200	-1.01894200
C	-3.04755300	0.83060100	-0.52619500
C	-4.27785000	1.08012600	-1.12880800
C	-5.18990100	0.04201400	-1.36987800
H	-4.51156200	2.10701700	-1.40272500
H	-6.14074200	0.28040700	-1.84491900
N	-1.52060300	-0.73622400	0.42946400
O	-2.18794200	1.78825800	-0.27557100
C	0.07687800	-2.20430400	1.56223000
H	0.93997700	-1.94871200	0.93714500
H	0.13822400	-1.58982600	2.47039700
H	0.16139900	-3.25437400	1.86162200
C	0.24707600	2.84780700	0.34955100
O	0.63109300	3.93018600	0.28746000
C	1.53546700	0.43759800	0.60297900
C	2.67710400	0.10932400	0.27947900
C	3.96711300	-0.28968500	-0.14821000
C	4.23646200	-1.64112300	-0.42652600
C	4.99497700	0.65771700	-0.29622900
C	5.50013500	-2.03094100	-0.84197200
H	3.43908700	-2.37415300	-0.31392000
C	6.25612800	0.25868700	-0.71185800
H	4.78267200	1.70347500	-0.08150900
C	6.51169300	-1.08343700	-0.98508900
H	5.69997700	-3.07902000	-1.05742900
H	7.04586000	0.99882400	-0.82663300
H	7.50293400	-1.39238500	-1.31220000
H	0.95943300	0.59071600	1.58759200

TS6-s

SCF energy in gas phase: -1047.507034 a.u.
Enthalpy in gas phase: -1047.21237 a.u.
Free energy in gas phase: -1047.285292 a.u.
SCF energy in solution: -1047.808111 a.u.
Enthalpy in solution: -1047.513447 a.u.
Free energy in solution: -1047.586369 a.u.

Rh	0.38706500	-1.04341600	0.01737200
C	2.14154200	3.11807800	0.01460700
C	3.47913100	2.82618700	0.00131800
C	3.90575200	1.48346300	-0.00963200
C	2.88762400	0.49104200	-0.00445400
C	1.18103600	2.08180700	0.02009100
H	6.03421400	1.86922000	-0.02995100
H	1.79527300	4.14970100	0.02081300
H	4.22471900	3.62190300	-0.00265300
C	5.26312600	1.10036400	-0.02662100
C	3.22892200	-0.89904600	-0.02042900
C	4.58529100	-1.23029700	-0.03888400
C	5.57763000	-0.24186800	-0.04033700
H	4.84662900	-2.28676100	-0.05091200

H	6.62299700	-0.54899800	-0.05350300
N	1.54636800	0.80192100	0.01231000
O	2.29241200	-1.80219900	-0.01596500
C	-0.26827500	2.44725300	0.03101100
H	-0.78569600	2.03212600	-0.84189800
H	-0.76945500	2.05556600	0.92545100
H	-0.39031400	3.53630900	0.02249300
C	-0.30746700	-2.75108300	-0.00082800
O	-0.73410400	-3.82302800	-0.01612900
C	-1.47827700	-0.40084400	0.00175000
C	-2.70564600	-0.10829900	-0.03382000
C	-4.08437200	0.24604700	-0.02603800
C	-4.47198700	1.59675800	-0.04316800
C	-5.06610500	-0.75938900	-0.01063100
C	-5.81748400	1.93056000	-0.04132500
H	-3.70503200	2.36969400	-0.06066200
C	-6.40936200	-0.41588900	-0.01109300
H	-4.75373600	-1.80193400	-0.00322700
C	-6.78398300	0.92622700	-0.02469500
H	-6.11739500	2.97635700	-0.05449300
H	-7.16877200	-1.19485000	-0.00084300
H	-7.83935200	1.19291600	-0.02429100
H	-1.84560500	-0.27562000	1.12160300

TS7-s

SCF energy in gas phase: -1047.514614 a.u.
Enthalpy in gas phase: -1047.219782 a.u.
Free energy in gas phase: -1047.292451 a.u.
SCF energy in solution: -1047.812014 a.u.
Enthalpy in solution: -1047.517182 a.u.
Free energy in solution: -1047.589851 a.u.

Rh	0.43241500	-1.14679400	0.26243100
C	1.92635300	3.05520700	0.62514100
C	3.21306300	2.90060000	0.18320400
C	3.68259600	1.62340000	-0.18166100
C	2.75870500	0.55345300	-0.07940600
C	1.04991500	1.94884500	0.70785400
H	5.70230300	2.19925000	-0.70354000
H	1.55310800	4.03169600	0.92560600
H	3.88708500	3.75514700	0.12054100
C	5.00046100	1.37074600	-0.62320200
C	3.15409500	-0.77501000	-0.40508700
C	4.46057800	-0.98421500	-0.82971500
C	5.36752900	0.08246200	-0.93876900
H	4.75874400	-2.00146700	-1.07540100
H	6.38180100	-0.12292600	-1.27771800
N	1.45827000	0.73228900	0.34424200
O	2.28551900	-1.75771000	-0.29278200
C	-0.33552600	2.16556100	1.21844900
H	-1.08101300	2.00082700	0.43152500
H	-0.57791400	1.46316900	2.02441200
H	-0.44631300	3.18507800	1.60259000
C	-0.23907600	-2.89483100	0.21648600
O	-0.65605300	-3.96088300	0.20669800
C	-1.43381200	-0.52761700	0.09563300
C	-2.60800000	-0.20414900	-0.02915400
C	-3.94908300	0.23810100	-0.22287600
C	-5.03143000	-0.56094900	0.17676900
C	-4.21142200	1.48717100	-0.80802200
C	-6.33508100	-0.11957100	-0.00159200
H	-4.83151200	-1.53079100	0.62949400
C	-5.51748200	1.92201800	-0.98447400
H	-3.37346100	2.10560500	-1.12808300
C	-6.58364800	1.12194700	-0.58170400
H	-7.16542300	-0.74973200	0.31319700
H	-5.70522900	2.89238000	-1.44172200
H	-7.60733600	1.46525400	-0.72116600
H	-0.40953600	-0.88404500	1.54259800

6-s

SCF energy in gas phase: -1047.514894 a.u.
Enthalpy in gas phase: -1047.218658 a.u.
Free energy in gas phase: -1047.291911 a.u.
SCF energy in solution: -1047.812661 a.u.
Enthalpy in solution: -1047.516425 a.u.
Free energy in solution: -1047.589678 a.u.

Rh	-0.42896000	1.13462100	0.21944800
C	-1.94396000	-3.05096200	0.59423400
C	-3.24425600	-2.88495700	0.19919900
C	-3.71568300	-1.60354900	-0.14811000
C	-2.78049500	-0.54095000	-0.07675000
C	-1.05513100	-1.95256200	0.64773300
H	-5.75542300	-2.16426500	-0.60225200
H	-1.56815700	-4.03099800	0.87946000
H	-3.92711200	-3.73386500	0.16005800
C	-5.04542200	-1.34081700	-0.54492800
C	-3.17661300	0.79173400	-0.38654400
C	-4.49564700	1.01011800	-0.76850600
C	-5.41318900	-0.04954400	-0.84853200
H	-4.79430200	2.02969000	-1.00375800
H	-6.43672100	0.16349900	-1.15316900
N	-1.46709000	-0.73172500	0.29977900
O	-2.29757100	1.76547400	-0.30007700
C	0.34591100	-2.18601200	1.10305300
H	1.05663200	-2.06455100	0.27695000
H	0.64707300	-1.46222500	1.86835700
H	0.45009600	-3.19617100	1.51316000
C	0.28681300	2.86484500	0.21856500
O	0.73635100	3.91685500	0.24578500
C	1.44070400	0.50835600	0.09147100
C	2.61812000	0.19438100	-0.02719400
C	3.96484300	-0.24018000	-0.20330400
C	5.03797300	0.56532700	0.20827500
C	4.24321000	-1.48711600	-0.78561900
C	6.34659200	0.13276800	0.04483500
H	4.82653400	1.53398000	0.65834000
C	5.55395900	-1.91385100	-0.94676800
H	3.41375900	-2.11164400	-1.11602600
C	6.61044900	-1.10709800	-0.53204400
H	7.16890300	0.76894100	0.36868400
H	5.75300800	-2.88315600	-1.40159200
H	7.63796000	-1.44355800	-0.65974500
H	0.12125800	0.94023600	1.63786600

TS8-s

SCF energy in gas phase: -1047.465452 a.u.
Enthalpy in gas phase: -1047.172432 a.u.
Free energy in gas phase: -1047.243937 a.u.
SCF energy in solution: -1047.761304 a.u.
Enthalpy in solution: -1047.468284 a.u.
Free energy in solution: -1047.539789 a.u.

