Electronic Supplementary Information

Computational studies of Rh-catalyzed carboxylation of the C(sp^2)–H bond using CO_2

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Dissociation of cholor-bridged dimeric Rh(I) complex

The dimeric Rh(I) complex (**Rh–Cl dimer**) is indeed more stable than the reactant complex **6** in term of free energy (Fig. S1). However, **Rh–Cl dimer** is a species that lies off the catalytic cycle. In contrast, the monomeric **6** with the reactant coordination is reactive species at the outset of the reaction. Moreover, in term of enthalpic energy, the monomeric **6** is more favorable than **Rh–Cl dimer**. The large excess of the reactant **2** can facilitate the dissociation of the dimer species to form the reactive reactant complex **6**. Thus, we only considered the monomeric Rh(I) species involved in the reaction (Fig. 1 in the manuscript).

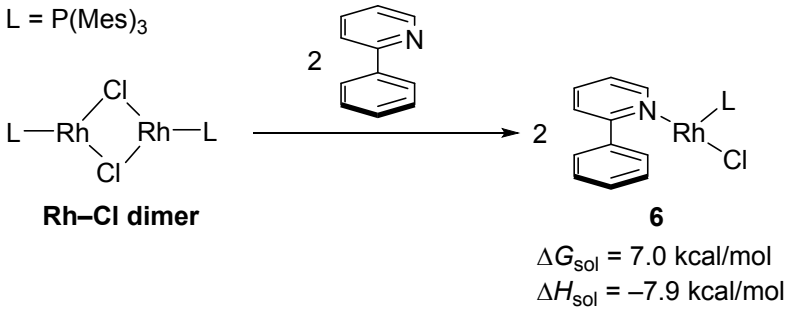


Fig. S1 Generation of monomeric reactant complex **6** from the cholor-bridged dimeric Rh(I) complex.

Energy profile of the formation of methylrhodium(I)

The formation of Rh(I)–Me from Rh(I)–Cl and $AlMe_2(OMe)$ occurs via the four-membered σ-bond metathesis transition state (**TS1**) (Fig. S2). This process has a low barrier of 12.9 kcal/mol. Note that, PCy_3 instead of $P(Mes)_3$ is used as the ligand because of the failure in calculating the transition state with $P(Mes)_3$ ligand.

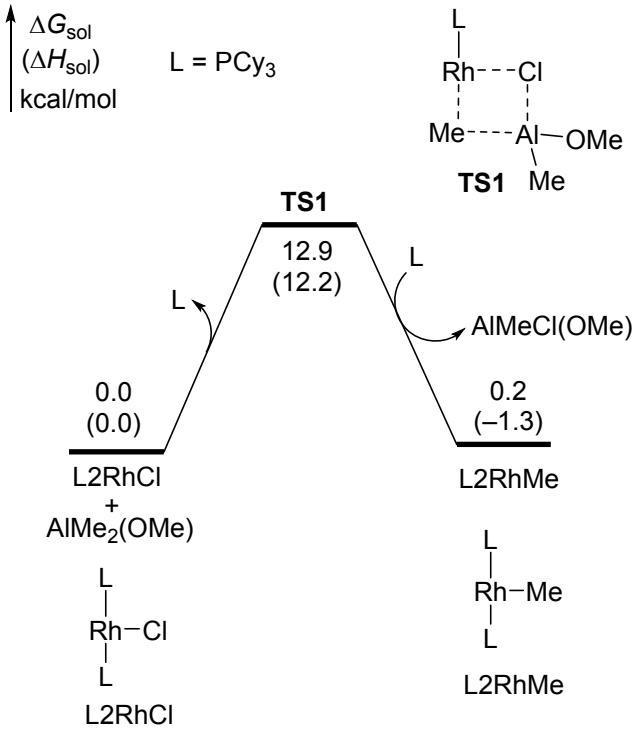
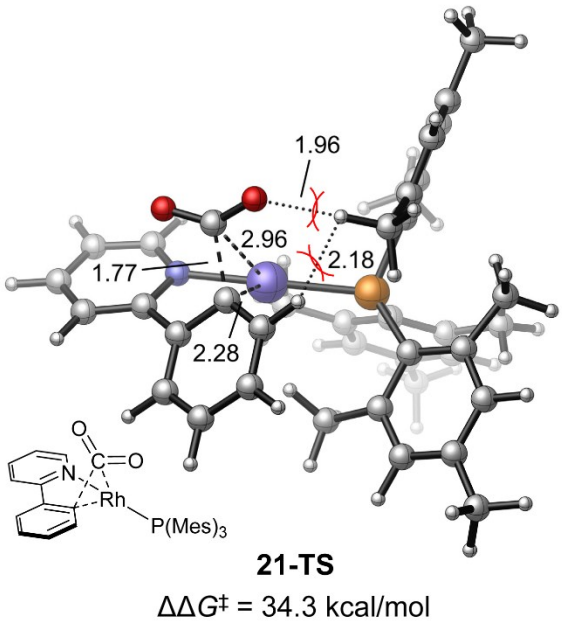


Fig. S2 Energy profiles of the formation of methylrhodium(I) by the reaction of Rh(I)–Cl with $AlMe_2(OMe)$.

Disfavored transition state 21-TS

As shown in Fig. S3, the high barrier of **21-TS** is majorly caused by the steric repulsions between the ortho-methyl group of the $P(Mes)_3$ ligand and the aryl group (short H···H distance, 2.18 Å), and between the ortho-methyl group of the $P(Mes)_2$ ligand and CO_2 (short H···O distance, 1.96 Å).



21-TS

$\Delta\Delta G^{\ddagger}$ = 34.3 kcal/mol

Fig. S3 Optimized geometries of the disfavored transition state **21-TS**.

CO_2 insertion into the Rh(III)–C(sp^2) bond

We calculated the CO_2 insertion into the Rh(III)–C(aryl) bond with and without $Me_2Al(OMe)$ using the $P(Mes)_3$ ligand. As shown in Fig. S4, the transition states of CO_2 insertion into the Rh(III)–C(aryl) bond (**30-TS**–**33-TS**, 32.6–47.6 kcal/mol) have higher barriers than those of the CO_2 insertion into the Rh(I)–C(aryl) bond (**20-TS**, 28.9 kcal/mol and **22-TS**, 22.7 kcal/mol in Fig. 3 in the manuscript). The high barriers are probably due to the steric congestion around the six-coordinated Rh(III) in the transitions states of **30-TS**–**33-TS**. It is also noted that the CO_2 insertion into the Rh(III)–C(aryl) bond is significantly less favorable than the reductive elimination from **10** and **11** to form the Rh(I) metallocycle (**14** in Fig. 2 in the manuscript). Therefore, the carboxylation is less possible to occur at the Rh(III) center.

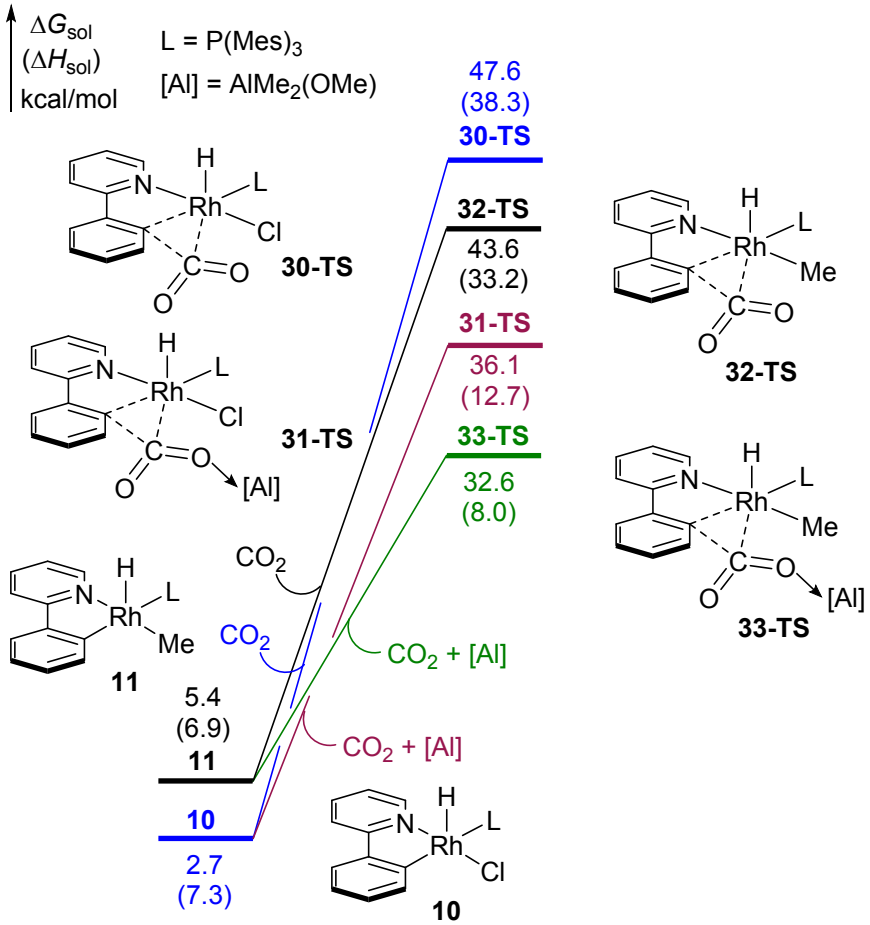
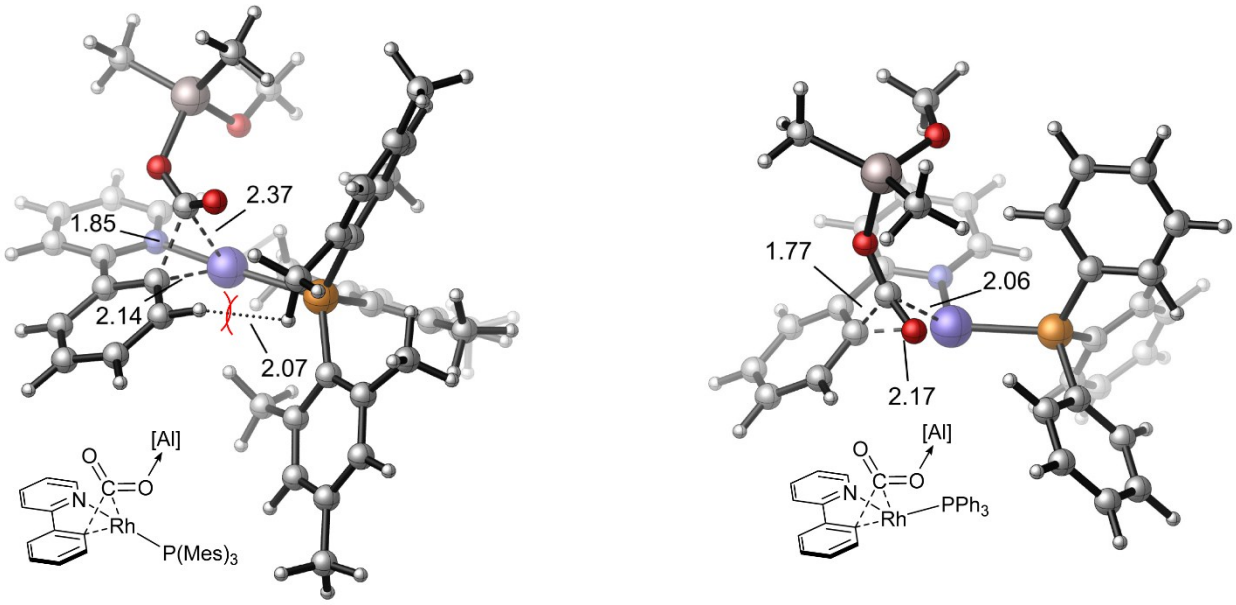


Fig. S4 Energy profile of CO_2 insertion into the Rh(III)–C(sp^2) bond.

Disfavored transition states 22-TSa and 27-TSa

As discussed in the manuscript, in the favored **22-TS** and **27-TS** (Fig. 5), the phosphine ligands are *cis* and *trans* to the aryl group, respectivly. In contrast, the disfaovred **22-TSa** and **27-TSa** hold the ligand geoemtry *trans* and *cis* to the aryl group (Fig. S5), respectivly. The origin of the high barrier of **22-TSa** is due to the steric repulsion between the ortho-methyl group of the $P(Mes)_3$ ligand and the aryl group in the substrate (short H···H distance, 2.07 Å). The disfavored **27-TSa** is majorly caused by the destablizing *trans* effect between the ligand and the aryl group.



22-TSa (disfavored)
$\Delta\Delta G^{\ddagger}$ = 29.8 kcal/mol

27-TSa (disfavored)
$\Delta\Delta G^{\ddagger}$ = 28.3 kcal/mol

Fig. S5 Optimized geometries of the disfavored conformers of the transition states **22-TS** and **27-TS**.

Topological analysis of the C–H···Rh interaction in 22-TS

The QTAIM analysis was performed to give a better understanding of the agostic interaction between the Rh center and the C–H bond. In the geometry of **22-TS** shown in Fig. S6, the C–H bond proximal to Rh is indeed elongated to 1.12 Å. We then performed topological analysis of **22-TS** implemented in the Multiwfn program. The bond critical point (BCP, shown in green) between the Rh and the H atoms was found. The values of the electron density and the laplacian at this BCP are 0.044 and 0.16 a.u., respectively. Both are in the ranges of the electron density (0.01−0.13 a.u.) and the laplacian (0.03−0.25 a.u.) of a series of reported agostic interactions. This indicates the interaction between the Rh and the C–H bond in **22-TS** is a typical agostic interaction.

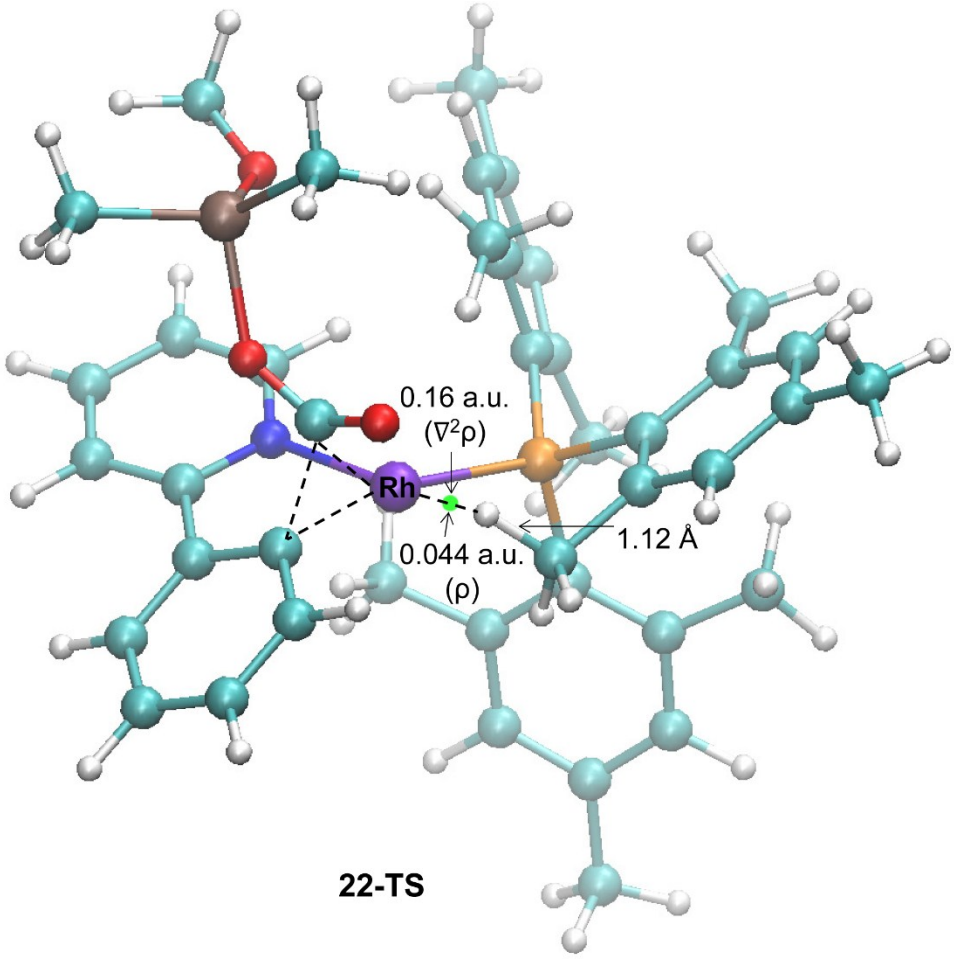


Fig. S6 Topological analysis of the C–H···Rh interaction in **22-TS**.

To investigate whether the agostic interaction of C–H with Rh can stabilize the CO_2 insertion transition state, we simply replace the methyl substituent in **22-TS** with the H atom in **22-TSb** (Fig. S7), and compare the barriers of these two transition states. The result shows that **22-TSb** without the agostic interaction is 4.7 kcal/mol higher than **22-TS**. This indicates the agnostic C–H···Rh interaction in **22-TS** is a stabilizing factor that can enhance the reactivity.

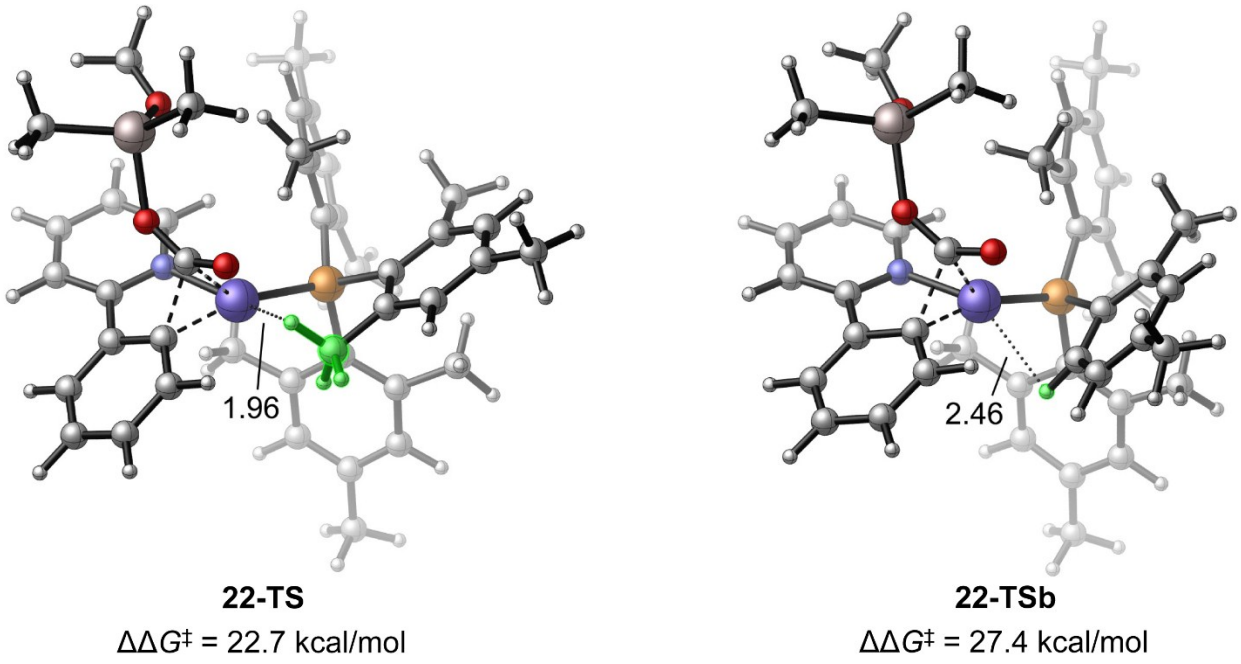


Fig. S7 Comparison of the transition states with and without the agostic C–H···Rh interaction.