Rh	0.15080500	-1.04289500	-0.30546100
C	2.03495300	3.03968000	-0.50757500
C	3.30997200	2.74050500	-0.11234200
C	3.64980000	1.41238100	0.21348600
C	2.61557700	0.44679900	0.10986200
C	1.04509400	2.03224700	-0.59100700
H	5.72693700	1.76851800	0.69705100
H	1.75555200	4.05917200	-0.76423700
H	4.07141200	3.51787600	-0.04497400
C	4.94193900	1.01779900	0.62126100
C	2.87903600	-0.91844800	0.41499700
C	4.16538200	-1.27050600	0.80914200
C	5.18004700	-0.30717400	0.91004600
H	4.35948800	-2.31652400	1.03751400
H	6.17424000	-0.62212300	1.22374800
N	1.33338700	0.76519100	-0.29030800
O	1.91732100	-1.81062000	0.32012200
C	-0.32894000	2.42078400	-1.02290800
H	-0.65197800	1.83647200	-1.89243700
H	-1.06815000	2.23944500	-0.23134100
H	-0.36025600	3.48557100	-1.27687300
C	-0.62112500	-2.73394600	-0.18198200
O	-1.08866400	-3.77784800	-0.09857600
C	-1.45128600	-0.48497200	-1.63694600
C	-2.25522300	-0.16437800	-0.69086000
C	-3.46077100	0.26276500	-0.02812900
C	-3.45639500	0.68059900	1.30886200
C	-4.66392900	0.28073000	-0.75042100
C	-4.63321800	1.10453600	1.91214000
H	-2.52384000	0.66524700	1.87463500
C	-5.83071800	0.71889300	-0.14212800
H	-4.66522900	-0.05154800	-1.78693300
C	-5.82179100	1.12866000	1.18963400
H	-4.61973200	1.42002200	2.95378100
H	-6.75851400	0.73264600	-0.71134200
H	-6.74250700	1.46382500	1.66342200
H	-1.23702200	-0.35862100	0.31272700

TS9-s

SCF energy in gas phase: -1163.139572 a.u.
Enthalpy in gas phase: -1162.787442 a.u.
Free energy in gas phase: -1162.864409 a.u.
SCF energy in solution: -1163.475236 a.u.
Enthalpy in solution: -1163.123106 a.u.
Free energy in solution: -1163.200073 a.u.

Rh	0.25344200	0.44102300	-0.26966700
C	4.46956500	1.85589000	0.50272700
C	5.14556500	0.66463100	0.48860200
C	4.44833300	-0.53968200	0.26399100
C	3.04687400	-0.43587600	0.06445200
C	3.07238400	1.88824300	0.29537000
H	6.14776900	-1.87622700	0.37893700
H	4.99385100	2.79428700	0.67153100
H	6.22400200	0.63313100	0.64681100
C	5.07198000	-1.80591900	0.22569200
C	2.25388100	-1.60438500	-0.17413100
C	2.91519300	-2.83194600	-0.20882200
C	4.30106300	-2.92226900	-0.01031500
H	2.32140400	-3.72391900	-0.40151400
H	4.77245000	-3.90391100	-0.04788500
N	2.38478600	0.76809900	0.08540200
O	0.96540600	-1.49255200	-0.35218800
C	2.36409600	3.20452800	0.31204800
H	1.61260300	3.24448500	1.11036200
H	1.84762400	3.39022100	-0.63772500
H	3.07309000	4.02344200	0.47603600
C	-0.44970100	2.13692200	-0.19688400
O	-0.94716200	3.18269300	-0.16311400
C	-1.54121800	-0.15619100	-0.61230500
C	-2.78774100	0.32182300	-1.05390300
C	-4.05607800	0.06554000	-0.30603700
C	-5.28468600	0.11070200	-0.97851300
C	-4.06045900	-0.18490100	1.07383900
C	-6.47598200	-0.09577600	-0.29689800
H	-5.29239100	0.30991600	-2.05049100
C	-5.25496500	-0.41306300	1.74974700
H	-3.11891500	-0.15382800	1.62402300
C	-6.46690900	-0.37090200	1.06894600
H	-7.42029500	-0.05084300	-0.83752600
H	-5.23728100	-0.60001200	2.82258600
H	-7.40197400	-0.53785000	1.60053600
O	-1.82501600	-1.60208200	-0.65220600
C	-1.67018600	-2.47499700	0.48868200
H	-0.93053800	-2.01865800	1.15057800
H	-1.30003600	-3.43215900	0.11765000
H	-2.64440600	-2.57472600	0.98018200
H	-2.75284600	-1.16895000	-1.26360900
H	-2.78438500	1.24420300	-1.64095600

7-s

SCF energy in gas phase: -1163.258837 a.u.
Enthalpy in gas phase: -1162.977895 a.u.
Free energy in gas phase: -1140.532437 a.u.
SCF energy in solution: -1163.58809 a.u.
Enthalpy in solution: -1163.229199 a.u.
Free energy in solution: -1163.307148 a.u.

Rh	0.29192500	0.61859400	0.16819100
C	4.70277400	1.36619100	-0.39579600
C	5.17945300	0.08313300	-0.43238800
C	4.29152200	-1.00314800	-0.29193300
C	2.91868300	-0.68570500	-0.11849300
C	3.32172700	1.61158400	-0.22220900
H	5.75783500	-2.58729800	-0.45140000
H	5.37504900	2.21540300	-0.50001400
H	6.24339400	-0.11352200	-0.56833600
C	4.70291000	-2.35347100	-0.31605400
C	1.94382500	-1.72288200	0.03812700
C	2.39654500	-3.04061200	0.00443000
C	3.75593600	-3.34234100	-0.16911500
H	1.65901600	-3.83358400	0.11704400
H	4.06178300	-4.38794400	-0.18752500
N	2.45880000	0.60823600	-0.08885600
O	0.68457800	-1.41437700	0.20910100
C	2.82751100	3.02175900	-0.18920300
H	2.13397100	3.21701900	-1.01694100
H	2.29194000	3.23335200	0.74454400
H	3.65982800	3.72929600	-0.27192800
C	-0.15234000	2.39777800	0.05343100
O	-0.50213900	3.50036100	-0.04376800
C	-1.61126400	0.20659000	0.31708300
C	-2.62028800	0.62153200	-0.72378900
H	-2.64934000	1.72355600	-0.69249700
C	-4.00295700	0.04353100	-0.61970700
C	-5.01603200	0.73953100	0.03855900
C	-4.28843200	-1.20784700	-1.16743800
C	-6.29276100	0.19860100	0.14700700
H	-4.80139200	1.72019800	0.46622500
C	-5.56278500	-1.75231200	-1.06033900
H	-3.49942900	-1.75727800	-1.68336100
C	-6.56858600	-1.04935900	-0.40314800
H	-7.07597600	0.75482800	0.65976900
H	-5.77257400	-2.72839400	-1.49503900
H	-7.56799000	-1.47374000	-0.32167600
O	-2.15273100	-0.54274600	1.22526400
C	-1.36966200	-1.00208600	2.34457000
H	-0.66940200	-1.76329700	1.99551400
H	-0.82046100	-0.15672400	2.77221800
H	-2.09269800	-1.40589500	3.05602600
H	-2.15413200	0.39095700	-1.69557800

TS10-s

SCF energy in gas phase: -1163.138173 a.u.
Enthalpy in gas phase: -1162.786254 a.u.
Free energy in gas phase: -1162.86351 a.u.
SCF energy in solution: -1163.476033 a.u.
Enthalpy in solution: -1163.124114 a.u.
Free energy in solution: -1163.20137 a.u.

Rh	-0.36649600	-0.86744800	-0.26180900
C	-4.80504200	-0.49508000	0.44093400
C	-4.95492400	0.86658200	0.40555700
C	-3.83599500	1.69543800	0.18536600
C	-2.58667400	1.04291000	0.01317200
C	-3.53202000	-1.07911900	0.25831000
H	-4.86759400	3.59662100	0.26415800
H	-5.65974400	-1.14721000	0.60880900
H	-5.93568100	1.32276500	0.54505200
C	-3.90527300	3.10437700	0.13149500
C	-1.39122300	1.79846900	-0.21355000
C	-1.50956900	3.18720900	-0.25870400
C	-2.74945900	3.82082400	-0.08905000
H	-0.60495700	3.76707700	-0.43281200
H	-2.79214100	4.90862700	-0.13408000
N	-2.45605200	-0.32414100	0.05207700
O	-0.25038000	1.18404100	-0.37013200
C	-3.39521900	-2.56746600	0.29541900
H	-2.71203100	-2.88431300	1.09333400
H	-2.99579500	-2.95248700	-0.65110900
H	-4.36624000	-3.04353300	0.47114000
C	-0.36006900	-2.70011400	-0.18716000
O	-0.28263100	-3.85674000	-0.13668500
C	1.52456900	-0.85315100	-0.54501200
C	2.41945600	0.01665300	-1.17546700
H	2.00454900	0.64975600	-1.96310500
C	3.58648600	0.60324800	-0.44357600
C	4.77049000	0.91723000	-1.12195600
C	3.49987500	0.89461600	0.92533400
C	5.83977900	1.49636700	-0.45135300
H	4.84253200	0.70040100	-2.18812400
C	4.58176300	1.45316900	1.59915300
H	2.55367800	0.72063400	1.44051400
C	5.75486400	1.75491500	0.91494900
H	6.75022300	1.74013100	-0.99696500
H	4.49611200	1.67766500	2.66149200
H	6.59560500	2.20468400	1.44021800
O	2.46567800	-1.95777400	-0.18763200
H	3.11317800	-1.31660000	-0.95099400
C	2.66515700	-2.34116900	1.18818200
H	2.97647100	-3.38792400	1.19866200
H	3.42152800	-1.68946300	1.63871400
H	1.70182700	-2.21436400	1.69526800

TS11-s

SCF energy in gas phase: -1163.14859 a.u.
Enthalpy in gas phase: -1162.796624 a.u.
Free energy in gas phase: -1162.874241 a.u.
SCF energy in solution: -1163.486839 a.u.
Enthalpy in solution: -1163.134873 a.u.

Free energy in solution: -1163.21249 a.u.

Rh	0.00703800	0.17169400	-0.39253000
C	-3.41392000	-2.77327500	-0.27061100
C	-4.42674300	-1.96974900	0.18130100
C	-4.17731200	-0.61053700	0.45996400
C	-2.85235700	-0.14913300	0.24182600
C	-2.11659000	-2.24843700	-0.46671900
H	-6.17611800	-0.08605100	1.10316300
H	-3.58896600	-3.82558100	-0.48542500
H	-5.42962100	-2.36984500	0.33403400
C	-5.16334600	0.27901400	0.93919500
C	-2.50304700	1.21362900	0.50785100
C	-3.50884100	2.05400800	0.98350500
C	-4.81535300	1.58738800	1.19143600
H	-3.24660500	3.08904800	1.19639600
H	-5.56635200	2.28235900	1.56602100
N	-1.85032200	-0.96779700	-0.22069000
O	-1.28006100	1.62504100	0.30689300
C	-1.03085000	-3.15010500	-0.95798600
H	-0.17587900	-3.15155700	-0.27100600
H	-0.66178200	-2.83076200	-1.94073800
H	-1.39335900	-4.17953100	-1.05308200
C	1.17637700	-1.05324500	-1.11627000
O	1.92032900	-1.78167700	-1.62251400
C	1.47457500	1.42377600	-0.36274900
C	2.86984400	1.49436600	-0.22125400
H	2.31885800	2.88600900	0.04265200
C	3.70115500	0.44103200	0.36382100
C	4.98591700	0.18524400	-0.12933700
C	3.23584200	-0.32090200	1.44497200
C	5.77828500	-0.80904100	0.42892900
H	5.35984000	0.77226600	-0.96952100
C	4.02498200	-1.32261000	1.99553300
H	2.24474200	-0.11388900	1.84926600
C	5.29897200	-1.57061300	1.49135300
H	6.77404400	-0.99427100	0.02877700
H	3.64666300	-1.90641800	2.83334600
H	5.91956500	-2.35051900	1.92938800
H	3.36630500	2.10645200	-0.99441800
O	1.18248300	2.86446000	-0.31235900
C	0.44128900	3.49004800	-1.38499200
H	0.39748600	4.55494800	-1.14966700
H	0.94688000	3.31506700	-2.34137300
H	-0.55544800	3.04290200	-1.36389700

8-s
SCF energy in gas phase: -1163.262095 a.u.
Enthalpy in gas phase: -1162.902805 a.u.
Free energy in gas phase: -1162.978648 a.u.
SCF energy in solution: -1163.59092 a.u.
Enthalpy in solution: -1163.23163 a.u.
Free energy in solution: -1163.307473 a.u.

Rh	0.29507500	0.29321700	-0.82297800
C	-3.31177200	-2.41196900	-0.68285300
C	-4.13874100	-1.69661300	0.14145200
C	-3.71840600	-0.45293900	0.65679300
C	-2.42389500	-0.01144400	0.27616300
C	-2.03223800	-1.91374200	-1.01895300
H	-5.50347500	-0.00205200	1.79494200
H	-3.62256800	-3.37177300	-1.09063200
H	-5.12616000	-2.07574200	0.40672900
C	-4.51229300	0.34597400	1.50793500
C	-1.91395300	1.24219200	0.74619300
C	-2.73394400	1.99603000	1.58447600
C	-4.01119700	1.54844000	1.95457000
H	-2.35042400	2.94817600	1.94770500
H	-4.61599100	2.17323300	2.61122200
N	-1.60683100	-0.74553400	-0.54795100
O	-0.72305800	1.64021300	0.38318000
C	-1.14594400	-2.71525500	-1.91723800
H	-0.22981600	-3.02227500	-1.39680900
H	-0.84565800	-2.13544300	-2.79881900
H	-1.65727300	-3.62052800	-2.26277400
C	1.30960900	-0.88285500	-1.81002800
O	2.01542400	-1.58969300	-2.40042900
C	1.84533600	1.46356300	-0.74797600
C	3.19585200	1.04942500	-0.23379200
H	3.76091100	1.94438100	0.07089000
C	3.12987600	0.02320100	0.86481200
C	3.80093300	-1.19236900	0.75086600
C	2.38631000	0.28425100	2.01904000
C	3.73740300	-2.13443100	1.77375900
H	4.36685100	-1.40940000	-0.15620700
C	2.32137700	-0.65505200	3.04081200
H	1.83703000	1.22346400	2.10476000
C	2.99821000	-1.86671300	2.92074800
H	4.26471400	-3.08154200	1.67072100
H	1.73383800	-0.44213300	3.93231800
H	2.94528000	-2.60289700	3.72122600
H	3.72668300	0.62703300	-1.10522700
O	1.85191500	2.73514700	-1.02831400
C	0.69229400	3.33739200	-1.63816000
H	1.02548200	4.31554400	-1.99101200
H	0.35373600	2.70904600	-2.46867300
H	-0.09685000	3.41902000	-0.88791900

TS12-s
SCF energy in gas phase: -1163.144788 a.u.
Enthalpy in gas phase: -1162.79333 a.u.
Free energy in gas phase: -1162.871685 a.u.
SCF energy in solution: -1163.48649 a.u.
Enthalpy in solution: -1163.135032 a.u.
Free energy in solution: -1163.213387 a.u.

Rh	-0.04255600	-1.05141800	-0.06384700
C	-4.34222500	-0.14872300	0.93533900
C	-4.47064500	1.10419700	0.39560100
C	-3.37348500	1.71338000	-0.24672200
C	-2.16973500	0.96195800	-0.29621200
C	-3.11501600	-0.84263900	0.84772100
H	-4.34873800	3.57101900	-0.78088400
H	-5.17887500	-0.62987300	1.43808300
H	-5.41648200	1.64335700	0.45884500
C	-3.42135900	3.00169600	-0.82197200
C	-0.99621900	1.49788400	-0.91852100
C	-1.09179000	2.77507800	-1.47176100
C	-2.28704900	3.50672200	-1.41979300
H	-0.20214800	3.18937700	-1.94271300
H	-2.31212700	4.50080600	-1.86536400
N	-2.06259700	-0.29694000	0.24380600
O	0.10242400	0.79667800	-0.95121000
C	-2.99786900	-2.20827500	1.44440400
H	-2.19262500	-2.24700200	2.18829000
H	-2.77217200	-2.95922600	0.67669100
H	-3.93148200	-2.50017300	1.93792700
C	-0.09791800	-2.75815200	0.61426200
O	-0.07628100	-3.85701100	0.98533900
C	1.80966600	-1.28696400	-0.50983000
C	2.96188100	-0.49941700	-0.54398900
O	2.42066300	-2.60515500	-0.88439800
C	2.02231300	-3.15331900	-2.15427700
H	2.39231700	-2.52039600	-2.96979200
H	0.92686800	-3.16825100	-2.16221700
H	2.43105900	-4.16333400	-2.22073500
H	3.38523900	-1.94394200	-0.60340600
C	3.17052300	0.73590400	0.21410800
C	4.00538900	1.73954300	-0.28738900
C	2.57776000	0.92304000	1.46967600
C	4.23291700	2.90461400	0.43437200
H	4.47503000	1.60381000	-1.26292200
C	2.79764200	2.09100400	2.18618700
H	1.93589600	0.14093800	1.87632500
C	3.62669800	3.08606100	1.67364000
H	4.88514400	3.67507900	0.02583100
H	2.32412300	2.22329100	3.15794800
H	3.80359800	3.99827600	2.24110600
H	3.52527200	-0.55899800	-1.49347600

TS13-s
SCF energy in gas phase: -1163.179479 a.u.
Enthalpy in gas phase: -1162.827101 a.u.
Free energy in gas phase: -1162.904074 a.u.
SCF energy in solution: -1163.514328 a.u.
Enthalpy in solution: -1163.16195 a.u.
Free energy in solution: -1163.238923 a.u.