Cartesian coordinates (Å) and energies of the optimized structures

```
 1
B3LYP SCF energy:                    -479.33520445 a.u.
B3LYP enthalpy:                      -479.155249 a.u.
B3LYP free energy:                   -479.199794 a.u.
M06 SCF energy in solution:          -479.09778143 a.u.
M06 enthalpy in solution:            -478.917826 a.u.
M06 free energy in solution:         -478.962371 a.u.
Three lowest frequencies (cm-1):      42.2727     95.2702    156.4448

Cartesian coordinates
ATOM       X           Y           Z
C       -0.763164    0.031256   -0.000262
C       -2.700261   -1.206292   -0.203474
C       -3.520052   -0.091187   -0.022866
C       -2.901183    1.139132    0.194468
C       -1.510813    1.203202    0.211856
C        0.725258    0.029001   -0.004018
C        1.417554   -1.179765    0.181548
C        2.810039   -1.209019    0.192093
C        3.541726   -0.032716    0.010082
C        2.866224    1.172859   -0.187683
C        1.472077    1.203367   -0.195334
H       -3.138340   -2.190560   -0.365246
H       -4.601117   -0.189198   -0.044140
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H       -1.014515    2.147248    0.408529
H        0.841480   -2.088547    0.315088
H        3.326666   -2.153278    0.343490
H        4.628221   -0.056108    0.016853
H        3.424482    2.092109   -0.344373
H        0.968438    2.148014   -0.377564
N       -1.366874   -1.157952   -0.195519



 3
B3LYP SCF energy:                    -518.64783762 a.u.
B3LYP enthalpy:                      -518.438496 a.u.
B3LYP free energy:                   -518.486241 a.u.
M06 SCF energy in solution:          -518.38941459 a.u.
M06 enthalpy in solution:            -518.180073 a.u.
M06 free energy in solution:         -518.227818 a.u.
Three lowest frequencies (cm-1):      56.5314     89.0336    119.4249
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Cartesian coordinates

ATOM	X	Y	Z
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C	3.593107	-0.068981	-0.083137
C	2.971624	-1.131251	0.572735
C	1.580773	-1.178934	0.606437
C	-0.650662	-0.213886	-0.042240
C	-1.457185	0.927357	0.187298
C	-2.848799	0.770221	0.153556
C	-3.450587	-0.461475	-0.105258
C	-2.653824	-1.581984	-0.332710
C	-1.267277	-1.450345	-0.295913
H	3.222774	1.753466	-1.182283
H	4.674616	0.012356	-0.135862
H	3.559653	-1.906215	1.057590
H	1.066615	-1.980202	1.127425
H	-3.474344	1.640018	0.340865
H	-4.534265	-0.542069	-0.127323
H	-3.103785	-2.548561	-0.542379
H	-0.642904	-2.317511	-0.494021
N	1.443340	0.868483	-0.644655
C	-0.882764	2.293155	0.489783
H	-0.103007	2.245587	1.257707
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H	-1.670086	2.966630	0.844518

4

B3LYP SCF energy: -3349.94808296 a.u.
B3LYP enthalpy: -3348.825788 a.u.
B3LYP free energy: -3348.993386 a.u.
M06 SCF energy in solution: -3349.94614752 a.u.
M06 enthalpy in solution: -3348.823853 a.u.
M06 free energy in solution: -3348.991451 a.u.
Three lowest frequencies (cm-1): 13.7813 16.5388 24.0661

Cartesian coordinates

ATOM	X	Y	Z
Rh	-0.058930	-0.307498	-0.141816
P	-2.501188	-0.205856	0.004567
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C	-2.764493	1.611839	-2.142034

C	-2.969548	2.864577	-2.730207
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C	-3.494535	3.948251	-2.027803
C	-3.878475	3.719924	-0.709850
H	-4.351419	4.527039	-0.154033
C	-3.710624	2.484647	-0.064339
C	-2.267117	0.513873	-3.050453
H	-2.113475	0.902051	-4.062159
H	-2.980015	-0.315024	-3.119000
H	-1.328875	0.068472	-2.712490
C	-3.654364	5.303482	-2.673470
H	-3.899908	5.214948	-3.737560
H	-2.726288	5.886925	-2.603637
H	-4.443481	5.888641	-2.189159
C	-4.307085	2.417091	1.329889
H	-3.557799	2.439882	2.125963
H	-4.906555	1.517257	1.482340
H	-4.967069	3.277400	1.478863
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C	-5.316623	-2.638607	-1.942354
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C	-3.692871	-4.038680	-0.910894
H	-3.301315	-5.028264	-0.685756
C	-3.055618	-2.929529	-0.345220
C	-5.497389	-0.200293	-1.630825
H	-5.056438	0.429164	-2.408881
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H	-6.517003	-0.442707	-1.946977
C	-5.435700	-5.127761	-2.390354
H	-5.338549	-6.018522	-1.760001
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H	-4.638310	-0.999026	4.569319
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H	3.126341	-2.951300	3.941952
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H	1.137961	-2.822346	2.945204
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C	4.640535	-1.652517	-3.861915
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H	5.225036	0.363403	-4.284809
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H	3.592505	-3.183355	-0.016144
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H	4.486585	-2.347734	-5.902755
H	5.668000	-3.230590	-4.933365
C	4.348837	1.790757	-2.354253
H	4.312212	2.171691	-1.338090
H	3.628587	2.370351	-2.941992
H	5.341870	2.015255	-2.758383
C	2.343291	1.887654	0.154409
C	2.705005	2.579641	1.346047
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C	2.099794	4.732987	0.324189
C	1.671248	4.033849	-0.803496
H	1.238266	4.584042	-1.636628
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H	2.011745	6.596444	1.424461
H	1.142975	6.624057	-0.121724
H	2.906095	6.696532	-0.096046
C	1.132827	2.034853	-2.144634
H	0.094493	1.758747	-1.929720
H	1.619554	1.129703	-2.505893
H	1.124331	2.768059	-2.959277
Cl	0.037153	-1.780778	-2.006056

5

B3LYP SCF energy: -2929.60987979 a.u.
B3LYP enthalpy: -2928.452400 a.u.
B3LYP free energy: -2928.621767 a.u.
M06 SCF energy in solution: -2929.57282429 a.u.
M06 enthalpy in solution: -2928.415345 a.u.
M06 free energy in solution: -2928.584712 a.u.
Three lowest frequencies (cm-1): 10.6180 14.0763 22.2803

Cartesian coordinates

ATOM	X	Y	Z
Rh	-0.058985	-0.242132	-0.253663

C	0.009515	-1.561899	-1.826104
H	0.602670	-1.133372	-2.643855
H	-0.987542	-1.811295	-2.197234
H	0.485143	-2.490122	-1.501286
P	-2.458358	-0.231648	-0.038921
C	-3.360375	1.183223	-0.917505
C	-3.023143	1.420858	-2.281924
C	-3.472445	2.576792	-2.927628
H	-3.198456	2.724645	-3.970376
C	-4.263055	3.531570	-2.289129
C	-4.664467	3.246687	-0.987413
H	-5.344856	3.932517	-0.486144
C	-4.260071	2.094271	-0.294582
C	-2.244747	0.439728	-3.123958
H	-2.241434	0.758017	-4.171355
H	-2.675719	-0.566675	-3.083691
H	-1.212480	0.346773	-2.784458
C	-4.683270	4.801808	-2.988086
H	-4.879750	4.628672	-4.052213
H	-3.897060	5.566439	-2.925955
H	-5.587461	5.227392	-2.539889
C	-4.925281	1.907395	1.057142
H	-4.296117	2.218996	1.896117
H	-5.211827	0.870396	1.239721
H	-5.838575	2.510434	1.091464
C	-3.284234	-1.860294	-0.470810
C	-4.448388	-2.008679	-1.277102
C	-4.827376	-3.289070	-1.706754
H	-5.718178	-3.380061	-2.324945
C	-4.130258	-4.444031	-1.360254
C	-3.039989	-4.294238	-0.505774
H	-2.504316	-5.179573	-0.169348
C	-2.605053	-3.044597	-0.049975
C	-5.398404	-0.894261	-1.675610
H	-5.004166	-0.251033	-2.467089
H	-5.650712	-0.242070	-0.836316
H	-6.331787	-1.331331	-2.044329
C	-4.544216	-5.799749	-1.879778
H	-4.329574	-6.591316	-1.153339
H	-4.003375	-6.051606	-2.802089
H	-5.614260	-5.831295	-2.112183
C	-1.458461	-3.051565	0.933147
H	-1.079049	-4.069543	1.068109
H	-1.760956	-2.673994	1.916756
H	-0.633807	-2.402220	0.599225

C	-2.686062	0.115761	1.792958
C	-3.491534	-0.627725	2.697159
C	-3.432064	-0.333533	4.068417
H	-4.050406	-0.919206	4.745822
C	-2.644717	0.688383	4.592623
C	-1.917902	1.460482	3.685385
H	-1.331283	2.299905	4.053600
C	-1.918459	1.199262	2.311587
C	-4.502584	-1.690291	2.308283
H	-4.044950	-2.653208	2.064079
H	-5.100216	-1.402279	1.440181
H	-5.190435	-1.857621	3.143342
C	-2.585299	0.956679	6.077386
H	-3.481733	0.588563	6.587671
H	-2.488999	2.027619	6.288362
H	-1.720969	0.458229	6.536800
C	-1.153064	2.178072	1.443994
H	-1.834681	2.832338	0.887452
H	-0.514767	1.709776	0.672860
H	-0.504676	2.811280	2.056624
P	2.421233	0.089973	-0.117793
C	3.286548	-0.608156	1.407723
C	4.637096	-1.055299	1.436031
C	5.110647	-1.744506	2.561821
H	6.146686	-2.078277	2.561148
C	4.322571	-1.998972	3.682557
C	3.027580	-1.483643	3.676808
H	2.401212	-1.609329	4.557615
C	2.501850	-0.793494	2.578891
C	5.674389	-0.799580	0.359184
H	5.563879	0.181034	-0.106292
H	5.638792	-1.541362	-0.444595
H	6.674317	-0.843226	0.803955
C	4.852546	-2.786210	4.856733
H	4.395590	-2.460557	5.797635
H	5.939031	-2.683936	4.951890
H	4.635579	-3.857248	4.745028
C	1.118090	-0.219564	2.737756
H	0.414486	-0.637694	1.995772
H	1.115306	0.867983	2.603023
H	0.719477	-0.428949	3.734644
C	3.394932	-0.659822	-1.539067
C	3.284567	-2.074892	-1.676252
C	3.787428	-2.705128	-2.819541
H	3.681774	-3.785354	-2.900987

C	4.425122	-2.004867	-3.842092
C	4.614712	-0.638388	-3.649459
H	5.176424	-0.076111	-4.393101
C	4.140869	0.049150	-2.522214
C	2.760139	-2.996776	-0.592273
H	2.401751	-3.932498	-1.032920
H	1.948148	-2.563961	-0.006963
H	3.562929	-3.248514	0.112387
C	4.905172	-2.700103	-5.093361
H	5.744893	-2.167116	-5.552528
H	4.106041	-2.757739	-5.844739
H	5.226499	-3.726690	-4.884871
C	4.577598	1.500360	-2.430016
H	4.841395	1.798013	-1.413768
H	3.814749	2.205796	-2.772228
H	5.460491	1.647763	-3.060451
C	2.605345	1.970879	-0.112763
C	3.263917	2.744085	0.885281
C	3.179568	4.145748	0.835023
H	3.690434	4.716674	1.607331
C	2.489982	4.834000	-0.157930
C	1.870032	4.068591	-1.144484
H	1.335988	4.570240	-1.949010
C	1.902826	2.671181	-1.142862
C	4.104359	2.207224	2.029123
H	4.904524	1.547621	1.688725
H	3.521490	1.643919	2.762384
H	4.572108	3.044096	2.556935
C	2.412259	6.341890	-0.169323
H	3.110870	6.784335	0.548251
H	1.404378	6.690690	0.091731
H	2.644050	6.747759	-1.161297
C	1.160747	1.985532	-2.262949
H	0.315198	1.408652	-1.848527
H	1.772083	1.266729	-2.816582
H	0.774439	2.722454	-2.974388

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B3LYP SCF energy:	-2439.19678323 a.u.
B3LYP enthalpy:	-2438.451272 a.u.
B3LYP free energy:	-2438.573589 a.u.
M06 SCF energy in solution:	-2439.48927988 a.u.
M06 enthalpy in solution:	-2438.743769 a.u.

M06 free energy in solution: -2438.866086 a.u.
Three lowest frequencies (cm-1): 25.4183 26.5160 30.8755

Cartesian coordinates

ATOM	X	Y	Z
Rh	1.490007	-0.276274	-0.460517
N	2.269325	1.662833	-0.247039
C	4.056639	3.666969	0.543989
C	1.823345	2.877103	0.125449
C	3.611942	1.443156	-0.255810
C	4.526223	2.414189	0.144656
C	2.682987	3.899344	0.522867
H	0.751099	3.017213	0.119096
H	5.586771	2.184811	0.124598
H	2.267281	4.857738	0.817210
H	4.749467	4.443577	0.854467
C	3.981196	0.075432	-0.701850
C	4.791875	-2.433030	-1.661794
C	4.836360	-0.742921	0.069545
C	3.548083	-0.378114	-1.971701
C	3.968501	-1.634241	-2.440982
C	5.228912	-1.984574	-0.404495
H	5.164762	-0.396159	1.045624
H	3.639039	-1.974668	-3.417945
H	5.869481	-2.616846	0.203625
H	5.102147	-3.408877	-2.023948
P	-0.787334	-0.153861	0.067842
C	-0.923712	-1.202200	1.619566
C	-0.163098	-0.778196	2.746929
C	-0.224502	-1.502655	3.939922
H	0.350738	-1.145801	4.792057
C	-0.973838	-2.671359	4.066158
C	-1.617080	-3.135871	2.922599
H	-2.143981	-4.086700	2.965985
C	-1.589646	-2.456478	1.695340
C	0.793768	0.393202	2.727882
H	0.379772	1.304844	2.291277
H	1.672829	0.131222	2.123206
H	1.126701	0.628920	3.744640
C	-1.062030	-3.411688	5.378915
H	-0.136212	-3.313619	5.956638
H	-1.254772	-4.478756	5.224962
H	-1.876751	-3.019972	6.003537
C	-2.213281	-3.201356	0.531171
H	-1.558933	-3.186875	-0.342068

H	-3.188769	-2.809795	0.230948
H	-2.356302	-4.248226	0.816538
C	-1.478967	1.598572	0.372146
C	-2.072661	2.117574	1.560318
C	-2.493125	3.459089	1.595405
H	-2.944114	3.824196	2.516074
C	-2.382128	4.326811	0.516098
C	-1.832658	3.803899	-0.652972
H	-1.746984	4.442164	-1.530168
C	-1.385147	2.481666	-0.752926
C	-2.355694	1.373424	2.854747
H	-1.531671	1.481231	3.568767
H	-2.527414	0.309513	2.730576
H	-3.244610	1.804808	3.326559
C	-2.833651	5.765096	0.600891
H	-3.390434	6.063451	-0.294915
H	-1.977912	6.447821	0.689054
H	-3.476944	5.931613	1.470948
C	-0.821728	2.096876	-2.105937
H	-0.612050	2.997841	-2.691270
H	-1.528491	1.486619	-2.676343
H	0.105121	1.521168	-2.022133
C	-2.067755	-0.705409	-1.222901
C	-3.464138	-0.595234	-0.946375
C	-4.401113	-0.898584	-1.939078
H	-5.457802	-0.816575	-1.691868
C	-4.033758	-1.308782	-3.219474
C	-2.673239	-1.425636	-3.476511
H	-2.351496	-1.757433	-4.461089
C	-1.681509	-1.141274	-2.522283
C	-4.057534	-0.201901	0.389217
H	-4.082023	0.884079	0.519424
H	-3.509190	-0.624778	1.230953
H	-5.088468	-0.563784	0.455734
C	-5.069826	-1.601091	-4.277921
H	-5.913220	-2.167857	-3.866851
H	-4.644811	-2.177788	-5.105750
H	-5.480403	-0.673377	-4.698652
C	-0.266846	-1.360296	-3.004421
H	-0.249304	-1.399542	-4.099079
H	0.142715	-2.296219	-2.612451
H	0.422872	-0.581097	-2.666664
H	3.010023	0.293785	-2.632308
Cl	1.325862	-2.667090	-0.338376

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B3LYP SCF energy: -2018.85261487 a.u.
B3LYP enthalpy: -2018.072615 a.u.
B3LYP free energy: -2018.196590 a.u.
M06 SCF energy in solution: -2019.11253351 a.u.
M06 enthalpy in solution: -2018.332534 a.u.
M06 free energy in solution: -2018.456509 a.u.
Three lowest frequencies (cm-1): 19.4973 22.5871 28.7001

Cartesian coordinates

ATOM	X	Y	Z
Rh	-1.446654	-0.549797	0.421948
C	-1.128103	-2.572587	0.144265
H	-1.385863	-2.779755	-0.904948
H	-1.820943	-3.117884	0.796065
H	-0.119508	-2.967044	0.314321
N	-2.605056	1.453006	0.256275
C	-4.814311	2.748935	-0.855592
C	-2.493028	2.691298	-0.245636
C	-3.818632	0.850467	0.233867
C	-4.943948	1.466915	-0.320688
C	-3.569401	3.375550	-0.812246
H	-1.503575	3.134084	-0.204580
H	-5.899557	0.952556	-0.313152
H	-3.425225	4.374595	-1.211680
H	-5.674297	3.252971	-1.288265
C	-3.809859	-0.514056	0.813871
C	-4.114428	-2.971327	2.163699
C	-4.569751	-1.569261	0.240545
C	-3.185470	-0.725727	2.079870
C	-3.376696	-1.957176	2.747989
C	-4.708198	-2.777292	0.897457
H	-5.034777	-1.416549	-0.730182
H	-2.940293	-2.095051	3.733633
H	-5.280243	-3.579697	0.439725
H	-4.248855	-3.916670	2.682673
P	0.816941	-0.176425	-0.071877
C	1.172211	-1.204476	-1.607482
C	0.318912	-0.979677	-2.729815
C	0.497569	-1.720139	-3.901221
H	-0.153553	-1.512280	-4.748077
C	1.460091	-2.722998	-4.014159
C	2.212981	-3.005143	-2.878468

H	2.925977	-3.826233	-2.912207
C	2.084031	-2.294201	-1.674249
C	-0.842610	-0.012138	-2.721116
H	-0.584384	0.996748	-2.391897
H	-1.616854	-0.370433	-2.022316
H	-1.283883	0.061535	-3.721185
C	1.662203	-3.478716	-5.305497
H	0.714212	-3.630772	-5.833834
H	2.113767	-4.460739	-5.129022
H	2.327601	-2.931449	-5.987278
C	2.913737	-2.834710	-0.523724
H	2.321117	-2.975585	0.382920
H	3.757436	-2.194209	-0.255901
H	3.320943	-3.811119	-0.804180
C	1.144582	1.671181	-0.399456
C	1.596168	2.288266	-1.601021
C	1.686018	3.689652	-1.669699
H	2.033058	4.130878	-2.602399
C	1.382115	4.527974	-0.603731
C	0.987912	3.913844	0.584696
H	0.771173	4.532147	1.453872
C	0.860863	2.525979	0.713505
C	2.056183	1.593887	-2.872142
H	1.249143	1.523073	-3.610169
H	2.429883	0.586996	-2.716693
H	2.856706	2.183225	-3.331831
C	1.474085	6.030678	-0.722129
H	1.886140	6.480100	0.188588
H	0.484804	6.480140	-0.883044
H	2.108058	6.327984	-1.564016
C	0.445259	2.038859	2.086973
H	-0.000352	2.862034	2.655077
H	1.304556	1.668432	2.655939
H	-0.286546	1.226555	2.032722
C	2.183928	-0.468146	1.216592
C	3.512253	0.007822	1.003042
C	4.455704	-0.059052	2.033350
H	5.462210	0.304634	1.834574
C	4.159677	-0.581748	3.291684
C	2.876839	-1.083606	3.478450
H	2.619931	-1.528950	4.437285
C	1.888706	-1.052356	2.480680
C	4.037029	0.551253	-0.308959
H	3.820128	1.616717	-0.429739
H	3.619048	0.030519	-1.170981

H	5.124619	0.430433	-0.348229
C	5.187819	-0.598504	4.397110
H	6.184242	-0.847287	4.014251
H	4.930160	-1.326238	5.173550
H	5.265344	0.384475	4.881001
C	0.580305	-1.703666	2.862966
H	0.489197	-1.751072	3.953557
H	0.527972	-2.731555	2.483507
H	-0.290999	-1.190226	2.444235
H	-2.793497	0.121019	2.633406

8-TS

B3LYP SCF energy: -2439.18012207 a.u.
B3LYP enthalpy: -2438.439546 a.u.
B3LYP free energy: -2438.561599 a.u.
M06 SCF energy in solution: -2439.46939650 a.u.
M06 enthalpy in solution: -2438.728820 a.u.
M06 free energy in solution: -2438.850873 a.u.
Three lowest frequencies (cm-1): -762.7738 18.2258 24.8480
Imaginary frequency: -762.7738 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Rh	1.656096	-0.381427	-0.537721
N	2.484271	1.508449	-0.084718
C	3.806004	3.901908	0.509102
C	1.809617	2.594729	0.331742
C	3.847228	1.580059	-0.177591
C	4.516471	2.780316	0.102471
C	2.421004	3.804221	0.639017
H	0.739630	2.484869	0.423193
H	5.594636	2.824711	0.002736
H	1.812600	4.641303	0.964192
H	4.324284	4.831586	0.726121
C	4.509952	0.330779	-0.551870
C	5.632081	-2.139585	-1.211491
C	5.903886	0.161203	-0.537792
C	3.661335	-0.755069	-0.883175
C	4.246323	-1.984381	-1.228039
C	6.464019	-1.069430	-0.864870
H	6.557628	0.980994	-0.253329
H	2.561871	-0.373195	-1.843571
H	3.603028	-2.813759	-1.497592

H	7.543318	-1.193899	-0.852704
H	6.067194	-3.102112	-1.469233
P	-0.970975	-0.162638	-0.000357
C	-1.086820	-1.511165	1.299034
C	-0.234627	-1.357370	2.427460
C	-0.256692	-2.303285	3.455019
H	0.392672	-2.151357	4.314931
C	-1.063401	-3.439064	3.401865
C	-1.804962	-3.634369	2.239607
H	-2.381369	-4.550797	2.133107
C	-1.817692	-2.723434	1.172764
C	0.777200	-0.240247	2.564278
H	0.381945	0.755137	2.347416
H	1.626338	-0.411747	1.881979
H	1.189218	-0.220063	3.578691
C	-1.111541	-4.425016	4.544067
H	-1.375191	-5.429212	4.195626
H	-1.861767	-4.131860	5.291355
H	-0.147436	-4.487171	5.060735
C	-2.543000	-3.191158	-0.073375
H	-1.919316	-3.062209	-0.960267
H	-3.490789	-2.678510	-0.253552
H	-2.762890	-4.258937	0.021957
C	-1.607127	1.487312	0.706615
C	-2.134164	1.754905	2.005101
C	-2.497076	3.068904	2.343932
H	-2.893428	3.244315	3.342163
C	-2.389990	4.145230	1.468859
C	-1.893219	3.872887	0.196683
H	-1.800676	4.684478	-0.522341
C	-1.506758	2.587596	-0.202009
C	-2.381393	0.750115	3.116798
H	-1.492374	0.605386	3.739552
H	-2.681538	-0.233838	2.767134
H	-3.171944	1.128700	3.772688
C	-2.827351	5.534496	1.867373
H	-2.704907	5.700914	2.943021
H	-3.887399	5.698900	1.631790
H	-2.255588	6.303179	1.336127
C	-0.998976	2.476662	-1.626009
H	-0.701477	3.463817	-1.993833
H	-1.772110	2.090765	-2.297894
H	-0.134723	1.813507	-1.719591
C	-2.283773	-0.400753	-1.341158
C	-3.672702	-0.297060	-1.033969

C	-4.620766	-0.352869	-2.060558
H	-5.673666	-0.285007	-1.793684
C	-4.268546	-0.499464	-3.401377
C	-2.912714	-0.608277	-3.690346
H	-2.603495	-0.735769	-4.725359
C	-1.912512	-0.565328	-2.705369
C	-4.243232	-0.160154	0.360903
H	-4.243658	0.880374	0.700465
H	-3.693066	-0.746633	1.096591
H	-5.280787	-0.509167	0.371834
C	-5.313985	-0.520346	-4.490382
H	-4.944321	-1.021230	-5.391049
H	-5.606154	0.498572	-4.778445
H	-6.223621	-1.035807	-4.162545
C	-0.502006	-0.721507	-3.222472
H	-0.479233	-0.544040	-4.302710
H	-0.118355	-1.727127	-3.027223
H	0.210486	-0.042791	-2.748659
Cl	1.063899	-2.672506	-0.938768

9-TS

B3LYP SCF energy: -2018.83531567 a.u.
B3LYP enthalpy: -2018.059221 a.u.
B3LYP free energy: -2018.181213 a.u.
M06 SCF energy in solution: -2019.09371629 a.u.
M06 enthalpy in solution: -2018.317622 a.u.
M06 free energy in solution: -2018.439614 a.u.
Three lowest frequencies (cm-1): -770.2587 16.2355 20.7148
Imaginary frequency: -770.2587 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Rh	1.556964	-0.504708	-0.632534
C	0.980093	-2.422750	-1.199626
H	1.377449	-3.112351	-0.440909
H	1.403200	-2.695448	-2.174319
H	-0.099309	-2.594146	-1.262808
N	2.606163	1.423560	-0.019714
C	4.193121	3.668151	0.503302
C	2.075719	2.561197	0.455355
C	3.953246	1.363774	-0.203499
C	4.759021	2.491191	0.030733
C	2.819331	3.702641	0.738484

H	1.006120	2.555166	0.614557
H	5.824089	2.443438	-0.163247
H	2.324053	4.589338	1.120693
H	4.814577	4.540570	0.686469
C	4.483835	0.060860	-0.631829
C	5.447255	-2.456881	-1.376998
C	5.861186	-0.217119	-0.604174
C	3.554389	-0.945759	-1.016516
C	4.079035	-2.193791	-1.404717
C	6.346787	-1.467091	-0.972588
H	6.565103	0.537784	-0.265884
H	2.484999	-0.484888	-1.939770
H	3.403524	-2.977238	-1.726588
H	7.414431	-1.667029	-0.943594
H	5.812805	-3.438800	-1.668871
P	-0.954580	-0.191390	-0.033299
C	-1.156097	-1.650169	1.138680
C	-0.233860	-1.688302	2.225750
C	-0.281548	-2.733258	3.150050
H	0.422580	-2.723313	3.979764
C	-1.181617	-3.792903	3.031023
C	-2.004831	-3.798171	1.909979
H	-2.671474	-4.643537	1.753415
C	-2.005732	-2.773304	0.948388
C	0.869619	-0.671285	2.417384
H	0.542912	0.368241	2.341790
H	1.660246	-0.816937	1.659214
H	1.343924	-0.802071	3.395827
C	-1.240312	-4.892778	4.063409
H	-0.236782	-5.198452	4.380993
H	-1.757816	-5.777031	3.677520
H	-1.776827	-4.564309	4.963806
C	-2.899252	-3.031481	-0.251640
H	-2.407996	-2.799721	-1.197584
H	-3.831178	-2.460195	-0.226514
H	-3.170288	-4.091563	-0.272443
C	-1.417858	1.430722	0.841129
C	-1.867998	1.624328	2.179424
C	-2.111320	2.927961	2.642672
H	-2.458286	3.046789	3.667311
C	-1.952182	4.063116	1.854148
C	-1.536304	3.862702	0.539616
H	-1.414505	4.722758	-0.116060
C	-1.263448	2.591493	0.020504
C	-2.158291	0.544574	3.206766

H	-1.263447	0.273274	3.777258
H	-2.548268	-0.375910	2.780425
H	-2.893415	0.919828	3.925958
C	-2.205299	5.448107	2.399993
H	-1.279468	5.902242	2.778468
H	-2.919110	5.427382	3.230275
H	-2.601003	6.117118	1.627953
C	-0.810017	2.559417	-1.426033
H	-0.474255	3.555221	-1.732218
H	-1.622821	2.261750	-2.095890
H	0.018436	1.862878	-1.591473
C	-2.339236	-0.210827	-1.326629
C	-3.702196	0.003891	-0.957691
C	-4.688000	0.090176	-1.944789
H	-5.719371	0.240465	-1.631158
C	-4.402558	-0.015257	-3.306268
C	-3.075022	-0.226990	-3.656810
H	-2.815245	-0.320628	-4.709213
C	-2.039197	-0.327297	-2.712423
C	-4.208350	0.121260	0.463885
H	-4.076165	1.132501	0.860024
H	-3.707416	-0.565797	1.145957
H	-5.278556	-0.107369	0.495378
C	-5.488269	0.113216	-4.347380
H	-5.168369	-0.293426	-5.312154
H	-5.761290	1.164876	-4.507380
H	-6.400283	-0.412402	-4.041916
C	-0.671177	-0.573397	-3.307337
H	-0.614050	-0.125180	-4.305227
H	-0.484064	-1.647765	-3.419838
H	0.148750	-0.188118	-2.698823

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B3LYP SCF energy: -2439.19357910 a.u.
B3LYP enthalpy: -2438.451288 a.u.
B3LYP free energy: -2438.576660 a.u.
M06 SCF energy in solution: -2439.47572273 a.u.
M06 enthalpy in solution: -2438.733432 a.u.
M06 free energy in solution: -2438.858804 a.u.
Three lowest frequencies (cm-1): 12.7462 20.9599 24.6980

Cartesian coordinates

ATOM	X	Y	Z

Rh	1.874142	-0.436061	-0.587354
N	2.598821	1.492303	-0.202281
C	3.785827	3.961236	0.286816
C	1.854114	2.561203	0.122776
C	3.957609	1.612329	-0.268651
C	4.563272	2.855189	-0.032061
C	2.400759	3.813287	0.376145
H	0.788193	2.395499	0.187266
H	5.641684	2.944645	-0.093677
H	1.747937	4.639824	0.634585
H	4.254661	4.923960	0.470310
C	4.656823	0.365586	-0.567484
C	5.841157	-2.096447	-1.103377
C	6.056244	0.260116	-0.650740
C	3.836215	-0.775302	-0.748467
C	4.449242	-2.003851	-1.025407
C	6.648230	-0.968685	-0.918051
H	6.685424	1.134603	-0.505972
H	2.006040	-0.190450	-2.084025
H	3.836452	-2.883703	-1.179071
H	7.729793	-1.049132	-0.983428
H	6.299917	-3.059381	-1.316193
P	-1.172092	-0.148520	-0.028187
C	-1.209015	-1.541429	1.227716
C	-0.252845	-1.457137	2.277331
C	-0.186155	-2.454386	3.252365
H	0.544534	-2.351783	4.052510
C	-1.004167	-3.582475	3.217419
C	-1.865868	-3.703634	2.130862
H	-2.469928	-4.603759	2.039978
C	-1.977167	-2.732749	1.123977
C	0.781968	-0.356325	2.389021
H	0.423408	0.636932	2.114531
H	1.658512	-0.588227	1.758370
H	1.170016	-0.296550	3.411538
C	-0.945355	-4.632460	4.300490
H	-1.265280	-5.610850	3.926855
H	-1.602142	-4.373760	5.142454
H	0.068770	-4.737582	4.701438
C	-2.869566	-3.109427	-0.042318
H	-2.347920	-3.007464	-0.996937
H	-3.782894	-2.513772	-0.105764
H	-3.168520	-4.157281	0.057220
C	-1.683459	1.488537	0.776101
C	-2.087772	1.731227	2.120468

C	-2.320445	3.049579	2.543203
H	-2.625765	3.206551	3.576153
C	-2.198456	4.154433	1.704920
C	-1.830930	3.906387	0.383730
H	-1.741247	4.741618	-0.308409
C	-1.577471	2.615783	-0.096413
C	-2.336031	0.679924	3.186200
H	-1.424270	0.432990	3.740692
H	-2.723877	-0.256495	2.791879
H	-3.057885	1.066286	3.913143
C	-2.494231	5.552040	2.194917
H	-2.209881	5.678106	3.245340
H	-3.566021	5.780031	2.120107
H	-1.961236	6.305522	1.605085
C	-1.217378	2.517036	-1.566153
H	-0.921566	3.499628	-1.947214
H	-2.066200	2.169831	-2.164276
H	-0.392365	1.823479	-1.755523
C	-2.569503	-0.337718	-1.275695
C	-3.937411	-0.119293	-0.948720
C	-4.903502	-0.145962	-1.960423
H	-5.944615	0.012099	-1.685174
C	-4.584479	-0.384435	-3.297736
C	-3.246680	-0.622035	-3.601719
H	-2.967892	-0.833409	-4.631601
C	-2.234741	-0.603172	-2.630805