Rh	0.34816300	0.64599000	-0.14072800
C	4.80813800	1.29412600	0.05237700
C	5.25551000	-0.00023400	0.02575900
C	4.33373000	-1.06465700	-0.04715800

C	2.95888100	-0.71388900	-0.08746000
C	3.42352200	1.57315800	0.00771300
H	5.76743600	-2.68655500	-0.05248400
H	5.50740200	2.12594000	0.10726000
H	6.32252000	-0.22221200	0.05924900
C	4.71091800	-2.42462800	-0.08251700
C	1.94811900	-1.72460200	-0.16171000
C	2.36795900	-3.05225600	-0.19594200
C	3.73015100	-3.38814500	-0.15693200
H	1.60455700	-3.82548600	-0.26176700
H	4.01076800	-4.44036800	-0.18696100
N	2.53011500	0.58997400	-0.06020000
O	0.68415500	-1.38424600	-0.20281700
C	2.96066900	2.99417100	0.04276000
H	2.34228900	3.18963200	0.92814000
H	2.36005000	3.24212900	-0.84087600
H	3.81455400	3.67980200	0.07164700
C	-0.08658100	2.43785600	-0.09750600
O	-0.39686200	3.55104500	-0.07664300
C	-1.62669800	0.26926400	-0.02664400
C	-2.70908000	0.17862500	-0.80148000
H	-2.50002100	0.35298000	-1.85962200
C	-4.10569100	-0.12626800	-0.47371200
C	-4.94472900	-0.59424800	-1.49447300
C	-4.65936600	0.06435900	0.80130300
C	-6.27981800	-0.88671500	-1.24886300
H	-4.53101600	-0.73180200	-2.49402900
C	-5.99610200	-0.22476200	1.04446100
H	-4.03592800	0.46360800	1.59906900
C	-6.81191700	-0.70663900	0.02429900
H	-6.90965400	-1.25392200	-2.05782100
H	-6.40729300	-0.06421600	2.04019800
H	-7.85898300	-0.93257000	0.21912400
O	-1.72126300	0.01932500	1.43213400
H	-0.46376800	0.41186400	1.37196500
C	-1.83335300	-1.38328500	1.76456800
H	-1.04578700	-1.93917500	1.24354900
H	-2.82622800	-1.73200500	1.46340700
H	-1.72287100	-1.45339600	2.84966900

9-s

SCF energy in gas phase: -1163.215272 a.u.
Enthalpy in gas phase: -1162.861811 a.u.
Free energy in gas phase: -1162.938461 a.u.
SCF energy in solution: -1163.553714 a.u.
Enthalpy in solution: -1163.200253 a.u.
Free energy in solution: -1163.276903 a.u.

Rh	-0.34576100	-0.74040900	-0.02131800
C	-4.92319100	-0.77137000	-0.28450200
C	-5.18653900	0.56506600	-0.13406600
C	-4.12498300	1.48088800	0.01508300
C	-2.81320600	0.93934100	0.00178000
C	-3.58960700	-1.23840700	-0.29272100
H	-5.31585800	3.28048100	0.18800500
H	-5.73037900	-1.49183600	-0.40052600
H	-6.21261800	0.93364800	-0.12725700
C	-4.30660600	2.87178900	0.17789600
C	-1.67498700	1.78865000	0.15690000
C	-1.89881500	3.15207000	0.31808800
C	-3.20084600	3.67862300	0.32405800
H	-1.03358800	3.80114300	0.43714800
H	-3.33030500	4.75256300	0.45147400
N	-2.56843200	-0.39920600	-0.15393000
O	-0.46563900	1.27652200	0.13083700
C	-3.31960800	-2.70064700	-0.44966600
H	-2.83025900	-3.10893100	0.44451000
H	-2.66604100	-2.89820400	-1.30810100
H	-4.25090000	-3.25665300	-0.60267700
C	-0.17917100	-2.57582000	-0.25448700
O	-0.06652200	-3.71515200	-0.37241900
C	1.67276700	-0.65970300	0.07180700
C	2.32288500	0.49450300	-0.18171400
H	1.69042100	1.36799200	-0.33868600
C	3.76499400	0.74221100	-0.24101500
C	4.19147800	2.07984000	-0.26967200
C	4.74863700	-0.26042900	-0.27896900
C	5.53961000	2.40792900	-0.30939100
H	3.44005400	2.86991700	-0.25186000
C	6.09636800	0.07040100	-0.32624600
H	4.44534000	-1.30351900	-0.28676500
C	6.50153400	1.40244900	-0.33574700
H	5.84072000	3.45453700	-0.32334200
H	6.84082000	-0.72422600	-0.36019100
H	7.56014700	1.65522200	-0.36912100
H	-0.25804200	-1.04090300	1.48622500
O	2.35429800	-1.82249500	0.33167500
C	2.54390000	-2.07400900	1.70647200
H	1.57322200	-2.20101700	2.21852800
H	3.09110000	-1.24806500	2.18543500
H	3.11962900	-3.00057900	1.78993700

TS16-s

SCF energy in gas phase: -1163.178136 a.u.
Enthalpy in gas phase: -1162.826663 a.u.
Free energy in gas phase: -1162.905217 a.u.
SCF energy in solution: -1163.518159 a.u.
Enthalpy in solution: -1163.166686 a.u.
Free energy in solution: -1163.24524 a.u.

Rh	0.00965100	0.68943700	-0.14051500
C	4.20609000	0.82998600	1.51174400
C	4.73022800	-0.31151000	0.96350300
C	3.93304400	-1.12890400	0.13679900
C	2.59632600	-0.70159200	-0.07872200
C	2.86586100	1.19666300	1.25536800
H	5.42135700	-2.63863800	-0.29820300
H	4.80994900	1.47157000	2.15036700
H	5.76427800	-0.59774600	1.15801300
C	4.39494900	-2.31737600	-0.46863300
C	1.70979000	-1.46380200	-0.90284000
C	2.20937300	-2.62835100	-1.48136600
C	3.53228200	-3.04187100	-1.26157700
H	1.53796300	-3.21159800	-2.10865000
H	3.87883900	-3.96086100	-1.73296000
N	2.08805400	0.44459700	0.48171000
O	0.47690900	-1.06376000	-1.08176200
C	2.31591600	2.44882000	1.85904300
H	1.49468800	2.23053700	2.55371900
H	1.92599200	3.12182900	1.08554100
H	3.09130300	2.98612500	2.41596800
C	-0.56583800	2.22797800	0.70082100
O	-0.96543100	3.18291100	1.21880500
C	-1.74372100	0.63340500	-1.12572300
C	-2.95689400	0.08478000	-1.12709800
H	-3.59778100	0.25339500	-1.99933700
C	-3.52125900	-0.73408400	-0.05456400
C	-4.90812900	-0.91377500	0.00911300
C	-2.72306700	-1.36194100	0.91281900
C	-5.48636300	-1.67188100	1.01983600
H	-5.53844700	-0.44298200	-0.74659300
C	-3.30189400	-2.11558500	1.92451600
H	-1.63804000	-1.27575100	0.84312000
C	-4.68518600	-2.27138900	1.98623500
H	-6.56783900	-1.79593400	1.05167500
H	-2.66561200	-2.59897300	2.66456900
H	-5.13489900	-2.86786700	2.77837300
H	-0.22250500	1.47318600	-1.67695500
O	-1.35150100	1.40244900	-2.33709200
C	-2.00192500	2.67213600	-2.46086000
H	-1.87818800	3.25553000	-1.53735700
H	-3.06718200	2.51130200	-2.65225500
H	-1.54186500	3.18699600	-3.30795400

10-s

SCF energy in gas phase: -1163.224144 a.u.
Enthalpy in gas phase: -1162.86985 a.u.
Free energy in gas phase: -1162.947131 a.u.
SCF energy in solution: -1163.555648 a.u.
Enthalpy in solution: -1163.201354 a.u.
Free energy in solution: -1163.278635 a.u.

Rh	0.40433900	0.38000700	-0.58956300
C	-3.27473900	-2.24977800	-0.85409100
C	-4.20771900	-1.43216000	-0.27197200
C	-3.82977500	-0.17034700	0.23572500
C	-2.46319100	0.18723500	0.08817600
C	-1.93068000	-1.82632100	-0.97068100
H	-5.76607700	0.44552600	0.98239200
H	-3.55015500	-3.23074600	-1.23637700
H	-5.24763700	-1.74855300	-0.18576700
C	-4.71796500	0.72043900	0.87454600

C	-1.96804900	1.43064900	0.59773000
C	-2.88233300	2.27624300	1.22371000
C	-4.23271500	1.91859700	1.35282500
H	-2.51427600	3.22346900	1.61322800
H	-4.91104800	2.61248300	1.84815100
N	-1.55471800	-0.63503600	-0.52351600
O	-0.69844400	1.72971700	0.48602900
C	-0.90952100	-2.72412700	-1.59260500
H	-0.07853000	-2.91395600	-0.89830300
H	-0.48605400	-2.27550900	-2.50108800
H	-1.34998500	-3.68837800	-1.86922400
C	1.49814900	-0.71002300	-1.62585100
O	2.19460400	-1.35087000	-2.28082000
C	2.02451600	1.55646200	-0.27626200
C	2.95066700	1.10151700	0.60151300
H	3.87616000	1.63430700	0.82665700
C	2.72942500	-0.22700800	1.17513800
C	3.73103600	-1.20839000	1.18299000
C	1.43829800	-0.60093700	1.60983500
C	3.43691200	-2.52108500	1.52533700
H	4.73781600	-0.93797300	0.86414400
C	1.14258600	-1.92998700	1.92889500
H	0.69684900	0.17933300	1.80633500
C	2.13650800	-2.89738000	1.87298700
H	4.22649900	-3.27113600	1.50063500
H	0.13205800	-2.19109300	2.24386800
H	1.91470700	-3.93306900	2.12385500
O	2.04598800	2.72296600	-0.93184100
C	3.09046900	3.62209300	-0.61369500
H	4.06780000	3.20544500	-0.89840400
H	3.09280600	3.84923300	0.46177000
H	2.89985400	4.53371000	-1.18470600
H	0.03853400	1.14321300	-1.87465700

TS17-s

SCF energy in gas phase: -1165.581732 a.u.
Enthalpy in gas phase: -1165.182254 a.u.
Free energy in gas phase: -1165.263293 a.u.
SCF energy in solution: -1165.922328 a.u.
Enthalpy in solution: -1165.52285 a.u.
Free energy in solution: -1165.603889 a.u.

Rh	-0.40953600	-0.79664300	0.02814000
C	-4.82877200	-0.63793600	-1.10964200
C	-5.17052500	0.61567000	-0.67830900
C	-4.19744500	1.44404000	-0.07871900
C	-2.89069900	0.90495800	0.04605100
C	-3.50366000	-1.10858900	-0.95146600
H	-5.47089800	3.15556900	0.28075800
H	-5.56352400	-1.28991100	-1.57761500
H	-6.18809900	0.98924200	-0.79419100
C	-4.46493500	2.75134400	0.38502600
C	-1.85802800	1.68799600	0.63817700
C	-2.15729600	2.96117700	1.08959800
C	-3.45403700	3.48784500	0.95635400
H	-1.35787200	3.54413100	1.54227600
H	-3.65278900	4.49592000	1.31609700
N	-2.56948400	-0.35456600	-0.38565400
O	-0.61288300	1.20727500	0.73465300
C	-3.13980800	-2.48213100	-1.41609200
H	-2.25721600	-2.46004300	-2.06688300
H	-2.90190900	-3.13287600	-0.56390200
H	-3.96468900	-2.94349800	-1.97000300
C	-0.28220500	-2.62846900	0.09840500
O	-0.21427500	-3.77703100	0.20742300
C	1.58687200	-0.70186500	0.28308500
C	2.19587700	0.31133800	-0.37224300
H	1.53614100	0.97640800	-0.93581600
C	3.61514400	0.64929000	-0.46182700
C	3.99318200	1.60778500	-1.33106800
C	4.62927100	-0.04074700	0.41774000
C	5.40605500	2.04077300	-1.56524600
H	3.22050000	2.10640900	-1.92201800
C	5.97095700	0.68274000	0.44116900
H	4.23060700	-0.12329000	1.43913400
C	6.40629800	1.06080700	-0.96603200
H	5.58342800	2.16354200	-2.64526100
H	5.88201800	1.60140500	1.04500900
H	6.44537200	0.15167000	-1.58832300
O	2.31194300	-1.65316700	0.94165100
C	2.01632600	-1.79065500	2.31056300
H	2.18662000	-0.84111400	2.84417600
H	0.96976500	-2.09800200	2.47001400
H	2.68492100	-2.55961600	2.70916400
H	-0.54918400	-0.02447100	1.45293300
H	4.76168500	-1.08100200	0.07946700
H	6.72561600	0.05438800	0.93452600
H	7.41708500	1.49207300	-0.96846500
H	5.56421700	3.04509700	-1.13075400

TS18-s

SCF energy in gas phase: -1165.584015 a.u.
Enthalpy in gas phase: -1165.18476 a.u.
Free energy in gas phase: -1165.26495 a.u.
SCF energy in solution: -1165.925445 a.u.
Enthalpy in solution: -1165.52619 a.u.
Free energy in solution: -1165.60638 a.u.

Rh	-0.28265200	-0.96731100	-0.18778500
C	3.45467100	0.69601900	-2.17060900
C	4.19473900	1.08671300	-1.08691900
C	3.69059400	0.89946600	0.21854300
C	2.41092900	0.29318000	0.32749500
C	2.18845600	0.09320300	-1.98579100
H	5.36481300	1.75692100	1.28522200
H	3.82567000	0.83859400	-3.18349900
H	5.17388300	1.54839500	-1.21661900
C	4.38584700	1.28986400	1.38359700
C	1.83411700	0.08301100	1.61608700
C	2.54930900	0.47496400	2.73618600
C	3.81266500	1.07779100	2.61581200
H	2.09783200	0.30944500	3.71232000
H	4.34170400	1.37720300	3.51905700
N	1.69377200	-0.10339400	-0.77056800
O	0.62371500	-0.46365000	1.74034600
C	1.38341500	-0.33597100	-3.17036600
H	0.38786100	0.12648000	-3.15966700
H	1.23620600	-1.42392700	-3.17172800
H	1.88024600	-0.05983300	-4.10682500
C	-0.76205400	-2.17598200	-1.47727400
O	-1.04119400	-2.99399100	-2.24535600
C	-2.07237200	-1.35177300	0.67520700
C	-2.97778400	-0.35944500	0.84415800
O	-2.48382300	-2.60420400	1.01608800
C	-1.54425500	-3.45726400	1.62235600
H	-1.05310700	-2.96753000	2.47763400
H	-0.77363300	-3.78730400	0.90729100
H	-2.09750700	-4.33336600	1.97443600
C	-2.91571600	1.03136500	0.42467700
C	-4.01751600	1.80441900	0.50416800
C	-1.61950400	1.60170000	-0.09444800
C	-4.10574800	3.21799700	0.02130100
H	-4.92571600	1.36660400	0.92519300
C	-1.64417000	3.11530700	-0.29739900
H	-1.35847800	1.10560200	-1.05636900
C	-2.95755000	3.56198800	-0.91798900
H	-4.10261400	3.91582200	0.87904300
H	-0.78385500	3.42489200	-0.90725300
H	-3.10363500	3.04103600	-1.87875300
H	-3.91475100	-0.66623900	1.32132900
H	-0.81331500	1.36143300	0.61899400
H	-1.52809400	3.60803600	0.68179600
H	-2.94320400	4.63872600	-1.13661800
H	-5.07367400	3.37858500	-0.47788600
H	0.50828100	-1.69137700	1.01583500

TS19-s

SCF energy in gas phase: -1165.604386 a.u.
Enthalpy in gas phase: -1165.202725 a.u.
Free energy in gas phase: -1165.282489 a.u.
SCF energy in solution: -1165.940968 a.u.
Enthalpy in solution: -1165.539307 a.u.
Free energy in solution: -1165.619071 a.u.