C	-4.456057	0.098329	0.455494
H	-4.319067	1.131327	0.789463
H	-3.958518	-0.548121	1.181140
H	-5.527366	-0.123309	0.496307
C	-5.648501	-0.377921	-4.369070
H	-5.315379	-0.907506	-5.267484
H	-5.903470	0.647760	-4.667979
H	-6.573386	-0.850014	-4.018780
C	-0.832079	-0.883157	-3.114080
H	-0.841395	-1.111665	-4.184563
H	-0.366065	-1.721743	-2.590142
H	-0.167408	-0.025267	-2.965627
Cl	1.249194	-2.704139	-0.902960

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B3LYP SCF energy: -2018.85087847 a.u.

B3LYP enthalpy: -2018.072550 a.u.

B3LYP free energy: -2018.195774 a.u.
M06 SCF energy in solution: -2019.10308718 a.u.
M06 enthalpy in solution: -2018.324759 a.u.
M06 free energy in solution: -2018.447983 a.u.
Three lowest frequencies (cm-1): 17.6455 22.9958 26.6043

Cartesian coordinates

ATOM	X	Y	Z
Rh	-1.684104	-0.534730	0.659603
C	-1.150635	-2.479793	1.137355
H	-1.559807	-3.132721	0.352378
H	-1.559632	-2.803171	2.100985
H	-0.067636	-2.642568	1.159317
N	-2.636917	1.457124	0.095550
C	-4.136273	3.764576	-0.366197
C	-2.059162	2.588866	-0.332599
C	-3.985757	1.430904	0.271081
C	-4.749311	2.592690	0.056493
C	-2.757966	3.765745	-0.580537
H	-0.988888	2.546869	-0.485576
H	-5.820185	2.574911	0.219775
H	-2.229547	4.648643	-0.925034
H	-4.727360	4.661528	-0.531544
C	-4.550083	0.130324	0.659186
C	-5.586935	-2.373901	1.321706
C	-5.939701	-0.061513	0.779039
C	-3.646474	-0.947885	0.870573
C	-4.207900	-2.191811	1.206706
C	-6.461966	-1.305489	1.110453
H	-6.626746	0.761997	0.604848
H	-1.797949	-0.321398	2.169189
H	-3.562266	-3.043348	1.385972
H	-7.536508	-1.441258	1.199739
H	-5.979588	-3.354937	1.581533
P	1.060379	-0.184186	0.067439
C	1.165275	-1.660935	-1.095115
C	0.164012	-1.715727	-2.107238
C	0.132493	-2.778779	-3.010920
H	-0.632281	-2.779556	-3.785309
C	1.029190	-3.845466	-2.937011
C	1.936783	-3.832909	-1.883250
H	2.607888	-4.680160	-1.760459
C	2.019708	-2.786832	-0.948499
C	-0.951468	-0.697974	-2.246903
H	-0.654020	0.337682	-2.076930

H	-1.784948	-0.934253	-1.559437
H	-1.393051	-0.752445	-3.248056
C	0.997180	-4.969279	-3.944336
H	-0.030651	-5.276624	-4.168905
H	1.541790	-5.847103	-3.582014
H	1.457210	-4.664994	-4.894141
C	2.996523	-3.024035	0.188637
H	2.551612	-2.827343	1.166266
H	3.898963	-2.411700	0.119755
H	3.312709	-4.071555	0.176214
C	1.462808	1.416440	-0.861131
C	1.832558	1.590396	-2.225118
C	2.042145	2.887557	-2.720608
H	2.330895	2.993297	-3.764583
C	1.919444	4.033694	-1.940131
C	1.574278	3.852326	-0.602104
H	1.480668	4.721812	0.045704
C	1.338831	2.587251	-0.051616
C	2.062945	0.489121	-3.243383
H	1.131743	0.184833	-3.733589
H	2.502661	-0.411994	-2.821779
H	2.731864	0.855753	-4.028505
C	2.135640	5.411109	-2.520031
H	2.528086	6.105049	-1.768824
H	1.195370	5.836987	-2.895703
H	2.837986	5.386602	-3.360038
C	0.958492	2.561984	1.415502
H	0.661973	3.563458	1.742282
H	1.794281	2.239992	2.044901
H	0.121507	1.884609	1.615503
C	2.519947	-0.207292	1.269122
C	3.858317	0.041029	0.853503
C	4.879366	0.124563	1.807872
H	5.895584	0.302937	1.461519
C	4.646438	-0.026089	3.173388
C	3.336449	-0.285851	3.569235
H	3.122078	-0.424542	4.626595
C	2.272956	-0.376833	2.660247
C	4.301016	0.185180	-0.585999
H	4.131605	1.196955	-0.966632
H	3.780694	-0.505451	-1.250962
H	5.372714	-0.023215	-0.667705
C	5.763318	0.100069	4.181350
H	6.729424	-0.177341	3.746226
H	5.587770	-0.535410	5.055981

H	5.854173	1.133047	4.543528
C	0.914632	-0.659576	3.259147
H	0.991280	-0.714255	4.349565
H	0.491252	-1.601809	2.905770
H	0.182026	0.112813	3.012444

12-TS

B3LYP SCF energy: -2439.15298066 a.u.
B3LYP enthalpy: -2438.413728 a.u.
B3LYP free energy: -2438.539131 a.u.
M06 SCF energy in solution: -2439.43893927 a.u.
M06 enthalpy in solution: -2438.699687 a.u.
M06 free energy in solution: -2438.825090 a.u.
Three lowest frequencies (cm-1): -151.7210 11.3225 20.1184
Imaginary frequency: -151.7210 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Rh	1.594342	0.075191	-0.632356
N	2.414489	1.924749	-0.962813
C	3.714096	4.355584	-1.362056
C	1.766398	2.972227	-1.502675
C	3.741279	2.046301	-0.639123
C	4.396943	3.271078	-0.826795
C	2.371610	4.203576	-1.718157
H	0.731194	2.798539	-1.768857
H	5.444950	3.357343	-0.561994
H	1.800248	5.015643	-2.154620
H	4.222584	5.303824	-1.510643
C	4.338982	0.811651	-0.149578
C	5.284376	-1.680862	0.658473
C	5.671927	0.672504	0.273814
C	3.465396	-0.302575	-0.152381
C	3.958103	-1.552543	0.239995
C	6.141099	-0.571465	0.681810
H	6.342605	1.528642	0.284524
H	1.966412	-0.607498	-2.026267
H	3.308768	-2.422174	0.206368
H	7.171112	-0.683349	1.008852
H	5.658908	-2.655653	0.962995
P	-1.246115	-0.007458	0.044249
C	-0.462981	-1.456231	0.926491
C	0.476681	-1.121610	1.950412

C	1.159457	-2.145541	2.620546
H	1.865570	-1.868903	3.400631
C	0.975042	-3.490724	2.315624
C	0.102063	-3.796739	1.269230
H	-0.021621	-4.836848	0.976010
C	-0.606764	-2.824973	0.556132
C	0.774726	0.291867	2.427621
H	0.708751	1.044312	1.635476
H	1.789381	0.333570	2.834070
H	0.085261	0.611113	3.216991
C	1.694545	-4.579318	3.075500
H	1.024381	-5.071585	3.793122
H	2.543457	-4.179391	3.639406
H	2.070621	-5.357030	2.401256
C	-1.443280	-3.317814	-0.604752
H	-1.131699	-2.850721	-1.542275
H	-2.511701	-3.132465	-0.474741
H	-1.306258	-4.396967	-0.720225
C	-2.157369	1.043269	1.314258
C	-2.545469	0.678801	2.631197
C	-3.150567	1.639492	3.460132
H	-3.438941	1.334967	4.464958
C	-3.409596	2.942854	3.052225
C	-3.055042	3.281095	1.744479
H	-3.261367	4.285900	1.380858
C	-2.438894	2.373696	0.881405
C	-2.397807	-0.687639	3.278699
H	-1.599605	-0.682977	4.031193
H	-2.172268	-1.488662	2.583081
H	-3.325373	-0.943574	3.803219
C	-4.040410	3.954978	3.978218
H	-4.492158	3.473080	4.851210
H	-4.819779	4.533529	3.468701
H	-3.296184	4.673475	4.346759
C	-2.106240	2.873976	-0.506961
H	-2.405063	3.921145	-0.615573
H	-2.615295	2.300017	-1.288259
H	-1.032057	2.809846	-0.704086
C	-2.604553	-0.462654	-1.167793
C	-3.890584	-0.948359	-0.798559
C	-4.866860	-1.140412	-1.781351
H	-5.838183	-1.525165	-1.477043
C	-4.639836	-0.865870	-3.130254
C	-3.379394	-0.391596	-3.481893
H	-3.167637	-0.178624	-4.527221

C	-2.360194	-0.181564	-2.541924
C	-4.288756	-1.312343	0.612587
H	-4.431905	-0.426102	1.238054
H	-3.540994	-1.939121	1.103183
H	-5.230400	-1.869824	0.605681
C	-5.726143	-1.056298	-4.161293
H	-5.306912	-1.215795	-5.160055
H	-6.377880	-0.173832	-4.216607
H	-6.363375	-1.913532	-3.917863
C	-1.043324	0.320088	-3.094049
H	-1.162371	0.603322	-4.144796
H	-0.265072	-0.448500	-3.045584
H	-0.671097	1.193281	-2.551987
Cl	1.563761	-2.239629	-2.427733

13-TS

B3LYP SCF energy: -2018.84316967 a.u.
B3LYP enthalpy: -2018.068120 a.u.
B3LYP free energy: -2018.201725 a.u.
M06 SCF energy in solution: -2019.08444574 a.u.
M06 enthalpy in solution: -2018.309396 a.u.
M06 free energy in solution: -2018.443001 a.u.
Three lowest frequencies (cm-1): -812.1291 8.3637 9.3740
Imaginary frequency: -812.1291 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Rh	3.354498	-1.434118	0.520824
C	2.901730	-2.911318	1.991590
H	1.963047	-3.388233	1.680801
H	2.709526	-2.192026	2.798452
H	3.561152	-3.690126	2.389227
N	3.558212	0.282150	-0.729264
C	4.027170	2.616366	-2.155450
C	2.682310	0.704487	-1.654233
C	4.688033	1.003065	-0.480529
C	4.936665	2.183151	-1.196926
C	2.872740	1.867316	-2.393815
H	1.806809	0.079962	-1.804068
H	5.835983	2.756306	-1.001179
H	2.134572	2.167149	-3.129601
H	4.217138	3.530473	-2.711459
C	5.549411	0.424613	0.553893

C	7.095689	-0.788276	2.535727
C	6.768562	0.997320	0.952176
C	5.086223	-0.779571	1.156871
C	5.885253	-1.367981	2.149754
C	7.542404	0.395765	1.939440
H	7.118851	1.917223	0.490445
H	3.823914	-2.925822	0.702759
H	5.563035	-2.287135	2.628696
H	8.485033	0.843150	2.241943
H	7.696470	-1.265470	3.306970
P	-2.281274	-0.042148	0.333273
C	-3.843440	-1.032268	0.497939
C	-4.221801	-1.293670	1.846042
C	-5.312790	-2.125838	2.114235
H	-5.591906	-2.301016	3.151459
C	-6.043707	-2.743415	1.097995
C	-5.665860	-2.477720	-0.217852
H	-6.234335	-2.928559	-1.029185
C	-4.594232	-1.635456	-0.545094
C	-3.497580	-0.682165	3.027775
H	-3.926345	-1.044438	3.967419
H	-3.565313	0.412287	3.032083
H	-2.429746	-0.929385	3.018368
C	-7.188803	-3.676971	1.411683
H	-6.833569	-4.706108	1.558139
H	-7.921853	-3.699663	0.598145
H	-7.708368	-3.381088	2.329654
C	-4.342603	-1.407877	-2.020816
H	-3.447923	-1.927744	-2.378581
H	-4.205570	-0.349535	-2.259618
H	-5.193388	-1.773947	-2.604479
C	-2.639183	1.759397	0.610296
C	-3.909163	2.393010	0.605425
C	-4.004564	3.737937	0.989854
H	-4.984946	4.210417	0.976116
C	-2.897337	4.495649	1.369167
C	-1.650978	3.866857	1.352587
H	-0.765354	4.433828	1.633198
C	-1.500609	2.523029	0.998156
C	-5.195381	1.720834	0.175493
H	-5.556199	0.996856	0.913003
H	-5.081995	1.176853	-0.766300
H	-5.979804	2.471367	0.034916
C	-3.040931	5.936050	1.800268
H	-3.085511	6.020606	2.894548

H	-3.956971	6.384796	1.401640
H	-2.191668	6.542165	1.465339
C	-0.101866	1.942727	1.025617
H	0.613676	2.683270	1.396379
H	0.235606	1.629094	0.030643
H	-0.043806	1.057020	1.668579
C	-1.544010	-0.310369	-1.350923
C	-1.497147	0.612093	-2.427363
C	-0.766721	0.286032	-3.580763
H	-0.755505	1.000105	-4.402480
C	-0.085514	-0.921890	-3.728646
C	-0.149483	-1.829091	-2.666995
H	0.358644	-2.787443	-2.755739
C	-0.846926	-1.547152	-1.487894
C	-2.224085	1.939719	-2.441307
H	-1.751901	2.682896	-1.790240
H	-3.259668	1.845377	-2.104513
H	-2.237421	2.347719	-3.457198
C	0.703114	-1.236125	-4.978092
H	0.562954	-2.277589	-5.289014
H	1.779839	-1.092042	-4.816188
H	0.406721	-0.590608	-5.811509
C	-0.849489	-2.605794	-0.404175
H	-0.216452	-3.450720	-0.693376
H	-1.856094	-2.995179	-0.211358
H	-0.482739	-2.207412	0.549163

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B3LYP SCF energy: -1978.37231334 a.u.
B3LYP enthalpy: -1977.642888 a.u.
B3LYP free energy: -1977.759310 a.u.
M06 SCF energy in solution: -1978.64913797 a.u.
M06 enthalpy in solution: -1977.919713 a.u.
M06 free energy in solution: -1978.036135 a.u.
Three lowest frequencies (cm-1): 16.7236 27.2580 29.0442

Cartesian coordinates

ATOM	X	Y	Z
C	3.916347	0.853644	-0.054029
C	2.968972	3.427493	0.399659
C	2.504141	1.042735	0.051603
C	4.813688	1.929773	0.058288
C	4.346808	3.219316	0.283197

C	2.074658	2.361409	0.287298
H	5.884663	1.763032	-0.030277
H	5.043638	4.048740	0.369067
H	1.016805	2.571954	0.381300
H	2.585726	4.430154	0.579468
C	4.362608	-0.519751	-0.270732
C	4.924432	-3.212290	-0.633531
C	5.694066	-0.953067	-0.370323
N	3.341982	-1.421097	-0.363495
C	3.627767	-2.724072	-0.533257
C	5.979648	-2.299994	-0.554119
H	6.499981	-0.231472	-0.298974
H	2.774089	-3.391823	-0.589260
H	7.010153	-2.635655	-0.630849
H	5.096095	-4.274831	-0.770495
Rh	1.414199	-0.614699	-0.196298
P	-0.902818	0.035056	0.053268
C	-1.377513	1.822899	-0.202927
C	-0.867323	2.426525	-1.391981
C	-1.067455	3.793841	-1.610821
H	-0.671682	4.232281	-2.524523
C	-1.747282	4.607026	-0.704596
C	-2.269974	3.996396	0.433514
H	-2.837711	4.599183	1.139324
C	-2.115922	2.629056	0.704614
C	-0.140190	1.662552	-2.476075
H	0.251647	2.355218	-3.227239
H	-0.803741	0.954999	-2.986674
H	0.697111	1.075489	-2.074430
C	-1.905785	6.089133	-0.945848
H	-2.049544	6.309745	-2.009462
H	-1.013548	6.640410	-0.619799
H	-2.760151	6.496333	-0.394805
C	-2.826486	2.125913	1.945803
H	-2.139485	1.861493	2.754484
H	-3.433346	1.238347	1.748588
H	-3.493732	2.906236	2.324897
C	-1.836122	-0.939416	-1.261401
C	-2.991343	-0.519722	-1.973134
C	-3.529632	-1.362043	-2.957725
H	-4.411822	-1.022181	-3.496419
C	-3.003680	-2.617277	-3.257529
C	-1.891693	-3.034109	-2.525446
H	-1.463343	-4.016063	-2.717214
C	-1.300218	-2.219394	-1.556916

C	-3.749374	0.772423	-1.740108
H	-3.248049	1.636808	-2.186523
H	-3.879780	1.001201	-0.680538
H	-4.744544	0.698836	-2.190253
C	-3.603288	-3.484202	-4.338433
H	-3.517057	-4.548556	-4.093403
H	-3.091388	-3.330267	-5.297926
H	-4.662731	-3.255195	-4.494785
C	-0.062502	-2.747089	-0.873674
H	0.111071	-3.801078	-1.114264
H	-0.091775	-2.664594	0.219977
H	0.827991	-2.207279	-1.283979
C	-1.504539	-0.619892	1.725136
C	-2.618481	-1.483878	1.931884
C	-2.816951	-2.058469	3.197315
H	-3.670940	-2.719412	3.330075
C	-1.992254	-1.803044	4.288726
C	-0.949382	-0.899605	4.093938
H	-0.310184	-0.636197	4.934098
C	-0.686565	-0.310766	2.853206
C	-3.694448	-1.820105	0.916284
H	-3.356460	-2.516374	0.144274
H	-4.075107	-0.933110	0.406489
H	-4.540901	-2.285871	1.430543
C	-2.220567	-2.467230	5.624985
H	-1.998184	-1.786735	6.454564
H	-1.572236	-3.345570	5.745985
H	-3.255655	-2.808609	5.732281
C	0.468474	0.658526	2.806873
H	0.833295	0.863894	3.818441
H	0.199934	1.616134	2.350765
H	1.294510	0.254215	2.208029

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B3LYP SCF energy: -2018.85529395 a.u.
B3LYP enthalpy: -2018.076812 a.u.
B3LYP free energy: -2018.200002 a.u.
M06 SCF energy in solution: -2019.10488786 a.u.
M06 enthalpy in solution: -2018.326406 a.u.
M06 free energy in solution: -2018.449596 a.u.
Three lowest frequencies (cm-1): 19.2513 20.5355 28.5205

Cartesian coordinates

ATOM	X	Y	Z
Rh	1.621197	-0.518364	0.210285
C	2.020868	-0.788615	2.209236
H	2.452306	0.137740	2.605983
H	2.721079	-1.611563	2.369748
H	1.080147	-1.018447	2.714769
N	2.633995	1.494668	0.216834
C	4.254572	3.747334	0.427889
C	2.111802	2.696772	0.502662
C	3.978234	1.371823	0.043556
C	4.805611	2.504541	0.142709
C	2.875550	3.853648	0.618566
H	1.034581	2.725190	0.636124
H	5.877293	2.404993	0.015316
H	2.401110	4.801135	0.851984
H	4.894580	4.621857	0.509452
C	4.462262	0.004613	-0.209065
C	5.327470	-2.623551	-0.602607
C	5.802603	-0.263696	-0.543770
C	3.522419	-1.056332	-0.090027
C	3.994134	-2.367139	-0.275696
C	6.236141	-1.569910	-0.743798
H	6.515783	0.548631	-0.659234
H	1.164267	-2.024635	0.303188
H	3.306441	-3.199644	-0.161347
H	7.272867	-1.765963	-1.004051
H	5.660943	-3.649397	-0.745933
P	-1.005071	-0.125724	-0.019836
C	-1.546429	-1.043022	1.508803
C	-1.373382	-0.364270	2.750291
C	-1.722690	-1.008658	3.941531
H	-1.593888	-0.468198	4.877398
C	-2.202000	-2.317947	3.972784
C	-2.249841	-3.005370	2.761141
H	-2.540428	-4.054047	2.761694
C	-1.907364	-2.416042	1.536086
C	-0.780243	1.025905	2.877284
H	0.106943	1.138047	2.246958
H	-0.471178	1.200459	3.912502
H	-1.475389	1.822823	2.600218
C	-2.621587	-2.971837	5.267489
H	-2.035618	-2.597619	6.114187
H	-2.500263	-4.059547	5.225182
H	-3.678410	-2.770816	5.490856
C	-1.861827	-3.341624	0.336619

H	-0.919540	-3.234066	-0.208819
H	-2.672069	-3.176767	-0.378364
H	-1.931374	-4.379798	0.676167
C	-1.961888	1.520393	-0.103382
C	-3.099137	1.918542	0.656833
C	-3.607852	3.221315	0.509719
H	-4.476601	3.495661	1.106004
C	-3.067404	4.161477	-0.358302
C	-1.985324	3.748777	-1.135139
H	-1.555211	4.440992	-1.856250
C	-1.433768	2.468384	-1.035611
C	-3.892744	1.084924	1.652197
H	-3.675377	1.390119	2.682642
H	-3.713668	0.018545	1.594083
H	-4.962724	1.257784	1.490334
C	-3.621447	5.562319	-0.459218
H	-3.645475	5.910523	-1.498138
H	-3.004923	6.274964	0.105020
H	-4.638463	5.620748	-0.057860
C	-0.309193	2.162556	-2.001004
H	-0.010397	3.071265	-2.532365
H	-0.617765	1.427409	-2.751733
H	0.577169	1.766207	-1.501350
C	-1.605067	-0.931856	-1.622515
C	-2.980461	-1.147873	-1.929472
C	-3.346581	-1.668753	-3.173256
H	-4.403711	-1.832951	-3.372999
C	-2.412943	-1.980580	-4.163010
C	-1.075248	-1.752017	-3.864300
H	-0.321146	-1.978335	-4.614948
C	-0.648526	-1.243372	-2.626422
C	-4.113685	-0.861198	-0.974206
H	-4.287491	0.213965	-0.872906
H	-3.921592	-1.259789	0.023722
H	-5.040290	-1.314238	-1.339861
C	-2.844799	-2.544168	-5.495341
H	-3.295716	-3.537988	-5.378822
H	-1.998135	-2.641493	-6.182070
H	-3.596823	-1.905496	-5.974510
C	0.852032	-1.099491	-2.490421
H	1.321913	-1.034405	-3.477770
H	1.292150	-1.958164	-1.976197
H	1.154719	-0.182120	-1.964116

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B3LYP SCF energy: -2018.82189816 a.u.
B3LYP enthalpy: -2018.045400 a.u.
B3LYP free energy: -2018.167916 a.u.
M06 SCF energy in solution: -2019.08386021 a.u.
M06 enthalpy in solution: -2018.307362 a.u.
M06 free energy in solution: -2018.429878 a.u.
Three lowest frequencies (cm-1): -437.4638 17.1346 21.4239
Imaginary frequency: -437.4638 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Rh	-1.115802	-0.331475	-1.317732
C	-2.601225	-0.501068	-2.978593
H	-3.578128	-0.016641	-2.975222
H	-2.593373	-1.358529	-3.647049
H	-1.865972	0.229407	-3.361432
N	-2.584914	1.144343	-0.462431
C	-4.716460	2.685628	0.461094
C	-2.451070	2.465668	-0.274008
C	-3.783972	0.554307	-0.201812
C	-4.868633	1.319590	0.263511
C	-3.481813	3.279129	0.184946
H	-1.470595	2.876538	-0.489996
H	-5.825694	0.842338	0.443169
H	-3.317338	4.343002	0.320840
H	-5.552116	3.283728	0.814693
C	-3.843486	-0.885277	-0.467157
C	-3.875011	-3.635190	-0.979521
C	-4.812328	-1.713946	0.124992
C	-2.845168	-1.438751	-1.333392
C	-2.913730	-2.832763	-1.580081
C	-4.835765	-3.081535	-0.119984
H	-5.534390	-1.284794	0.815660
H	-0.268896	-1.453801	-2.041762
H	-2.187499	-3.275002	-2.255174
H	-5.586071	-3.710528	0.350269
H	-3.881336	-4.704096	-1.181764
P	0.923887	-0.096077	-0.011377
C	2.204013	0.114859	-1.379646
C	2.006065	1.186611	-2.300464
C	2.896638	1.373434	-3.359959
H	2.728214	2.210091	-4.035059
C	3.973631	0.517633	-3.591474

C	4.098276	-0.579945	-2.746283
H	4.889358	-1.301855	-2.937573
C	3.235944	-0.820830	-1.664213
C	0.827747	2.131040	-2.241636
H	0.733112	2.657999	-1.289944
H	-0.111496	1.573635	-2.390739
H	0.899003	2.881477	-3.035652
C	4.945436	0.764018	-4.720126
H	5.503871	-0.143266	-4.972710
H	5.678604	1.536933	-4.452418
H	4.430986	1.108575	-5.624520
C	3.467555	-2.136375	-0.944441
H	2.544777	-2.709990	-0.830717
H	3.896379	-2.017403	0.053679
H	4.162776	-2.747012	-1.528866
C	0.843372	1.429271	1.122698
C	1.632537	2.610473	1.079980
C	1.315250	3.688661	1.925908
H	1.935712	4.581444	1.863797
C	0.272961	3.654986	2.842755
C	-0.457529	2.468234	2.921955
H	-1.259304	2.387640	3.653275
C	-0.200966	1.366882	2.101566
C	2.872626	2.859532	0.235962
H	2.684306	3.622490	-0.529433
H	3.252988	1.981344	-0.272496
H	3.671182	3.247902	0.878684
C	-0.054298	4.838567	3.721529
H	-0.178043	4.538352	4.768847
H	-0.993585	5.316354	3.412821
H	0.732319	5.598940	3.678782
C	-1.046929	0.139100	2.365835
H	-1.913675	0.406175	2.978312
H	-0.477655	-0.623015	2.909278
H	-1.415610	-0.322308	1.446277
C	1.547629	-1.367905	1.243656
C	2.650228	-1.085818	2.099470
C	2.988629	-1.984049	3.118924
H	3.839365	-1.745592	3.754329
C	2.292043	-3.170616	3.337478
C	1.250704	-3.463011	2.460770
H	0.710294	-4.399804	2.576677
C	0.866344	-2.603750	1.421702
C	3.563381	0.112232	1.964152
H	3.142052	1.005608	2.434229

H	3.771706	0.354636	0.921018
H	4.521432	-0.096678	2.450760
C	2.651873	-4.098505	4.472579
H	3.717814	-4.038587	4.717838
H	2.415416	-5.140001	4.229661
H	2.094192	-3.842571	5.383655
C	-0.254742	-3.097398	0.541838
H	-0.583027	-4.088299	0.871421
H	0.044516	-3.166295	-0.507342
H	-1.117954	-2.430124	0.554463

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B3LYP SCF energy: -1979.54872839 a.u.
B3LYP enthalpy: -1978.799720 a.u.
B3LYP free energy: -1978.921353 a.u.
M06 SCF energy in solution: -1979.82765591 a.u.
M06 enthalpy in solution: -1979.078648 a.u.
M06 free energy in solution: -1979.200281 a.u.
Three lowest frequencies (cm-1): 14.5771 17.8286 29.7555

Cartesian coordinates

ATOM	X	Y	Z
Rh	1.403614	-0.456652	-0.662165
N	2.688324	1.442919	-0.388923
C	5.019262	2.646597	0.552912
C	2.667555	2.700026	0.073506
C	3.864067	0.771505	-0.408937
C	5.049905	1.340517	0.063314
C	3.810206	3.341886	0.553296
H	1.699190	3.190770	0.077813
H	5.973000	0.770723	0.029308
H	3.744661	4.359937	0.924200
H	5.927622	3.116027	0.920917
C	3.736949	-0.610576	-0.936548
C	3.800281	-3.156040	-2.152131
C	4.395692	-1.702876	-0.306812
C	3.097882	-0.822722	-2.197317
C	3.155214	-2.112619	-2.787355
C	4.421726	-2.949292	-0.901441
H	4.876822	-1.542605	0.654868
H	2.702448	-2.261146	-3.764120
H	4.921561	-3.775543	-0.403063
H	3.835815	-4.138037	-2.616215

P	-0.805848	-0.188033	0.054573
C	-1.002608	-1.425322	1.457602
C	-0.083157	-1.313765	2.543248
C	-0.151340	-2.215326	3.608700
H	0.550785	-2.096288	4.431610
C	-1.065564	-3.267804	3.642799
C	-1.885670	-3.427641	2.529660
H	-2.563849	-4.277806	2.494507
C	-1.867133	-2.553938	1.431076
C	1.040194	-0.304867	2.585394
H	0.716115	0.731495	2.463566
H	1.738281	-0.507632	1.755265
H	1.585751	-0.379999	3.532292
C	-1.147634	-4.201566	4.826450
H	-0.161385	-4.369351	5.273823
H	-1.561161	-5.175079	4.541853
H	-1.793888	-3.790966	5.614466
C	-2.745893	-2.968606	0.265900
H	-2.200082	-2.965838	-0.680878
H	-3.622292	-2.329798	0.131719
H	-3.107078	-3.988180	0.433247
C	-1.121229	1.588871	0.658362
C	-1.502723	2.025752	1.957254
C	-1.569428	3.402596	2.236115
H	-1.861168	3.703395	3.241024
C	-1.305074	4.385410	1.290966
C	-0.985150	3.949824	0.004263
H	-0.810919	4.688219	-0.776480
C	-0.888112	2.595744	-0.333903
C	-1.903667	1.153872	3.135517
H	-1.081428	1.048008	3.853062
H	-2.213981	0.151255	2.861939
H	-2.732917	1.631460	3.668944
C	-1.365390	5.855208	1.632349
H	-1.868567	6.429973	0.846071
H	-0.359034	6.280368	1.746331
H	-1.900726	6.025986	2.572111
C	-0.568702	2.307513	-1.787019
H	-0.229805	3.222478	-2.283829
H	-1.449520	1.943718	-2.326255
H	0.213646	1.547549	-1.895543
C	-2.254726	-0.348344	-1.157838
C	-3.571671	0.062398	-0.800055
C	-4.581424	0.099093	-1.768662
H	-5.578305	0.410748	-1.462497

C	-4.361914	-0.259582	-3.097125
C	-3.087553	-0.711434	-3.426267
H	-2.892082	-1.038505	-4.445206
C	-2.036674	-0.776623	-2.498603
C	-4.014344	0.417824	0.602895
H	-3.785561	1.456485	0.858724
H	-3.547269	-0.217463	1.356602
H	-5.097914	0.288102	0.690959
C	-5.458634	-0.162388	-4.130029
H	-6.440286	-0.380587	-3.694890
H	-5.291531	-0.857305	-4.959804
H	-5.511805	0.848468	-4.556633
C	-0.744947	-1.354122	-3.027418
H	-0.792306	-1.441974	-4.118341
H	-0.552972	-2.351304	-2.615883
H	0.129406	-0.756765	-2.746416
H	2.824169	0.027137	-2.816191
H	0.943965	-1.955827	-0.716411

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B3LYP SCF energy: -2166.95382248 a.u.
B3LYP enthalpy: -2166.207009 a.u.
B3LYP free energy: -2166.331613 a.u.
M06 SCF energy in solution: -2167.21278277 a.u.
M06 enthalpy in solution: -2166.465969 a.u.
M06 free energy in solution: -2166.590573 a.u.
Three lowest frequencies (cm-1): 23.3349 26.3142 28.8446

Cartesian coordinates

ATOM	X	Y	Z
C	3.765519	1.362760	0.177038
C	2.531822	3.460837	1.524028
C	2.356251	1.295157	0.392398
C	4.522284	2.455078	0.632797
C	3.910942	3.505182	1.308586
C	1.775678	2.375947	1.071715
H	5.596074	2.486739	0.466593
H	4.501152	4.346106	1.662228
H	0.708987	2.389769	1.252093
H	2.037216	4.275609	2.048435
C	4.372046	0.234767	-0.530046
C	5.236116	-2.029664	-1.882671
C	5.721496	0.107459	-0.891749

N	3.493339	-0.753192	-0.849609
C	3.911732	-1.850987	-1.501862
C	6.154992	-1.025685	-1.569371
H	6.423190	0.895282	-0.643424
H	3.150099	-2.598394	-1.695302
H	7.199944	-1.126117	-1.849384
H	5.533083	-2.933238	-2.404090
Rh	1.492214	-0.379828	-0.338994
C	1.606097	-2.172705	0.684901
O	1.138507	-2.734670	-0.321559
O	2.048467	-2.367695	1.784973
P	-0.927245	-0.088969	-0.002085
C	-1.587016	1.643984	0.400581
C	-1.195741	2.652374	-0.538645
C	-1.576821	3.981108	-0.337148
H	-1.262339	4.722479	-1.068498
C	-2.336424	4.389368	0.759246
C	-2.733378	3.400942	1.650167
H	-3.350692	3.677831	2.502798
C	-2.392102	2.044756	1.502862
C	-0.377954	2.390578	-1.785450
H	-0.091564	3.339418	-2.248498
H	-0.938852	1.814111	-2.527299
H	0.544327	1.842759	-1.565140
C	-2.703667	5.839477	0.962186
H	-3.075981	6.291651	0.035455
H	-1.832524	6.427867	1.278928
H	-3.475975	5.953972	1.729485
C	-2.980106	1.158275	2.587513
H	-2.381330	1.207556	3.504200
H	-3.061254	0.112062	2.316069
H	-3.982318	1.519829	2.841779
C	-1.983668	-0.427089	-1.547257
C	-3.398926	-0.263228	-1.518075
C	-4.140005	-0.378027	-2.700172
H	-5.219461	-0.253413	-2.643656
C	-3.554603	-0.657336	-3.932699
C	-2.178136	-0.862264	-3.944158
H	-1.692365	-1.117954	-4.883003
C	-1.383324	-0.763876	-2.792815
C	-4.215149	-0.023324	-0.268079
H	-4.189645	1.024778	0.042793
H	-3.869142	-0.628246	0.571407
H	-5.260931	-0.287252	-0.453533
C	-4.376164	-0.733369	-5.196636

H	-3.898287	-1.370519	-5.948181
H	-4.503785	0.261193	-5.644886
H	-5.378216	-1.130090	-5.000112
C	0.082532	-1.071865	-2.997986
H	0.278236	-1.281337	-4.054697
H	0.398125	-1.944963	-2.420074
H	0.732355	-0.237497	-2.705824
C	-1.345201	-1.345757	1.332513
C	-1.981727	-2.593138	1.077811
C	-2.237364	-3.455900	2.154083
H	-2.736738	-4.399082	1.943753
C	-1.855967	-3.174256	3.462773
C	-1.132110	-2.002127	3.673452
H	-0.752018	-1.783827	4.669038
C	-0.841669	-1.103208	2.644274
C	-2.345274	-3.144635	-0.287707
H	-1.524848	-3.027241	-0.998133
H	-3.234263	-2.684259	-0.726233
H	-2.544052	-4.216790	-0.195719