Rh	-0.48478100	-0.77038900	0.05363000
C	-4.90387800	-0.66688200	-0.74764300
C	-5.18970700	0.63607900	-0.44194800
C	-4.15670300	1.50457200	-0.03142900
C	-2.85114300	0.95340700	0.04427700
C	-3.57932700	-1.15323700	-0.65119900
H	-5.37499200	3.27258400	0.24183000
H	-5.68714300	-1.35037500	-1.06951000

H	-6.20883400	1.01735100	-0.51295300
C	-4.36836400	2.86102500	0.30018200
C	-1.74243600	1.76595500	0.44732300
C	-1.99891900	3.09815200	0.76463500
C	-3.29495800	3.63019900	0.68977000
H	-1.15840200	3.71735900	1.07389500
H	-3.44836200	4.67765000	0.94805800
N	-2.58436500	-0.36200200	-0.26030600
O	-0.54255800	1.24620300	0.49752400
C	-3.29918100	-2.57984300	-0.99483300
H	-2.55978700	-2.65555700	-1.80128500
H	-2.89647000	-3.12349100	-0.13114400
H	-4.21331400	-3.08839300	-1.32109700
C	-0.31085300	-2.52777100	-0.39386100
O	-0.15267400	-3.64228000	-0.69081900
C	1.53825400	-0.66748800	0.43573900
C	2.25409600	0.35738700	-0.21460700
H	1.60051300	1.04686200	-0.75328300
C	3.67424200	0.64848200	-0.28218900
C	4.02971900	1.64695300	-1.12144700
C	4.70306000	-0.12358400	0.50542100
C	5.43799500	2.02956400	-1.42559900
C	6.06462400	0.56189200	0.48940100
H	4.35141400	-0.25471300	1.53658700
C	6.43742700	0.99609500	-0.92050200
H	5.54709500	2.19380400	-2.50827800
H	6.03794600	1.44927100	1.14320100
H	6.42374000	0.11810500	-1.58598500
O	2.30888900	-1.56756400	1.10144500
C	1.66766000	-2.34334800	2.09952000
H	1.06601300	-1.70931900	2.76462100
H	1.02104500	-3.10980200	1.65682900
H	2.46704500	-2.82734800	2.66845500
H	1.41880400	0.40695100	1.03258800
H	5.64006300	3.01325500	-0.96502300
H	7.45597200	1.40402400	-0.95620100
H	6.82282200	-0.11302800	0.90766000
H	3.24155800	2.20470200	-1.63243300
H	4.78006100	-1.14490500	0.10099300

TS20-s

SCF energy in gas phase: -1165.602913 a.u.
Enthalpy in gas phase: -1165.20191 a.u.
Free energy in gas phase: -1165.282002 a.u.
SCF energy in solution: -1165.940887 a.u.
Enthalpy in solution: -1165.539884 a.u.
Free energy in solution: -1165.619976 a.u.

Rh	-0.04564300	-0.95685200	-0.12613200
C	-4.07747000	-0.24940000	1.71264700
C	-4.49415500	0.84660700	1.00708200
C	-3.66194300	1.40153700	0.01213500
C	-2.40845100	0.76907300	-0.19804200
C	-2.81409000	-0.83058800	1.45492100
H	-4.98616000	3.00240300	-0.59452900
H	-4.70794600	-0.69240300	2.48106000
H	-5.46700900	1.30002300	1.19983300
C	-4.02107600	2.52623100	-0.76219500
C	-1.50362900	1.26155900	-1.19507800
C	-1.90144100	2.37492600	-1.93332500
C	-3.14192800	2.99188100	-1.71407100
H	-1.21764300	2.75082500	-2.69273300
H	-3.41074500	3.85873700	-2.31723200
N	-2.00535100	-0.33039500	0.52588000
O	-0.35386900	0.66528300	-1.38113200
C	-2.38803600	-2.02745100	2.24150700
H	-1.46708200	-1.82737800	2.80300600
H	-2.18814800	-2.88180900	1.58323100
H	-3.16569300	-2.32069200	2.95554500
C	0.35885700	-2.37762500	0.94258300
O	0.66860700	-3.28229900	1.60569800
C	1.76598000	-1.25241700	-1.07091300
C	2.96456800	-0.53630500	-0.88424400
O	1.99622000	-2.33575500	-1.87331400
C	0.86048100	-2.91104200	-2.49435100
H	0.29599500	-2.15536200	-3.05909300
H	0.19191700	-3.37081300	-1.75490000
H	1.24359600	-3.67476700	-3.17792900
H	1.71064600	-0.21758500	-1.71575600
C	3.24646100	0.61878800	-0.06378800
C	4.54694100	0.98848300	-0.01014700
C	2.18389200	1.34750800	0.71402800
C	5.07734200	2.06547800	0.87214500
H	5.26968000	0.45552500	-0.63253600
C	2.69280100	2.67597700	1.26429500
H	1.82612300	0.69910300	1.53098500
C	4.05826100	2.50964000	1.91492500
H	5.37136200	2.92187900	0.23875400
H	1.96310400	3.08132400	1.97690900
H	3.99058800	1.74751900	2.70768900
H	3.81430800	-0.92056000	-1.46448500
H	1.30444000	1.50656600	0.07308700
H	2.77072600	3.40896300	0.44445200
H	4.38961300	3.43949200	2.39530100
H	6.01185900	1.72513600	1.34340700

TS21-s

SCF energy in gas phase: -1664.177984 a.u.
Enthalpy in gas phase: -1663.625139 a.u.
Free energy in gas phase: -1663.726017 a.u.
SCF energy in solution: -1664.666533 a.u.
Enthalpy in solution: -1664.113688 a.u.
Free energy in solution: -1664.214566 a.u.

Rh	-1.62685600	-0.90307400	0.34440700
C	-5.93732500	-0.75050600	-1.12472300
C	-6.25223900	0.56264200	-0.89974000
C	-5.28733500	1.43541100	-0.35191100
C	-4.01756200	0.87657600	-0.05358500
C	-4.64874500	-1.23798900	-0.80138800
H	-6.50669700	3.22218100	-0.33661500
H	-6.66482800	-1.43768500	-1.55191800
H	-7.24167200	0.94985300	-1.14359800
C	-5.52853200	2.80454400	-0.10228400
C	-2.99325800	1.70272500	0.49323600
C	-3.26762100	3.03748100	0.73385500
C	-4.52795200	3.58253600	0.43062400
H	-2.47690100	3.65500700	1.15509800
H	-4.70661600	4.63841500	0.62647500
N	-3.72470800	-0.44250200	-0.27798100
O	-1.77850000	1.19932100	0.74551300
C	-4.31725600	-2.67684900	-1.03522900
H	-3.33412400	-2.78540800	-1.50769700
H	-4.28874100	-3.22862900	-0.08509200
H	-5.06614400	-3.15568800	-1.67558100
C	-1.57187000	-2.70302900	0.70586900
O	-1.54294800	-3.82264700	0.99089300
C	0.35855800	-0.82383000	0.68485400
C	1.00443200	-0.02906400	-0.18407300
H	0.40442000	0.42409200	-0.97643200
C	2.50376900	0.20621100	-0.32684800
O	1.04005100	-1.56740100	1.59477800
C	0.56889500	-1.52806100	2.92229200
H	0.54037800	-0.49455200	3.29981700
H	-0.43743600	-1.96789300	3.00576500
H	1.27243400	-2.11017000	3.52435200
C	2.94356300	-0.92006200	-1.27500900
C	3.11860000	-2.22179000	-0.78587900
C	3.01349800	-0.72461600	-2.65625100
C	3.39494500	-3.27719500	-1.64490900
H	3.01196900	-2.40772400	0.28164500
C	3.28400000	-1.78380000	-3.51927600
H	2.85261000	0.27017100	-3.06861500
C	3.48519300	-3.06355600	-3.01844800
H	3.53311200	-4.27753800	-1.23632900
H	3.33590200	-1.60061700	-4.59186000
H	3.70268300	-3.89151300	-3.69157000
C	3.23976800	0.22701200	1.02221900
C	2.68956800	0.95229800	2.08416800
C	4.50597500	-0.33030100	1.19743100
C	3.35867600	1.07583700	3.29380000
H	1.71465200	1.42511300	1.95451600
C	5.18332900	-0.20435500	2.40870400
H	4.97389500	-0.87931600	0.38165300
C	4.61103500	0.49060300	3.46601000
H	2.90060200	1.63856200	4.10682200
H	6.16816200	-0.65654800	2.52049400
H	5.13814100	0.58577500	4.41416600
C	2.77374300	1.60282300	-0.91105300
C	4.04873600	1.90950200	-1.40168400
C	1.82190100	2.62246200	-0.87817900
C	4.35222500	3.17893300	-1.87267700

H	4.81310700	1.13245500	-1.42023900
C	2.12606700	3.90041600	-1.34456200
H	0.83132000	2.43150900	-0.46574200
C	3.38774600	4.18387400	-1.84967500
H	5.35022100	3.38598800	-2.25672900
H	1.36431400	4.67825100	-1.30679000
H	3.62351200	5.18159400	-2.21675200
H	-1.82279200	0.07471100	1.62474700

TS22-s

SCF energy in gas phase: -1664.192556 a.u.
Enthalpy in gas phase: -1663.640065 a.u.
Free energy in gas phase: -1663.738037 a.u.
SCF energy in solution: -1664.674408 a.u.
Enthalpy in solution: -1664.121917 a.u.
Free energy in solution: -1664.219889 a.u.