C	-2.185507	-4.108600	4.601535
H	-3.063002	-3.757748	5.161626
H	-1.355200	-4.178730	5.312972
H	-2.409722	-5.117537	4.240095
C	0.064607	0.051877	3.005212
H	0.103949	0.174650	4.092473
H	-0.237927	1.006332	2.575706
H	1.080918	-0.155043	2.654847

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B3LYP SCF energy: -2604.43613495 a.u.
B3LYP enthalpy: -2603.563506 a.u.
B3LYP free energy: -2603.713307 a.u.
M06 SCF energy in solution: -2604.62139793 a.u.
M06 enthalpy in solution: -2603.748769 a.u.
M06 free energy in solution: -2603.898570 a.u.
Three lowest frequencies (cm-1): 19.4279 24.1076 27.6122

Cartesian coordinates

ATOM	X	Y	Z
C	-1.522162	3.709479	-0.031769
C	0.861340	4.685746	-1.092139
C	-0.441805	2.806631	-0.239851
C	-1.399451	5.065267	-0.373576

C	-0.213748	5.556196	-0.910170
C	0.745487	3.331997	-0.759167
H	-2.232432	5.745195	-0.217011
H	-0.127431	6.606261	-1.174744
H	1.608256	2.696098	-0.902115
H	1.799972	5.056176	-1.497726
C	-2.732787	3.158057	0.578357
C	-4.859200	1.843315	1.772070
C	-3.904092	3.862952	0.881555
N	-2.645558	1.834037	0.875817
C	-3.676463	1.185472	1.446584
C	-4.970716	3.203186	1.483052
H	-3.977559	4.917894	0.644135
H	-3.567905	0.113470	1.612233
H	-5.882849	3.745326	1.716541
H	-5.671304	1.284693	2.223890
Rh	-0.826509	0.922053	0.354015
C	-1.885290	0.116107	-1.167187
O	-2.180313	-1.009023	-0.629214
O	-2.150019	0.653833	-2.210590
Al	-3.783143	-2.077064	-0.463163
C	-5.210884	-1.067272	-1.403064
H	-5.013158	-0.982943	-2.480312
H	-5.337881	-0.043480	-1.024509
H	-6.186643	-1.565033	-1.298742
C	-3.329146	-3.900379	-1.113932
H	-2.883880	-3.862009	-2.117974
H	-4.218441	-4.542778	-1.191181
H	-2.614191	-4.427360	-0.467115
O	-3.840995	-1.952950	1.321778
C	-4.349586	-2.914839	2.202174
H	-4.191793	-3.946879	1.846000
H	-5.433403	-2.792303	2.374752
H	-3.857705	-2.836463	3.186180
P	1.244742	-0.373142	-0.047316
C	2.861440	0.608655	-0.063852
C	3.021880	1.499216	1.046892
C	4.152589	2.314217	1.127285
H	4.247283	2.981182	1.981276
C	5.157332	2.307425	0.157863
C	5.005963	1.418739	-0.897920
H	5.783491	1.364035	-1.657688
C	3.898691	0.562489	-1.033372
C	2.039695	1.627910	2.192779
H	2.366509	2.416838	2.876494

H	1.955159	0.702673	2.769990
H	1.035124	1.901982	1.847009
C	6.351019	3.225400	0.262643
H	6.800622	3.184064	1.261752
H	6.064244	4.269661	0.083020
H	7.123192	2.963524	-0.467442
C	3.992873	-0.355069	-2.240527
H	3.840146	0.207950	-3.168908
H	3.282466	-1.173646	-2.240403
H	5.000946	-0.781752	-2.289479
C	1.604006	-1.520458	1.415737
C	2.824494	-2.246728	1.508365
C	3.114374	-2.967857	2.672460
H	4.051870	-3.518416	2.714801
C	2.245254	-3.026221	3.760486
C	1.028818	-2.360003	3.634606
H	0.306227	-2.420717	4.445081
C	0.687379	-1.618244	2.496017
C	3.841651	-2.366428	0.396099
H	4.518395	-1.507657	0.363268
H	3.370713	-2.456425	-0.584167
H	4.451915	-3.261790	0.549470
C	2.603633	-3.784043	5.015401
H	1.709349	-4.130493	5.543639
H	3.168550	-3.149042	5.711037
H	3.228136	-4.655909	4.792975
C	-0.685639	-0.988169	2.518348
H	-1.277317	-1.390408	3.346383
H	-1.274826	-1.200645	1.618054
H	-0.633391	0.098622	2.679617
C	0.958665	-1.382214	-1.606482
C	0.648607	-2.771738	-1.599193
C	0.407800	-3.417685	-2.821427
H	0.182294	-4.480853	-2.798770
C	0.415927	-2.759993	-4.047113
C	0.650240	-1.386312	-4.028211
H	0.625233	-0.829653	-4.962412
C	0.894987	-0.681300	-2.847669
C	0.480236	-3.650532	-0.374836
H	-0.199118	-3.206862	0.355431
H	1.419938	-3.869166	0.137677
H	0.040312	-4.603729	-0.679471
C	0.129787	-3.488108	-5.337761
H	0.808586	-3.168651	-6.136977
H	-0.892719	-3.286885	-5.682521

H	0.229772	-4.571538	-5.217733
C	1.035289	0.816972	-2.992282
H	1.236848	1.074638	-4.036808
H	1.836603	1.243018	-2.390281
H	0.103060	1.312615	-2.706151

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B3LYP SCF energy: -2565.13385193 a.u.
B3LYP enthalpy: -2564.291337 a.u.
B3LYP free energy: -2564.441479 a.u.
M06 SCF energy in solution: -2565.33768562 a.u.
M06 enthalpy in solution: -2564.495171 a.u.
M06 free energy in solution: -2564.645313 a.u.
Three lowest frequencies (cm-1): 14.2196 17.5610 21.6911

Cartesian coordinates

ATOM	X	Y	Z
C	1.341206	3.653052	-0.191972
C	-0.955916	4.517606	1.127377
C	0.335013	2.701060	0.133684
C	1.178065	5.007521	0.137114
C	0.033537	5.443855	0.796941
C	-0.805150	3.166426	0.797135
H	1.952299	5.727526	-0.113720
H	-0.082782	6.493232	1.052560
H	-1.606273	2.486322	1.055869
H	-1.855116	4.842491	1.645635
C	2.544345	3.141015	-0.852218
C	4.718590	1.873890	-2.012933
C	3.653337	3.894354	-1.256828
N	2.533330	1.796202	-1.053971
C	3.591482	1.169830	-1.598604
C	4.742222	3.258364	-1.844266
H	3.664386	4.967363	-1.104058
H	3.551457	0.081753	-1.660809
H	5.606659	3.838416	-2.155376
H	5.556808	1.334730	-2.440157
Rh	0.764626	0.831132	-0.457479
C	1.847472	0.200669	1.146447
O	2.183378	-0.979538	0.781105
O	2.078245	0.885567	2.107704
Al	3.831975	-1.969076	0.683517
C	5.208324	-0.873266	1.602902

H	5.004998	-0.765471	2.676965
H	5.285445	0.143299	1.192200
H	6.207497	-1.325355	1.513364
C	3.391208	-3.773366	1.394982
H	3.071471	-3.718304	2.445264
H	4.249331	-4.460554	1.366473
H	2.577717	-4.262570	0.840066
O	3.947372	-1.926734	-1.104828
C	4.574712	-2.887601	-1.905879
H	4.441445	-3.914701	-1.525617
H	5.661528	-2.713638	-1.998914
H	4.160111	-2.868429	-2.928017
P	-1.268004	-0.420466	0.046691
C	-2.829520	0.615496	-0.069179
C	-2.962975	1.342456	-1.292457
C	-4.055329	2.190643	-1.482769
H	-4.135536	2.726399	-2.426161
C	-5.036238	2.378819	-0.508118
C	-4.900837	1.658423	0.673307
H	-5.660768	1.767348	1.444254
C	-3.833688	0.778659	0.923260
C	-1.973738	1.265706	-2.436683
H	-2.318222	1.881827	-3.272581
H	-1.837964	0.246651	-2.809289
H	-0.986959	1.650002	-2.140343
C	-6.188455	3.328050	-0.731439
H	-6.647244	3.176186	-1.715455
H	-5.853143	4.372598	-0.691376
H	-6.965926	3.201088	0.028528
C	-3.900589	0.087911	2.273379
H	-3.334741	0.635354	3.034827
H	-3.512304	-0.928078	2.272854
H	-4.942276	0.050662	2.607711
C	-1.592412	-1.781779	-1.207570
C	-2.830187	-2.482391	-1.261823
C	-3.043698	-3.424232	-2.273661
H	-3.993631	-3.954572	-2.290850
C	-2.085515	-3.719959	-3.243750
C	-0.868011	-3.049135	-3.162177
H	-0.088209	-3.275391	-3.885665
C	-0.601599	-2.091214	-2.174975
C	-3.952050	-2.319351	-0.261034
H	-4.534789	-1.410737	-0.439084
H	-3.584513	-2.275272	0.766235
H	-4.636372	-3.170744	-0.326794

C	-2.361691	-4.723560	-4.336772
H	-1.433421	-5.119153	-4.761101
H	-2.929501	-4.265709	-5.157765
H	-2.954234	-5.566930	-3.965656
C	0.763645	-1.446170	-2.228443
H	1.439149	-2.012913	-2.875519
H	1.266758	-1.422148	-1.255063
H	0.713608	-0.430715	-2.650482
C	-1.035885	-1.127078	1.747730
C	-0.861658	-2.481567	2.122014
C	-0.613328	-2.758640	3.477819
H	-0.481458	-3.799440	3.764700
C	-0.495160	-1.776988	4.461985
C	-0.610408	-0.441565	4.059848
H	-0.477315	0.361874	4.779931
C	-0.860847	-0.132514	2.731121
C	-0.854224	-3.665880	1.178692
H	-0.136795	-3.528719	0.365160
H	-1.828730	-3.860940	0.723124
H	-0.558672	-4.565970	1.725126
C	-0.206848	-2.136059	5.899514
H	-0.951705	-1.700683	6.577103
H	0.773435	-1.754265	6.210733
H	-0.205938	-3.220012	6.050141
H	-0.901819	0.913589	2.447245

20-TS

B3LYP SCF energy: -2166.90721408 a.u.
B3LYP enthalpy: -2166.162968 a.u.
B3LYP free energy: -2166.285465 a.u.
M06 SCF energy in solution: -2167.18159109 a.u.
M06 enthalpy in solution: -2166.437345 a.u.
M06 free energy in solution: -2166.559842 a.u.
Three lowest frequencies (cm-1): -220.9736 21.0467 22.5632
Imaginary frequency: -220.9736 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.969719	-0.134505	0.179001
C	4.702824	-2.819481	0.405028
C	3.335357	-1.091052	-0.662381
C	4.945608	-0.517325	1.105359
C	5.315930	-1.859067	1.214179

C	3.728841	-2.434372	-0.516988
H	5.391877	0.222002	1.766569
H	6.078045	-2.152727	1.931272
H	3.292724	-3.164337	-1.192915
H	4.998394	-3.862964	0.483154
C	3.507409	1.258604	0.073790
C	2.461405	3.787377	-0.225280
C	4.337146	2.371245	0.236282
N	2.179914	1.404970	-0.195693
C	1.681111	2.642768	-0.348306
C	3.814571	3.650382	0.082276
H	5.389519	2.216740	0.447552
H	0.624359	2.709175	-0.568277
H	4.452825	4.523050	0.186806
H	2.006036	4.761191	-0.371501
Rh	1.208702	-0.407658	-0.391225
C	2.993534	-0.695487	-2.393276
O	3.424484	0.413099	-2.670546
O	2.508228	-1.662427	-2.979757
P	-1.053004	-0.035221	0.175749
C	-1.793832	1.641399	-0.183404
C	-1.544257	2.152753	-1.494135
C	-1.968411	3.447488	-1.820469
H	-1.767661	3.815815	-2.824186
C	-2.640229	4.268794	-0.916257
C	-2.921475	3.735975	0.340631
H	-3.485975	4.336327	1.051096
C	-2.531489	2.446746	0.729234
C	-0.879327	1.364732	-2.603647
H	-1.535460	0.569590	-2.975480
H	0.049102	0.874041	-2.282747
H	-0.643215	2.022435	-3.445122
C	-3.049057	5.674871	-1.283857
H	-3.950428	5.984657	-0.744274
H	-3.244733	5.767696	-2.357361
H	-2.257947	6.394975	-1.034718
C	-3.009903	2.013182	2.101613
H	-2.214622	2.019675	2.852462
H	-3.428380	1.004344	2.104560
H	-3.790055	2.698708	2.446466
C	-1.977484	-1.221863	-0.936221
C	-3.322883	-1.073853	-1.373402
C	-3.860281	-2.026486	-2.245494
H	-4.890696	-1.902534	-2.572474
C	-3.140063	-3.136109	-2.695669

C	-1.832526	-3.280713	-2.239008
H	-1.242707	-4.135655	-2.563246
C	-1.237912	-2.338456	-1.391293
C	-4.260811	0.035718	-0.943065
H	-4.063420	0.973692	-1.471864
H	-4.193901	0.253587	0.125175
H	-5.294866	-0.252713	-1.157019
C	-3.752539	-4.127342	-3.655353
H	-3.288792	-5.114774	-3.562120
H	-3.617990	-3.800963	-4.695158
H	-4.829289	-4.237308	-3.486438
C	0.213760	-2.573381	-1.053070
H	0.417050	-3.635106	-0.866700
H	0.531697	-2.142460	-0.050440
H	0.877502	-2.284073	-1.881819
C	-1.308806	-0.541973	1.973109
C	-2.141883	-1.603907	2.429019
C	-2.108197	-1.964150	3.785588
H	-2.752428	-2.777027	4.113178
C	-1.305408	-1.327402	4.726938
C	-0.514972	-0.273393	4.273098
H	0.112996	0.263377	4.981255
C	-0.489352	0.121444	2.932891
C	-3.118340	-2.406539	1.590800
H	-2.625601	-3.024272	0.835786
H	-3.839002	-1.775384	1.067460
H	-3.687290	-3.076037	2.242630
C	-1.280615	-1.764749	6.171361
H	-2.199185	-2.293246	6.446923
H	-1.162984	-0.910216	6.847039
H	-0.440835	-2.446001	6.363197
C	0.448940	1.257849	2.598187
H	0.760544	1.771256	3.513669
H	0.008473	2.007205	1.934524
H	1.342063	0.872674	2.097380

21-TS

B3LYP SCF energy:	-2166.88785275 a.u.
B3LYP enthalpy:	-2166.144066 a.u.
B3LYP free energy:	-2166.268367 a.u.
M06 SCF energy in solution:	-2167.17076318 a.u.
M06 enthalpy in solution:	-2166.426976 a.u.
M06 free energy in solution:	-2166.551277 a.u.

Three lowest frequencies (cm-1): -172.0749 16.7380 18.9880
Imaginary frequency: -172.0749 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.541793	1.169996	-0.055772
C	2.230918	3.489804	0.764928
C	2.535107	1.058842	0.959946
C	3.881828	2.398803	-0.626086
C	3.224394	3.560753	-0.215628
C	1.905530	2.262912	1.342582
H	4.635344	2.447494	-1.408930
H	3.490340	4.517342	-0.658120
H	1.192167	2.224431	2.156637
H	1.727448	4.395432	1.093321
C	4.172022	-0.089800	-0.482084
C	5.086631	-2.599848	-1.147747
C	5.508007	-0.250500	-0.856611
N	3.313413	-1.138081	-0.489228
C	3.760658	-2.362323	-0.798942
C	5.970576	-1.520062	-1.189229
H	6.174012	0.605402	-0.845140
H	3.032067	-3.165354	-0.754798
H	7.011460	-1.670573	-1.461061
H	5.412953	-3.609219	-1.374961
Rh	1.338571	-0.544850	-0.137390
C	2.894809	-0.009049	2.328396
O	3.950476	-0.607477	2.158404
O	2.085687	0.123352	3.242232
P	-1.022173	-0.114910	0.012785
C	-1.698654	1.654441	-0.085597
C	-1.048656	2.483228	-1.054007
C	-1.414525	3.826223	-1.179297
H	-0.900542	4.431815	-1.922429
C	-2.411488	4.412514	-0.399976
C	-3.072942	3.585802	0.499243
H	-3.884165	3.997217	1.097456
C	-2.756324	2.228107	0.672440
C	0.008749	2.001087	-2.022848
H	0.391452	2.842258	-2.607970
H	-0.395631	1.265061	-2.727256
H	0.856609	1.531632	-1.510642
C	-2.752950	5.877034	-0.531995
H	-2.714773	6.205301	-1.576820
H	-2.043107	6.500327	0.028082

H	-3.753829	6.092249	-0.143597
C	-3.653103	1.528219	1.679409
H	-3.429998	1.868794	2.696776
H	-3.574466	0.447103	1.677810
H	-4.697270	1.791753	1.475431
C	-1.752449	-0.823385	-1.584248
C	-3.115050	-0.713068	-1.973265
C	-3.515357	-1.205747	-3.221183
H	-4.563874	-1.113665	-3.496839
C	-2.636528	-1.827849	-4.110445
C	-1.314392	-1.975744	-3.699092
H	-0.605215	-2.486620	-4.347494
C	-0.869409	-1.485507	-2.466365
C	-4.206122	-0.151199	-1.094137
H	-4.151650	0.938007	-1.018526
H	-4.153006	-0.555142	-0.080193
H	-5.188126	-0.409089	-1.502104
C	-3.104482	-2.320278	-5.458433
H	-2.443571	-3.099137	-5.852669
H	-3.122663	-1.503426	-6.192200
H	-4.119584	-2.728930	-5.405750
C	0.576878	-1.707711	-2.125795
H	1.025232	-2.521726	-2.704622
H	0.685309	-2.084235	-1.053915
H	1.182117	-0.810926	-2.342032
C	-1.687285	-1.095667	1.472853
C	-2.166977	-2.433534	1.355402
C	-2.590023	-3.109582	2.508622
H	-2.961055	-4.126038	2.397932
C	-2.539522	-2.548010	3.781717
C	-2.000462	-1.268810	3.887721
H	-1.896855	-0.813949	4.870456
C	-1.555036	-0.542597	2.778565
C	-2.219663	-3.261483	0.084810
H	-1.265042	-3.264220	-0.447855
H	-2.981967	-2.927859	-0.623433
H	-2.445549	-4.300138	0.343981
C	-3.038152	-3.293830	4.995594
H	-2.380975	-3.136456	5.858009
H	-3.100374	-4.370672	4.807353
H	-4.040856	-2.952600	5.286773
C	-0.890921	0.775834	3.087357
H	-1.273865	1.182367	4.029703
H	-1.025196	1.535516	2.318858
H	0.185830	0.603839	3.206255

22-TS

B3LYP SCF energy: -2604.39404075 a.u.
B3LYP enthalpy: -2603.523649 a.u.
B3LYP free energy: -2603.670308 a.u.
M06 SCF energy in solution: -2604.58617272 a.u.
M06 enthalpy in solution: -2603.715781 a.u.
M06 free energy in solution: -2603.862440 a.u.
Three lowest frequencies (cm-1): -295.9755 19.6332 19.8213
Imaginary frequency: -295.9755 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.630401	-2.656007	-0.642484
C	-2.479904	-4.748732	1.207066
C	-2.052348	-2.419646	0.632827
C	-3.113227	-3.925608	-0.977739
C	-3.039192	-4.969430	-0.055033
C	-1.999400	-3.484440	1.547419
H	-3.518564	-4.113140	-1.968516
H	-3.419685	-5.951958	-0.319941
H	-1.622950	-3.294063	2.547708
H	-2.434615	-5.558733	1.930337
C	-2.635194	-1.525888	-1.577212
C	-2.555777	0.744257	-3.137514
C	-3.526275	-1.389371	-2.644720
N	-1.704598	-0.562408	-1.317859
C	-1.690284	0.551165	-2.065659
C	-3.485559	-0.247965	-3.438564
H	-4.263988	-2.163531	-2.822960
H	-0.961523	1.300862	-1.795963
H	-4.182364	-0.126723	-4.262649
H	-2.502644	1.667925	-3.702699
Rh	-0.524021	-0.958512	0.324924
C	-2.499954	-0.844060	1.570437
O	-3.418841	-0.252418	0.942550
O	-2.137706	-0.859496	2.731536
Al	-4.436054	1.372089	1.180369
C	-6.252314	0.823561	0.570781
H	-6.252955	0.420192	-0.452507
H	-6.976432	1.651278	0.583476
H	-6.668557	0.038488	1.218553
C	-4.189844	1.949532	3.063749

H	-4.565228	1.206230	3.780657
H	-4.729464	2.887161	3.265636
H	-3.136282	2.128344	3.317838
O	-3.600129	2.430650	0.009314
C	-4.217518	3.285395	-0.903893
H	-3.594740	3.406699	-1.808948
H	-4.373171	4.299218	-0.491360
H	-5.203074	2.921909	-1.243167
P	1.609952	0.240527	-0.081355
C	1.506426	1.838186	-1.029291
C	0.491964	2.741965	-0.596537
C	0.261961	3.915605	-1.328256
H	-0.523063	4.584956	-0.984042
C	1.000177	4.248246	-2.462004
C	2.021403	3.375065	-2.841842
H	2.639918	3.630698	-3.699875
C	2.301926	2.186589	-2.157120
C	-0.342309	2.563517	0.653916
H	0.144258	3.048241	1.510574
H	-0.495738	1.514021	0.924204
H	-1.340156	2.992288	0.522663
C	0.709949	5.501176	-3.252669
H	0.065599	5.283704	-4.115081
H	1.629507	5.951369	-3.642796
H	0.194962	6.249533	-2.642067
C	3.495426	1.400973	-2.663854
H	3.213496	0.481009	-3.184786
H	4.175699	1.108330	-1.860048
H	4.061936	2.015575	-3.369978
C	2.181383	0.665947	1.644059
C	2.881952	1.833510	2.038319
C	3.174469	2.015797	3.398699
H	3.705307	2.918873	3.692049
C	2.830157	1.091201	4.382881
C	2.175290	-0.072149	3.971152
H	1.902903	-0.823603	4.709082
C	1.839197	-0.286990	2.634780
C	3.389418	2.913861	1.104317
H	2.592309	3.588937	0.777838
H	3.850187	2.511180	0.199292
H	4.143248	3.517770	1.618854
C	3.135907	1.339566	5.839698
H	3.453500	0.420768	6.345226
H	2.246819	1.707940	6.367976
H	3.925286	2.087880	5.962922

C	1.089032	-1.554099	2.295394
H	1.053516	-2.239201	3.149123
H	1.513129	-2.116477	1.458135
H	-0.000495	-1.324573	2.173313
C	2.859849	-0.958549	-0.817257
C	4.136950	-1.263547	-0.264523
C	4.880293	-2.321895	-0.808859
H	5.851286	-2.541783	-0.370752
C	4.446088	-3.084012	-1.890142
C	3.225183	-2.731782	-2.462981
H	2.871897	-3.272894	-3.338249
C	2.429787	-1.701332	-1.954092
C	4.832731	-0.506708	0.850502
H	4.389090	-0.686181	1.833249
H	4.825478	0.572788	0.685430
H	5.879830	-0.820274	0.899687
C	5.262250	-4.236415	-2.422564
H	6.322602	-4.127048	-2.172432
H	5.174876	-4.320921	-3.511319
H	4.922085	-5.189463	-1.995900
C	1.136637	-1.432646	-2.687806
H	1.159384	-1.904176	-3.675547
H	0.940995	-0.366410	-2.835480
H	0.284732	-1.841113	-2.135264

22-TSa

B3LYP SCF energy: -2604.37847666 a.u.
B3LYP enthalpy: -2603.508092 a.u.
B3LYP free energy: -2603.653576 a.u.
M06 SCF energy in solution: -2604.57599450 a.u.
M06 enthalpy in solution: -2603.705610 a.u.
M06 free energy in solution: -2603.851094 a.u.
Three lowest frequencies (cm-1): -328.0358 20.3633 21.3452
Imaginary frequency: -328.0358 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.551348	-2.787789	0.530002
C	-0.795933	-3.840354	2.434422
C	-1.537075	-1.942778	1.074904
C	-2.683864	-4.114493	0.956067
C	-1.810051	-4.643139	1.904337
C	-0.678411	-2.512232	2.034421

H	-3.445399	-4.752346	0.515929
H	-1.918423	-5.675568	2.225045
H	0.060392	-1.877746	2.500115
H	-0.109837	-4.245341	3.173566
C	-3.376023	-2.236833	-0.549145
C	-4.736068	-0.991059	-2.593910
C	-4.638155	-2.708759	-0.921563
N	-2.807445	-1.186067	-1.189727
C	-3.480092	-0.565403	-2.169787
C	-5.322382	-2.085622	-1.960659
H	-5.083862	-3.537268	-0.382735
H	-3.016729	0.319483	-2.581523
H	-6.307727	-2.434627	-2.255354
H	-5.246953	-0.450061	-3.382972
Rh	-0.888479	-0.638222	-0.497319
C	-1.989393	-0.211684	1.560719
O	-3.168852	0.106084	1.194560
O	-1.273697	0.226734	2.432365
Al	-3.801927	1.856453	0.758679
C	-5.755786	1.571788	0.491333
H	-6.264884	1.356111	1.441895
H	-5.977064	0.733455	-0.184349
H	-6.253460	2.457355	0.068515
C	-3.238266	3.135673	2.171059
H	-3.711207	2.904632	3.136320
H	-3.514212	4.173004	1.927551
H	-2.153285	3.119421	2.336447
O	-2.920875	2.113778	-0.801891
C	-3.142878	3.274422	-1.555137
H	-2.902624	4.199893	-1.002161
H	-4.188999	3.367023	-1.900295
H	-2.508603	3.274824	-2.458798
P	1.397677	0.157316	-0.022319
C	2.768027	-1.134647	0.309041
C	2.632377	-2.349139	-0.440342
C	3.535754	-3.397798	-0.252584
H	3.397753	-4.305059	-0.836591
C	4.605509	-3.322562	0.638766
C	4.764153	-2.124039	1.318678
H	5.608125	-2.009637	1.996874
C	3.893213	-1.029184	1.175314
C	1.584842	-2.589149	-1.503319
H	1.678483	-3.604141	-1.901432
H	1.702498	-1.895057	-2.342934
H	0.563839	-2.472050	-1.116131

C	5.542632	-4.487659	0.843691
H	5.072253	-5.271646	1.451714
H	6.459520	-4.179075	1.356019
H	5.824517	-4.947398	-0.110614
C	4.341060	0.168047	1.999117
H	4.379221	-0.101193	3.059819
H	3.718053	1.048529	1.903844
H	5.361245	0.445754	1.709901
C	2.014162	0.828109	-1.688869
C	3.303797	1.380816	-1.910063
C	3.680781	1.761882	-3.203668
H	4.672383	2.187090	-3.343795
C	2.838430	1.635491	-4.308572
C	1.558656	1.139464	-4.074174
H	0.854714	1.064640	-4.900522
C	1.140455	0.747463	-2.797864
C	4.312677	1.639463	-0.820530
H	4.805197	0.714965	-0.508105
H	3.851908	2.091030	0.060292
H	5.088162	2.323034	-1.179051
C	3.294425	2.023917	-5.693910
H	2.446376	2.271882	-6.340587
H	3.842421	1.201710	-6.173277
H	3.967146	2.887962	-5.666715
C	-0.282445	0.283745	-2.669038
H	-0.872527	0.513864	-3.561435
H	-0.824940	0.836676	-1.855951
H	-0.345055	-0.818533	-2.568585
C	1.376243	1.575920	1.218145
C	1.075730	2.903479	0.780663
C	1.057464	3.943029	1.716733
H	0.840587	4.947078	1.359651
C	1.269621	3.744719	3.080185
C	1.464309	2.435115	3.500548
H	1.576206	2.229340	4.563332
C	1.489824	1.349470	2.615821
C	0.667167	3.303259	-0.623736
H	-0.168840	2.691060	-0.975105
H	1.475972	3.246716	-1.354493
H	0.307667	4.336076	-0.609178
C	1.216744	4.893999	4.056740
H	0.178172	5.187701	4.256723
H	1.733841	5.777771	3.665610
H	1.674335	4.627267	5.014984
C	1.576892	0.002522	3.301639

H	2.316717	0.027677	4.108340
H	1.835156	-0.822331	2.640633
H	0.602108	-0.212678	3.745863

22-TSb

B3LYP SCF energy: -2565.08519741 a.u.
B3LYP enthalpy: -2564.244726 a.u.
B3LYP free energy: -2564.392149 a.u.
M06 SCF energy in solution: -2565.29465562 a.u.
M06 enthalpy in solution: -2564.454184 a.u.
M06 free energy in solution: -2564.601607 a.u.
Three lowest frequencies (cm-1): -290.4281 13.3952 16.0378
Imaginary frequency: -290.4281 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.402597	-2.225983	-1.632544
C	-2.464480	-4.677081	-0.283038
C	-1.947459	-2.297357	-0.287871
C	-2.863816	-3.375646	-2.282416
C	-2.895215	-4.598490	-1.609800
C	-2.002834	-3.533439	0.371063
H	-3.171962	-3.329315	-3.323727
H	-3.258900	-5.485840	-2.120524
H	-1.721434	-3.571070	1.418132
H	-2.504005	-5.626369	0.245299
C	-2.307269	-0.918421	-2.296217
C	-2.037917	1.636792	-3.305961
C	-3.075026	-0.524859	-3.395298
N	-1.405669	-0.060631	-1.739277
C	-1.298908	1.189797	-2.216209
C	-2.935565	0.760020	-3.911442
H	-3.795595	-1.216424	-3.817180
H	-0.596952	1.836727	-1.705825
H	-3.536026	1.078122	-4.758591
H	-1.920134	2.658778	-3.648605
Rh	-0.421103	-0.813761	-0.105109
C	-2.453610	-0.944943	0.945349
O	-3.341616	-0.245117	0.377275
O	-2.197023	-1.204901	2.103488
Al	-4.397103	1.295751	0.766426
C	-6.157638	0.887495	-0.070713
H	-6.061772	0.617762	-1.132422

H	-6.860063	1.732623	-0.022181
H	-6.656146	0.042968	0.426697
C	-4.336281	1.610269	2.729451
H	-4.879265	0.833636	3.286458
H	-4.793644	2.572984	3.003880
H	-3.311103	1.620154	3.124472
O	-3.441546	2.481514	-0.178606
C	-3.938198	3.674030	-0.705977
H	-3.294874	4.030932	-1.529887
H	-3.975499	4.488067	0.041551
H	-4.955951	3.571599	-1.122217
P	1.665564	0.298219	0.154884
C	1.861891	2.145682	0.272574
C	0.729526	2.884835	0.725607
C	0.757551	4.285382	0.665714
H	-0.117084	4.825610	1.021692
C	1.849078	4.996735	0.179809
C	2.965564	4.260348	-0.220589
H	3.848353	4.793027	-0.567242
C	3.010218	2.862890	-0.183733
C	-0.536333	2.301088	1.317548
H	-0.814718	2.878363	2.207795
H	-0.457434	1.257704	1.619034
H	-1.390597	2.383835	0.630506
C	1.831754	6.503100	0.086631
H	1.525941	6.831220	-0.915865
H	2.822932	6.928719	0.278021
H	1.127075	6.940544	0.801039
C	4.327135	2.247762	-0.616172
H	4.255851	1.705859	-1.563455
H	4.724694	1.548408	0.122151
H	5.069477	3.040593	-0.747254
C	1.531295	-0.599316	1.759622
C	1.546204	-0.107944	3.091893
C	1.182821	-0.985520	4.113678
H	1.201049	-0.612208	5.136013
C	0.808402	-2.323244	3.899722
C	0.853981	-2.807195	2.597120
H	0.621350	-3.848580	2.391553
C	1.201711	-1.961143	1.536720
C	1.988875	1.287748	3.469876
H	1.200205	2.028271	3.305977
H	2.859530	1.617320	2.895074
H	2.253414	1.320507	4.531357
C	0.371513	-3.192135	5.052850

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H        0.465903   -4.256078    4.812676
H       -0.681032   -3.000771    5.298315
H        0.958880   -2.991334    5.955811
C        3.081707   -0.505341   -0.741458
C        4.202383   -1.075819   -0.083461
C        5.144422   -1.785269   -0.839599
H        6.000711   -2.215505   -0.324166
C        5.039870   -1.940156   -2.221483
C        3.959855   -1.326289   -2.858876
H        3.871105   -1.396344   -3.940931
C        2.982335   -0.619254   -2.153265
C        4.500345   -0.937247    1.395790
H        3.984841   -1.695561    1.994555
H        4.209466    0.037723    1.794887
H        5.574913   -1.057252    1.567072
C        6.056446   -2.739086   -3.000640
H        7.016829   -2.786664   -2.476956
H        6.229453   -2.309604   -3.993397
H        5.713793   -3.771714   -3.149927
C        1.864365    0.014519   -2.947541
H        2.084158   -0.030704   -4.018645
H        1.713143    1.068328   -2.686655
H        0.915463   -0.500865   -2.770669
H        1.338740   -2.398426    0.546809
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 23
B3LYP SCF energy:                    -2166.94063214 a.u.
B3LYP enthalpy:                      -2166.194691 a.u.
B3LYP free energy:                   -2166.321282 a.u.
M06 SCF energy in solution:          -2167.20438811 a.u.
M06 enthalpy in solution:            -2166.458447 a.u.
M06 free energy in solution:         -2166.585038 a.u.
Three lowest frequencies (cm-1):      13.6507     15.9603     25.4852

Cartesian coordinates
ATOM       X           Y           Z
C        4.149015   -0.271282    0.225629
C        4.583854   -3.031657    0.488172
C        3.526402   -1.163440   -0.672199
C        4.983548   -0.778855    1.237486
C        5.183919   -2.148606    1.388467
C        3.787080   -2.535193   -0.540361
H        5.469164   -0.084074    1.918510
```

H	5.814423	-2.520289	2.191589
H	3.357809	-3.205249	-1.278357
H	4.750988	-4.102004	0.577487
C	4.057451	1.208137	0.095482
C	3.923258	3.964439	-0.093628
C	5.236699	1.963581	-0.012770
N	2.849530	1.817863	0.113087
C	2.794925	3.161370	0.012438
C	5.174957	3.348766	-0.106861
H	6.188395	1.444592	-0.041658
H	1.797649	3.588098	0.015547
H	6.084337	3.935806	-0.199249
H	3.815218	5.041178	-0.172737
Rh	0.983390	0.768738	0.084504
C	2.682425	-0.752394	-1.875431
O	3.012652	-1.206730	-2.968556
O	1.644038	0.008057	-1.695991
P	-1.202070	-0.048316	0.016928
C	-2.241408	1.351371	-0.699262
C	-1.894959	1.769102	-2.019259
C	-2.514421	2.891798	-2.576799
H	-2.236403	3.180437	-3.588627
C	-3.461228	3.648476	-1.888546
C	-3.797529	3.225631	-0.606447
H	-4.545724	3.785794	-0.049773
C	-3.226959	2.097894	0.005642
C	-0.879296	1.071565	-2.896000
H	-0.901851	-0.016849	-2.819253
H	0.143541	1.355917	-2.638303
H	-1.052121	1.335331	-3.944896
C	-4.116137	4.852033	-2.523110
H	-4.635524	5.464936	-1.779217
H	-4.855685	4.551343	-3.277246
H	-3.380496	5.486074	-3.031535
C	-3.770009	1.790192	1.388377
H	-3.020401	1.890648	2.177629
H	-4.176992	0.779392	1.462771
H	-4.583651	2.484493	1.619102
C	-1.552966	-1.668389	-0.837991
C	-2.568910	-1.903022	-1.803814
C	-2.613910	-3.143183	-2.455703
H	-3.395563	-3.305296	-3.195232
C	-1.714024	-4.172916	-2.189810
C	-0.767617	-3.951350	-1.190193
H	-0.079015	-4.750458	-0.923719