Rh	0.98780300	-1.16069700	0.80462100
C	4.55538700	-0.20298200	-1.83978800
C	4.65141800	1.15228700	-1.67662900
C	3.81545200	1.81296000	-0.75033300
C	2.89566700	1.00399400	-0.03080100
C	3.60881700	-0.94407800	-1.09266200
H	4.55150800	3.81738800	-1.09537300
H	5.19830900	-0.73065100	-2.54148000
H	5.37038700	1.73555200	-2.25249600
C	3.84756300	3.20739000	-0.53087900
C	2.02711200	1.60494300	0.92916600
C	2.08293500	2.97690200	1.11360500
C	2.98481300	3.76782900	0.38198700
H	1.39687800	3.42317700	1.83135500
H	2.99631100	4.84359500	0.54980600
N	2.79612900	-0.34643500	-0.23095300
O	1.15941400	0.86691600	1.62178100
C	3.52251600	-2.42602500	-1.25893500
H	2.51181600	-2.72513500	-1.56563400
H	3.74385100	-2.93661400	-0.31228900
H	4.23384200	-2.78264000	-2.01232700
C	1.23798300	-2.97349800	0.94924600
O	1.39717000	-4.11101100	1.08736700
C	-0.79134800	-1.41205500	1.73725500
C	-1.90839600	-0.83987400	1.25700800
O	-0.93860100	-2.18576100	2.85627400
C	-0.03879600	-1.93033600	3.90646000
H	-0.04633700	-0.86396400	4.18604200
H	0.99124300	-2.21612800	3.63923300
H	-0.36754200	-2.53096800	4.75981200
C	-2.08596000	0.00663300	0.00991400
H	-2.79906900	-0.96398400	1.87793600
C	-2.16356400	1.50631300	0.37633500
C	-2.74557400	2.41357800	-0.51885300
C	-1.65229400	2.00402000	1.57383400
C	-2.79536200	3.77243200	-0.23647600
H	-3.16589700	2.04624800	-1.45589500
C	-1.71189700	3.36556900	1.86536000
H	-1.19272000	1.32067200	2.28277200
C	-2.27783200	4.25634000	0.96247700
H	-3.24847700	4.45590100	-0.95341200
H	-1.31475600	3.72667500	2.81405200
H	-2.32447700	5.31989700	1.19233100
C	-3.45087300	-0.36375800	-0.62302500
C	-4.60137000	-0.26747800	0.17050000
C	-3.61783300	-0.71246300	-1.96390300
C	-5.86018100	-0.54464500	-0.34205400
H	-4.51291600	0.05809900	1.20689200
C	-4.88241800	-0.98646500	-2.48463800
H	-2.75864500	-0.76453900	-2.63086100
C	-6.00836200	-0.91287800	-1.67707400
H	-6.73313800	-0.46482300	0.30414500
H	-4.97858400	-1.25595800	-3.53564600
H	-6.99496500	-1.12839700	-2.08401400
C	-0.95804500	-0.25698800	-1.00168300
C	-0.70698300	-1.58312100	-1.40998400
C	-0.26997500	0.76518900	-1.66804400
C	0.15344800	-1.86231200	-2.46976300
H	-1.26134000	-2.39245300	-0.93564300
C	0.60447700	0.48278800	-2.71461900
H	-0.42304200	1.80055700	-1.36875400
C	0.81108200	-0.82841100	-3.12993300
H	0.29549200	-2.89649500	-2.78398200
H	1.11979400	1.30296500	-3.21364800
H	1.48311300	-1.04441600	-3.96010200
H	1.63182600	-0.36910000	2.06410000

TS23-s

SCF energy in gas phase: -1664.198425 a.u.
Enthalpy in gas phase: -1663.644165 a.u.
Free energy in gas phase: -1663.745137 a.u.
SCF energy in solution: -1664.681466 a.u.
Enthalpy in solution: -1664.127206 a.u.
Free energy in solution: -1664.228178 a.u.

Rh	1.71804600	-0.92807000	-0.30952700
C	6.11471400	-0.48153000	0.48217700
C	6.25988700	0.87482500	0.37107900
C	5.14088800	1.68004800	0.07145500
C	3.90111400	1.01101500	-0.10007200
C	4.84871700	-1.08522500	0.30023900
H	6.16592400	3.58553800	0.06471900
H	6.96704500	-1.11775500	0.71229700
H	7.23354200	1.34598500	0.50953700
C	5.20822500	3.08383100	-0.06658700
C	2.71498300	1.75205800	-0.40748000
C	2.82957300	3.13373700	-0.53769000
C	4.06141900	3.78360400	-0.36682000
H	1.92989800	3.69959200	-0.77650400
H	4.10410200	4.86669900	-0.47712700
N	3.77469500	-0.35448800	0.01733200
O	1.57539200	1.12234100	-0.55044100
C	4.71885100	-2.56843300	0.42705000
H	4.03397900	-2.83864300	1.24045700
H	4.31905700	-3.00871000	-0.49472800
H	5.69156600	-3.02923300	0.63239100
C	1.69518300	-2.72932900	-0.03381800
O	1.61791400	-3.87500300	0.15244800
C	-0.32826000	-0.95150300	-0.61384900
C	-1.05173300	0.04455600	0.05515100
H	-0.41047300	0.75244800	0.58271500
C	-2.53124900	0.25892800	0.23393900
O	-1.07486100	-1.91440700	-1.21489600
C	-0.55245600	-2.45284100	-2.41373000
H	-0.63217600	-1.71480600	-3.22710200
H	0.50046300	-2.74117700	-2.29597600
H	-1.16136300	-3.32700600	-2.65876300
H	-0.22537800	0.09095600	-1.23651200
C	-2.68188300	-0.50017200	1.56730200
C	-2.69033500	-1.90237400	1.56998500
C	-2.65168000	0.17147700	2.79241200
C	-2.71913200	-2.60684900	2.76572500
H	-2.66313300	-2.43913200	0.62300000
C	-2.67805800	-0.53779200	3.98927300
H	-2.61067600	1.25876300	2.81407400
C	-2.71826700	-1.92671600	3.98108400
H	-2.73207500	-3.69505700	2.74659000
H	-2.66126000	0.00432900	4.93323500
H	-2.73770500	-2.48035700	4.91823000
C	-3.40327100	-0.25594600	-0.91465500
C	-3.08541200	0.12149900	-2.22249600
C	-4.57440200	-0.97952300	-0.70109500
C	-3.88535900	-0.25575400	-3.29116300
H	-2.19981200	0.73195500	-2.40977800
C	-5.38581300	-1.35137300	-1.77091400
H	-4.85924400	-1.26584800	0.31015000
C	-5.04133600	-1.00112900	-3.06955800
H	-3.61042100	0.04170700	-4.30199000
H	-6.29414300	-1.92080100	-1.57978700
H	-5.67244600	-1.29673200	-3.90584200
C	-2.84842100	1.75464000	0.35749100
C	-4.11623900	2.14085400	0.80615200
C	-1.95215200	2.74840700	-0.03754500
C	-4.46910000	3.48027400	0.88254600
H	-4.83541900	1.37690300	1.10315700
C	-2.31011400	4.09431500	0.03080000
H	-0.95848300	2.49146700	-0.40748700
C	-3.56395300	4.46626100	0.49420200
H	-5.45888500	3.75692600	1.24220600
H	-1.59413900	4.85235000	-0.28309400
H	-3.84041400	5.51771400	0.54890400

TS24-s

SCF energy in gas phase: -1664.194928 a.u.
Enthalpy in gas phase: -1663.641277 a.u.

Free energy in gas phase: -1663.740555 a.u.
SCF energy in solution: -1664.676912 a.u.
Enthalpy in solution: -1664.123261 a.u.
Free energy in solution: -1664.222539 a.u.