C	-0.668824	-2.735591	-0.506086
C	-3.673725	-0.934424	-2.180007
H	-3.343576	-0.185717	-2.906681
H	-4.070594	-0.383042	-1.325701
H	-4.501067	-1.488490	-2.634721
C	-1.761435	-5.476005	-2.950158
H	-1.475079	-6.322266	-2.315895
H	-1.066642	-5.458563	-3.800337
H	-2.761959	-5.672172	-3.350226
C	0.341518	-2.668274	0.617110
H	1.022683	-3.522386	0.568466
H	-0.154115	-2.691479	1.595795
H	0.941718	-1.751064	0.585159
C	-1.654934	-0.317226	1.816824
C	-2.684259	-1.170172	2.302174
C	-2.890502	-1.272349	3.682298
H	-3.683505	-1.927628	4.037214
C	-2.140488	-0.554853	4.618088
C	-1.139880	0.281764	4.130422
H	-0.533834	0.854958	4.829616
C	-0.872379	0.389310	2.760401
C	-3.616837	-1.977692	1.424229
H	-3.110335	-2.828606	0.959520
H	-4.046452	-1.382977	0.613927
H	-4.445999	-2.367217	2.023121
C	-2.395604	-0.700656	6.099057
H	-3.468606	-0.728194	6.320159
H	-1.952924	0.125338	6.665076
H	-1.963054	-1.633311	6.484801
C	0.316946	1.234410	2.372702
H	0.507057	2.035862	3.095225
H	0.155467	1.831585	1.411557
H	1.228428	0.617547	2.345856