Rh	1.19103200	-1.03383300	0.93716100
C	5.00558700	-0.46585200	-1.32356500
C	5.03010300	0.89768900	-1.43676200
C	4.04494900	1.67501000	-0.79187000
C	3.05863300	0.97094200	-0.05373500
C	3.98966700	-1.10570700	-0.57583600
H	4.76281400	3.61629000	-1.42644300
H	5.76426900	-1.08095300	-1.80373700
H	5.80856900	1.39746500	-2.01410000
C	4.00224900	3.08558000	-0.85544300
C	2.01855400	1.67962500	0.63041500
C	2.02459300	3.07132600	0.55108500
C	3.00216100	3.75601500	-0.18682500
H	1.23768200	3.61622900	1.07275300
H	2.96301600	4.84428500	-0.22678400
N	3.03854900	-0.40185300	0.02946900
O	1.11037900	1.01312300	1.29436400
C	3.99204500	-2.59540900	-0.46552800
H	3.18441300	-3.04199400	-1.06095500
H	3.84655700	-2.91364700	0.57330700
H	4.94017800	-3.01009400	-0.82672800
C	1.17903400	-2.84156700	0.69819800
O	1.10590500	-3.99495400	0.56124200
C	-0.74016300	-1.21886800	1.71425600
C	-1.92405600	-0.75421100	1.13451800
O	-1.02216300	-1.94018400	2.84335300
C	0.02127700	-2.06970200	3.79152800
H	0.36285400	-1.08487500	4.14127200
H	0.87966700	-2.60960200	3.37100700
H	-0.40119600	-2.63149600	4.62965100
H	-0.73354600	-0.03481200	1.87871300
C	-2.21795500	0.08049200	-0.09253400
H	-2.82568400	-0.95381000	1.72938200
C	-2.76616900	1.38960000	0.53011500
C	-4.13173600	1.67785900	0.56943500
C	-1.88635800	2.25261700	1.19772700
C	-4.60154600	2.81768200	1.21801600
H	-4.84517200	1.01007200	0.09142900
C	-2.35589200	3.39299900	1.83661000
H	-0.81760000	2.02521800	1.22526100
C	-3.71716400	3.68444400	1.84658600
H	-5.67112900	3.02123700	1.23160700
H	-1.64924700	4.05215800	2.33925000
H	-4.08577100	4.57540600	2.35221400
C	-3.30636200	-0.64348700	-0.90708800
C	-3.75261900	-1.93223800	-0.62072300
C	-3.82551300	0.00676200	-2.03276800
C	-4.71016100	-2.54982400	-1.42609100
H	-3.34661200	-2.48679800	0.22582200
C	-4.78383800	-0.60153100	-2.82839900
H	-3.46489200	1.00496500	-2.28255800
C	-5.23395900	-1.88616500	-2.52565900
H	-5.03913100	-3.55944600	-1.18598300
H	-5.17738500	-0.07401700	-3.69573200
H	-5.98224600	-2.36741900	-3.15280100
C	-1.04071500	0.26481300	-1.06459600
C	-0.48570000	-0.88453600	-1.64355900
C	-0.56520900	1.50512700	-1.48180400
C	0.53181200	-0.79695700	-2.58378900
H	-0.87466700	-1.86478600	-1.36714100
C	0.46935000	1.59616600	-2.41284000
H	-0.98687300	2.42245900	-1.07682900
C	1.02630900	0.44895300	-2.96191300
H	0.94544400	-1.70966000	-3.01210100
H	0.84248600	2.57911200	-2.69705000
H	1.83671700	0.52419900	-3.68588900

Phenylacetylene
SCF energy in gas phase: -308.1457409 a.u.
Enthalpy in gas phase: -308.0291989 a.u.
Free energy in gas phase: -308.0670059a.u.
SCF energy in solution: -308.2393599 a.u.
Enthalpy in solution: -308.1228179 a.u.
Free energy in solution: -308.1606249 a.u.

C	1.50743300	1.20489700	0.00001700
C	0.11980400	1.20872200	-0.00001700
C	-0.58905000	0.00000300	-0.00003300
C	0.11981500	-1.20872500	-0.00001800
C	1.50743300	-1.20489300	0.00001800
C	2.20466500	0.00000800	0.00003700
H	2.04966900	2.14880400	0.00003000
H	-0.43421100	2.14562900	-0.00003100
H	-0.43421500	-2.14562300	-0.00003300
H	2.04968900	-2.14878900	0.00003200
H	3.29311000	0.00000000	0.00006500
C	-2.01657800	-0.00002200	-0.00007800
C	-3.22520700	-0.00002700	-0.00009200
H	-4.29392700	0.00019600	0.00093300

MeOH
SCF energy in gas phase: -115.644053 a.u.
Enthalpy in gas phase: -115.588387 a.u.
Free energy in gas phase: -115.615487 a.u.
SCF energy in solution: -115.6982642 a.u.
Enthalpy in solution: -115.6425982 a.u.
Free energy in solution: -115.6696982 a.u.

C	0.65458200	-0.01994500	0.00000000
H	1.07957000	0.98901800	-0.00000100
H	1.03216500	-0.54407100	-0.89343600
H	1.03216500	-0.54407000	0.89343700
O	-0.74240300	0.12234100	0.00000000
H	-1.13216600	-0.75993300	0.00000000

CO
SCF energy in gas phase: -113.251769 a.u.
Enthalpy in gas phase: -113.243397 a.u.
Free energy in gas phase: -113.26584 a.u.
SCF energy in solution: -113.2838069 a.u.
Enthalpy in solution: -113.2754349 a.u.
Free energy in solution: -113.2978779 a.u.

C	0.00000000	0.00000000	-0.64995900
O	0.00000000	0.00000000	0.48747000

(*Z*)-PhCH=CHOMe
SCF energy in gas phase: -423.8547287 a.u.
Enthalpy in gas phase: -423.6779477 a.u.
Free energy in gas phase: -423.7238177 a.u.
SCF energy in solution: -423.986111 a.u.
Enthalpy in solution: -423.80933 a.u.
Free energy in solution: -423.8552 a.u.

C	-0.73817700	1.28837600	-0.00081600
C	-2.00771500	0.85857800	-0.00867500
H	-0.62877000	2.37312700	0.00563600
H	-2.83476800	1.57422900	-0.00610400
C	0.50627200	0.52878800	-0.00072500
C	1.71665700	1.23841700	0.00380100
C	0.56687800	-0.87387300	-0.00364000
C	2.93927100	0.58182600	0.00538400
H	1.68718200	2.32876700	0.00604900
C	1.79136400	-1.52820200	-0.00143700
H	-0.35462900	-1.44792500	-0.00732100
C	2.98279200	-0.80863400	0.00288200
H	3.86259800	1.15938200	0.00860800
H	1.81506700	-2.61712700	-0.00334900
H	3.93938800	-1.32855100	0.00421200
O	-2.37747600	-0.44289300	-0.02728400
C	-3.76824700	-0.66520700	0.02161500
H	-3.92197300	-1.74593800	-0.03005800
H	-4.20025800	-0.28454000	0.95904900
H	-4.27860800	-0.18869400	-0.82878500

(*E*)-PhCH=CHOMe
SCF energy in gas phase: -423.8533313 a.u.
Enthalpy in gas phase: -423.6769563 a.u.
Free energy in gas phase: -423.7240993 a.u.
SCF energy in solution: -423.9854159 a.u.
Enthalpy in solution: -423.8090409 a.u.
Free energy in solution: -423.8561839 a.u.

C	-4.15853500	0.44886100	0.23351300
H	-5.10797500	-0.05581700	0.03682300
H	-4.12428600	1.38446000	-0.34579900
H	-4.09520000	0.68964400	1.30520300

O	-3.13376900	-0.43412000	-0.15794900
C	-1.87945100	0.05167400	-0.02476100
C	-0.80586600	-0.73116500	-0.17739500
H	-1.81126900	1.11957700	0.20831600
H	-0.98645700	-1.79192700	-0.36093300
C	0.58432300	-0.29762900	-0.09185900
C	1.58852400	-1.26507400	0.04683000
C	0.97641000	1.04840000	-0.14753200
C	2.92660900	-0.90732400	0.14558400
H	1.30257800	-2.31678800	0.08263600
C	2.31237400	1.40680600	-0.04245300
H	0.22684200	1.82538100	-0.29686100
C	3.29653900	0.43267500	0.10612700
H	3.68516400	-1.68102900	0.25508200
H	2.59068200	2.45875700	-0.08928600
H	4.34451000	0.71735300	0.18009000