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B3LYP SCF energy: -2604.43584024 a.u.
B3LYP enthalpy: -2603.563010 a.u.
B3LYP free energy: -2603.713368 a.u.
M06 SCF energy in solution: -2604.62174335 a.u.
M06 enthalpy in solution: -2603.748913 a.u.
M06 free energy in solution: -2603.899271 a.u.
Three lowest frequencies (cm-1): 10.6600 14.3269 18.2338

Cartesian coordinates

ATOM	X	Y	Z
C	2.397516	2.462207	0.018077
C	3.500521	3.170026	2.509463
C	3.203716	1.544354	0.723652
C	2.179532	3.733553	0.572098
C	2.704553	4.081388	1.816358
C	3.762853	1.920514	1.951267
H	1.584597	4.455264	0.018698
H	2.502424	5.064764	2.231715
H	4.414854	1.215108	2.455027
H	3.930012	3.435331	3.471360
C	1.853443	2.230799	-1.356144
C	0.768488	2.002028	-3.888121
C	2.318254	3.045995	-2.397110
N	0.874334	1.314859	-1.580855
C	0.346822	1.220817	-2.819427
C	1.784486	2.930692	-3.676796
H	3.107568	3.758456	-2.184612
H	-0.449266	0.497807	-2.941255
H	2.152921	3.553080	-4.486837
H	0.306687	1.870416	-4.860921
Rh	0.576189	-0.224976	-0.235545
C	3.537297	0.173455	0.193033
O	4.713115	-0.237152	0.424468
O	2.662444	-0.496708	-0.424595
Al	5.507833	-1.991096	0.133817
C	7.227888	-1.759543	1.113263
H	7.851593	-0.946532	0.714649
H	7.841461	-2.671637	1.080333
H	7.063063	-1.534001	2.177660
C	4.193477	-3.291090	0.880333
H	3.758640	-2.948833	1.832817
H	4.650832	-4.270737	1.079262
H	3.366859	-3.457472	0.176897
O	5.657013	-2.168871	-1.610974
C	6.573249	-1.557811	-2.464061
H	6.210910	-0.581127	-2.837514
H	6.755004	-2.187565	-3.351388
H	7.556659	-1.376171	-1.994087
P	-1.704928	-0.241356	0.171780
C	-2.884386	-0.164855	-1.302654
C	-2.538983	-1.022041	-2.396856
C	-3.278767	-0.966225	-3.582698
H	-2.993151	-1.627253	-4.398086

C	-4.372697	-0.116637	-3.749519
C	-4.740544	0.658755	-2.655557
H	-5.620911	1.294247	-2.732619
C	-4.040177	0.652322	-1.438282
C	-1.436099	-2.060199	-2.358297
H	-1.670139	-2.863575	-1.651051
H	-0.469296	-1.640987	-2.048150
H	-1.311123	-2.513756	-3.345966
C	-5.126363	-0.053357	-5.055871
H	-4.616216	0.601464	-5.774956
H	-6.138269	0.340614	-4.916403
H	-5.206295	-1.041952	-5.521108
C	-4.662514	1.533224	-0.369357
H	-4.393349	2.585749	-0.512849
H	-4.383192	1.268398	0.645569
H	-5.753380	1.470973	-0.446457
C	-2.083111	-1.940642	0.872692
C	-3.387878	-2.455317	1.095539
C	-3.532655	-3.771037	1.549517
H	-4.538462	-4.149185	1.720346
C	-2.443721	-4.606922	1.810747
C	-1.168283	-4.079126	1.618688
H	-0.295459	-4.692495	1.831339
C	-0.974596	-2.775682	1.148501
C	-4.656801	-1.652490	0.925335
H	-4.910266	-1.498256	-0.127710
H	-4.577761	-0.666132	1.389852
H	-5.496539	-2.171430	1.397291
C	-2.643623	-6.029455	2.274000
H	-1.783635	-6.388308	2.848467
H	-2.769973	-6.706292	1.418510
H	-3.538013	-6.126336	2.898786
C	0.446300	-2.327222	0.937033
H	1.176219	-2.907086	1.508959
H	0.620739	-1.280101	1.346055
H	0.759121	-2.447358	-0.113373
C	-2.064998	1.101926	1.435589
C	-2.238974	0.856460	2.828674
C	-2.446437	1.943475	3.690780
H	-2.592421	1.735244	4.748161
C	-2.461633	3.267740	3.261621
C	-2.225905	3.494444	1.907651
H	-2.201095	4.517474	1.535855
C	-2.006583	2.455663	0.998850
C	-2.170624	-0.494809	3.515216

H	-1.255032	-1.039199	3.269685
H	-3.007355	-1.152617	3.268486
H	-2.179461	-0.347755	4.599126
C	-2.677842	4.409109	4.225796
H	-3.132643	4.063748	5.159737
H	-3.327845	5.179686	3.795808
H	-1.727641	4.895503	4.483237
C	-1.678728	2.897872	-0.412289
H	-2.251580	3.795209	-0.671097
H	-1.872156	2.147948	-1.176875
H	-0.618405	3.159902	-0.476805

25-TS

B3LYP SCF energy: -2604.40374096 a.u.
B3LYP enthalpy: -2603.531385 a.u.
B3LYP free energy: -2603.676253 a.u.
M06 SCF energy in solution: -2604.60877282 a.u.
M06 enthalpy in solution: -2603.736417 a.u.
M06 free energy in solution: -2603.881285 a.u.
Three lowest frequencies (cm-1): -33.6901 14.8047 23.0271
Imaginary frequency: -33.6901 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.282041	1.016946	-0.976901
C	3.062741	3.684674	-1.883206
C	3.028139	2.063979	-0.061685
C	3.450794	1.347441	-2.332798
C	3.338837	2.660096	-2.788478
C	2.915241	3.378550	-0.533506
H	3.673027	0.552852	-3.038729
H	3.474434	2.878040	-3.844788
H	2.727554	4.151340	0.204181
H	2.979022	4.713503	-2.223084
C	3.541474	-0.419891	-0.628342
C	4.147392	-3.086406	-0.197497
C	4.832433	-0.904199	-0.884870
N	2.571413	-1.255039	-0.175485
C	2.889792	-2.546678	0.042302
C	5.146451	-2.242135	-0.670132
H	5.584680	-0.208674	-1.240183
H	2.092482	-3.164253	0.435800
H	6.150554	-2.610714	-0.860077

H	4.329380	-4.135901	0.007742
Rh	0.536923	-0.731910	0.236591
C	2.905305	1.874501	1.434537
O	3.086447	0.639051	1.826178
O	2.665109	2.828087	2.163702
Al	2.223936	-0.492466	2.947767
C	1.536201	0.349420	4.594622
H	0.928074	1.244027	4.418545
H	2.388355	0.670006	5.210293
H	0.944546	-0.346433	5.205163
C	0.556813	-1.717495	2.283223
O	3.381821	-1.806744	3.147083
C	4.738848	-1.659204	3.467530
H	4.890370	-1.397726	4.528366
H	5.234218	-0.883525	2.860729
H	5.272048	-2.606055	3.288707
P	-1.689647	-0.087283	-0.104310
C	-0.766583	-0.316995	-1.697492
C	-0.244812	-1.649339	-1.913249
C	0.644292	-1.853895	-3.004142
H	1.019104	-2.862642	-3.165881
C	0.985854	-0.856148	-3.891877
C	0.472096	0.435681	-3.660279
H	0.756456	1.239290	-4.334889
C	-0.348765	0.740959	-2.585581
C	-0.779647	-2.958876	-1.340817
H	-1.384082	-2.853833	-0.444082
H	0.060579	-3.619706	-1.103911
H	-1.384644	-3.475243	-2.099487
C	1.871178	-1.123262	-5.084727
H	1.344635	-0.909528	-6.023592
H	2.201932	-2.166049	-5.114167
H	2.765026	-0.486601	-5.071582
C	-0.739459	2.193054	-2.421291
H	-0.386508	2.603373	-1.471201
H	-1.819774	2.350058	-2.458286
H	-0.287348	2.785290	-3.221722
C	-3.204130	-1.174728	0.092326
C	-3.890578	-1.881773	-0.926817
C	-4.959604	-2.721875	-0.574765
H	-5.469884	-3.259767	-1.372099
C	-5.393738	-2.886810	0.735921
C	-4.729134	-2.158603	1.726271
H	-5.053674	-2.248910	2.760902
C	-3.657532	-1.312323	1.438244

C	-3.623795	-1.801093	-2.419004
H	-3.506668	-2.806431	-2.838908
H	-2.742126	-1.224049	-2.685032
H	-4.484436	-1.348190	-2.926523
C	-6.532415	-3.815417	1.083328
H	-6.174399	-4.688860	1.643430
H	-7.039032	-4.182197	0.185023
H	-7.278376	-3.315389	1.712508
C	-3.058187	-0.542907	2.594509
H	-1.966439	-0.574463	2.592390
H	-3.402087	-0.957021	3.546862
H	-3.353172	0.512721	2.565400
C	-2.380685	1.629299	0.157492
C	-3.545789	2.097164	-0.513582
C	-4.053514	3.362488	-0.207351
H	-4.937729	3.707367	-0.739627
C	-3.461762	4.201265	0.739751
C	-2.311048	3.740320	1.372273
H	-1.810961	4.377386	2.098092
C	-1.757818	2.478463	1.109266
C	-4.276092	1.326974	-1.589680
H	-4.917241	0.547236	-1.166681
H	-3.592679	0.841756	-2.290199
H	-4.913441	2.003773	-2.167193
C	-4.053350	5.551710	1.063921
H	-4.881708	5.457442	1.778792
H	-4.454345	6.039432	0.168370
H	-3.309060	6.217915	1.511583
C	-0.515987	2.118345	1.883680
H	0.198732	1.551489	1.280932
H	-0.752784	1.495830	2.754191
H	-0.007455	3.013252	2.249099
H	-0.168721	-1.381227	3.026700
H	0.025301	-2.425900	1.628725
H	1.274354	-2.392398	2.782420

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B3LYP SCF energy:	-1064.91197057 a.u.
B3LYP enthalpy:	-1064.638523 a.u.
B3LYP free energy:	-1064.709942 a.u.
M06 SCF energy in solution:	-1064.58973032 a.u.
M06 enthalpy in solution:	-1064.316283 a.u.
M06 free energy in solution:	-1064.387702 a.u.

Three lowest frequencies (cm-1): 19.9051 26.5192 30.6694

Cartesian coordinates

ATOM	X	Y	Z
C	1.916612	0.721577	0.068088
C	1.925753	3.530796	-0.223884
C	0.718299	1.425442	-0.186531
C	3.100831	1.459125	0.193728
C	3.108673	2.848350	0.060433
C	0.736318	2.816870	-0.352071
H	4.034359	0.929433	0.360329
H	4.043854	3.392725	0.158952
H	-0.197903	3.327947	-0.559172
H	1.927324	4.610144	-0.343376
C	1.979039	-0.766312	0.101472
C	2.119517	-3.504530	0.024145
C	2.720229	-1.437831	1.084255
N	1.330237	-1.415879	-0.881448
C	1.404715	-2.748645	-0.907959
C	2.788934	-2.828934	1.042802
H	3.211646	-0.879096	1.874579
H	0.867936	-3.238294	-1.718821
H	3.349167	-3.374154	1.797565
H	2.144507	-4.587472	-0.049260
C	-0.609265	0.772550	-0.197907
O	-1.566603	1.227713	-0.927902
O	-0.910110	-0.215606	0.562091
Al	-2.676763	-0.160547	-0.197555
C	-3.100024	-1.633103	-1.414418
H	-3.896378	-1.367074	-2.121096
H	-3.434236	-2.528975	-0.875507
H	-2.220311	-1.916247	-2.005124
O	-3.792624	0.510945	0.915237
C	-5.103082	0.195049	1.301999
H	-5.770536	1.051239	1.127476
H	-5.139555	-0.041613	2.375288
H	-5.518213	-0.667132	0.756203

27-TS

B3LYP SCF energy: -2250.58810473 a.u.

B3LYP enthalpy: -2249.983268 a.u.

B3LYP free energy: -2250.101984 a.u.

M06 SCF energy in solution: -2250.95699638 a.u.

M06 enthalpy in solution: -2250.352160 a.u.
M06 free energy in solution: -2250.470876 a.u.
Three lowest frequencies (cm-1): -308.5354 16.5074 21.5849
Imaginary frequency: -308.5354 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.072397	-2.416838	-1.015285
C	0.516846	-3.175869	-3.217898
C	0.974924	-1.595185	-1.411057
C	2.377587	-3.582150	-1.726740
C	1.603814	-3.962322	-2.823690
C	0.219392	-2.003319	-2.527181
H	3.197209	-4.218387	-1.403162
H	1.849876	-4.868884	-3.369555
H	-0.558632	-1.336509	-2.883806
H	-0.079543	-3.465342	-4.079181
C	2.789236	-2.037616	0.211106
C	3.903063	-1.170916	2.582191
C	4.104989	-2.393884	0.522522
N	2.056305	-1.281755	1.066447
C	2.598007	-0.855723	2.214741
C	4.666775	-1.956374	1.718265
H	4.684894	-2.981950	-0.180095
H	1.960536	-0.243552	2.844333
H	5.692747	-2.212030	1.966189
H	4.308353	-0.795060	3.515445
Rh	0.149173	-0.752364	0.339413
C	1.235508	0.256720	-1.539682
O	2.386201	0.575107	-1.114985
O	0.442365	0.785535	-2.285617
Al	3.085477	2.388800	-1.054226
C	4.790081	2.111577	-0.054894
H	4.653586	1.638089	0.928318
H	5.331124	3.052717	0.121617
H	5.473585	1.463100	-0.622497
C	3.177267	3.026485	-2.928481
H	3.829690	2.398180	-3.552090
H	3.574795	4.050263	-2.988381
H	2.189183	3.036005	-3.406287
O	1.835748	3.235080	-0.104774
C	1.931988	3.652105	1.223640
H	1.862676	4.750865	1.306779
H	2.876469	3.351916	1.708967
H	1.111574	3.234568	1.836328

P	-1.957785	0.099013	0.060402
C	-2.370774	1.766859	-0.560617
C	-1.344254	2.725003	-0.646310
C	-3.673953	2.108352	-0.959315
C	-1.634165	4.012080	-1.099940
H	-0.313519	2.496165	-0.388535
C	-3.949749	3.395537	-1.421079
H	-4.472104	1.374541	-0.916579
C	-2.932021	4.349862	-1.487879
H	-0.825467	4.734009	-1.161198
H	-4.959959	3.649497	-1.731104
H	-3.149709	5.350788	-1.851510
C	-3.471064	-0.926777	-0.096683
C	-4.565577	-0.774292	0.771219
C	-3.526742	-1.900544	-1.104971
C	-5.697163	-1.576988	0.624119
H	-4.531926	-0.029916	1.562006
C	-4.663523	-2.696995	-1.254035
H	-2.675352	-2.042425	-1.764081
C	-5.748564	-2.536446	-0.390482
H	-6.537742	-1.453930	1.301636
H	-4.697297	-3.446872	-2.039524
H	-6.630748	-3.160725	-0.503371
C	-1.589635	0.218215	1.856242
C	-1.278012	-1.012083	2.490910
C	-1.345874	1.426096	2.547242
C	-0.757814	-1.017825	3.799100
H	-1.554079	-1.954617	2.023774
C	-0.843451	1.402292	3.841375
H	-1.557110	2.372784	2.060820
C	-0.543752	0.180017	4.468747
H	-0.542537	-1.966093	4.283763
H	-0.677600	2.336746	4.369994
H	-0.153569	0.175040	5.482983

27-TSa

B3LYP SCF energy:	-2250.59681684 a.u.		
B3LYP enthalpy:	-2249.991568 a.u.		
B3LYP free energy:	-2250.111681 a.u.		
M06 SCF energy in solution:	-2250.95269775 a.u.		
M06 enthalpy in solution:	-2250.347449 a.u.		
M06 free energy in solution:	-2250.467562 a.u.		
Three lowest frequencies (cm-1):	-262.7007	10.9920	21.8072

Imaginary frequency: -262.7007 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.742696	-2.165406	-0.486092
C	3.442754	-2.462223	-3.193727
C	2.234332	-1.256781	-1.455225
C	3.604012	-3.190333	-0.892961
C	3.972932	-3.323894	-2.233724
C	2.568395	-1.445906	-2.805380
H	3.951778	-3.923528	-0.170606
H	4.653174	-4.118600	-2.526756
H	2.169619	-0.751864	-3.538116
H	3.710334	-2.577850	-4.240287
C	2.211244	-2.142088	0.892917
C	1.029964	-2.133046	3.388056
C	2.927647	-2.599969	2.001640
N	0.934575	-1.672177	1.032481
C	0.366062	-1.681098	2.252281
C	2.338913	-2.594318	3.263022
H	3.950246	-2.934803	1.868756
H	-0.650625	-1.314791	2.307336
H	2.894788	-2.936407	4.130674
H	0.524346	-2.106206	4.347331
Rh	0.312114	-0.652968	-0.648990
C	1.935083	0.478743	-1.233912
O	2.859321	1.025684	-0.585461
O	1.100597	0.916781	-2.074320
Al	3.170289	2.819823	0.130292
C	5.156602	2.862062	0.209497
H	5.587234	2.027596	0.781063
H	5.529194	3.787390	0.672370
H	5.600195	2.816130	-0.795558
C	2.203707	4.099167	-1.033599
H	2.518874	4.027388	-2.083862
H	2.386208	5.136915	-0.718414
H	1.116612	3.946820	-1.015601
O	2.372537	2.680980	1.714765
C	2.893459	2.037617	2.841128
H	2.672065	0.953868	2.844102
H	2.452616	2.455906	3.761262
H	3.987933	2.142003	2.932060
P	-1.857443	0.043290	-0.084561
C	-2.848846	0.316049	-1.615563
C	-2.251262	1.057872	-2.650272

C	-4.155171	-0.166745	-1.782149
C	-2.956751	1.313057	-3.825907
H	-1.236226	1.428539	-2.538219
C	-4.853762	0.089049	-2.964453
H	-4.629783	-0.743480	-0.994585
C	-4.257213	0.828325	-3.986725
H	-2.485761	1.888314	-4.618197
H	-5.865317	-0.290293	-3.083441
H	-4.802765	1.025602	-4.905675
C	-2.839479	-1.178328	0.888517
C	-3.543456	-0.853606	2.057574
C	-2.828672	-2.515748	0.451480
C	-4.229089	-1.843775	2.767865
H	-3.557883	0.170708	2.415731
C	-3.522540	-3.498440	1.155427
H	-2.269597	-2.785240	-0.441684
C	-4.223722	-3.164196	2.317997
H	-4.769192	-1.577712	3.672578
H	-3.509483	-4.525836	0.801771
H	-4.758817	-3.931393	2.871026
C	-1.965392	1.640153	0.812013
C	-0.797986	2.195681	1.353721
C	-3.180717	2.341106	0.923999
C	-0.843013	3.428116	2.010989
H	0.165660	1.707681	1.245743
C	-3.223127	3.563382	1.592240
H	-4.086374	1.939755	0.476955
C	-2.054238	4.107166	2.137303
H	0.087758	3.839986	2.387749
H	-4.165107	4.099397	1.674920
H	-2.090785	5.068321	2.643635

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B3LYP SCF energy: -2312.35771513 a.u.
B3LYP enthalpy: -2311.531782 a.u.
B3LYP free energy: -2311.676381 a.u.
M06 SCF energy in solution: -2474.18250815 a.u.
M06 enthalpy in solution: -2473.356575 a.u.
M06 free energy in solution: -2473.501174 a.u.
Three lowest frequencies (cm-1): 13.4390 21.2111 24.5122

Cartesian coordinates

ATOM	X	Y	Z

C	1.091199	3.901107	0.238254
C	-1.281112	4.479549	1.573771
C	0.134641	2.859000	0.414738
C	0.855546	5.191629	0.738698
C	-0.325688	5.484289	1.411698
C	-1.050868	3.191406	1.080947
H	1.596794	5.974766	0.603255
H	-0.501104	6.483885	1.799298
H	-1.823713	2.447340	1.217227
H	-2.214734	4.694587	2.088651
C	2.306184	3.555998	-0.499234
C	4.476011	2.611487	-1.948654
C	3.370656	4.416206	-0.803508
N	2.344723	2.263435	-0.918494
C	3.396703	1.801736	-1.615129
C	4.457230	3.943627	-1.530507
H	3.344698	5.446967	-0.469412
H	3.369537	0.752058	-1.883745
H	5.284299	4.607579	-1.765725
H	5.306506	2.197348	-2.509601
Rh	0.684982	1.095539	-0.388863
C	2.029595	0.113244	0.801260
O	2.299339	-0.776398	-0.049796
O	2.390572	0.462610	1.896591
P	-1.194238	-0.463020	0.007297
C	-2.896677	0.297264	0.337461
C	-3.302718	1.271500	-0.631529
C	-4.517671	1.942312	-0.477526
H	-4.798626	2.677457	-1.228393
C	-5.376864	1.709021	0.597539
C	-4.986778	0.743060	1.515399
H	-5.644198	0.513940	2.352093
C	-3.782643	0.023742	1.414265
C	-2.500119	1.644426	-1.860504
H	-2.988356	2.469414	-2.387577
H	-2.409520	0.809435	-2.561353
H	-1.487295	1.977803	-1.605474
C	-6.668931	2.475198	0.747161
H	-7.238415	2.485833	-0.189676
H	-6.479700	3.521781	1.019149
H	-7.304584	2.040809	1.525136
C	-3.607305	-1.011603	2.511859
H	-3.358096	-0.530388	3.464999
H	-2.837919	-1.748777	2.314440
H	-4.554535	-1.541748	2.660721

C	-1.627474	-1.479968	-1.535580
C	-2.764102	-2.336518	-1.558068
C	-3.148201	-2.950503	-2.756324
H	-4.018610	-3.603240	-2.742679
C	-2.452463	-2.775675	-3.950514
C	-1.306496	-1.985528	-3.903745
H	-0.711434	-1.864164	-4.806105
C	-0.876736	-1.343855	-2.734665
C	-3.586354	-2.709832	-0.344773
H	-4.343789	-1.955367	-0.113278
H	-2.969381	-2.845781	0.544911
H	-4.107509	-3.654375	-0.529524
C	-2.915341	-3.419218	-5.234800
H	-2.075445	-3.621878	-5.907586
H	-3.613986	-2.764954	-5.773446
H	-3.436592	-4.363591	-5.045114
C	0.410578	-0.561710	-2.857701
H	0.886109	-0.763421	-3.823153
H	1.134853	-0.832010	-2.082391
H	0.241827	0.523165	-2.810566
C	-0.607032	-1.604779	1.379699
C	-0.152409	-2.937724	1.161893
C	0.310510	-3.681347	2.254858
H	0.644215	-4.700410	2.073531
C	0.398017	-3.166745	3.546557
C	0.021286	-1.839183	3.726581
H	0.118167	-1.388503	4.711573
C	-0.450148	-1.041671	2.679048
C	-0.038272	-3.636486	-0.179178
H	0.479469	-3.017293	-0.915196
H	-1.001112	-3.920811	-0.610330
H	0.548117	-4.551582	-0.055067
C	0.950417	-3.995192	4.680014
H	0.692204	-3.566840	5.653884
H	2.045138	-4.047043	4.618480
H	0.573711	-5.023991	4.647589
C	-0.709125	0.408600	3.015635
H	-0.793334	0.534075	4.099832
H	-1.616536	0.809520	2.566419
H	0.128912	1.024428	2.675374
Zn	4.221260	-2.087435	0.005530
C	4.177498	-3.030174	1.816242
H	3.469299	-3.869349	1.811763
H	5.161939	-3.427382	2.096614
H	3.855741	-2.332276	2.598638

C	4.975018	-1.636141	-1.852838
H	5.510208	-0.675453	-1.853337
H	5.691949	-2.395569	-2.192529
H	4.186681	-1.573942	-2.616523

29-TS

B3LYP SCF energy: -2312.31720313 a.u.
B3LYP enthalpy: -2311.493845 a.u.
B3LYP free energy: -2311.639085 a.u.
M06 SCF energy in solution: -2474.14558256 a.u.
M06 enthalpy in solution: -2473.322224 a.u.
M06 free energy in solution: -2473.467464 a.u.
Three lowest frequencies (cm-1): -255.4585 12.1213 18.2612
Imaginary frequency: -255.4585 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.525463	2.593150	0.553685
C	-2.687188	4.252937	-1.686616
C	-2.178528	2.067473	-0.721863
C	-2.937451	3.921552	0.696639
C	-3.019848	4.750781	-0.423566
C	-2.278205	2.926660	-1.830638
H	-3.161562	4.324020	1.681483
H	-3.343954	5.781614	-0.310051
H	-2.082460	2.521615	-2.819033
H	-2.764376	4.895490	-2.560087
C	-2.369647	1.680809	1.691167
C	-2.007796	-0.214277	3.659638
C	-3.110421	1.762155	2.874784
N	-1.444436	0.693635	1.510853
C	-1.284116	-0.231288	2.472729
C	-2.932923	0.808394	3.869926
H	-3.843181	2.553662	2.985705
H	-0.549752	-1.001199	2.280159
H	-3.516323	0.851855	4.784950
H	-1.844066	-0.995269	4.394358
Rh	-0.528089	0.733404	-0.333059
C	-2.892598	0.381904	-1.213349
O	-3.640922	-0.007963	-0.313676
O	-2.665472	0.116257	-2.380006
P	1.697206	-0.214511	-0.008824
C	1.888493	-1.557363	1.270231

C	0.914206	-2.600016	1.212629
C	0.906504	-3.589084	2.204730
H	0.155567	-4.373363	2.141931
C	1.825837	-3.607403	3.252880
C	2.802435	-2.611902	3.264082
H	3.560633	-2.628670	4.044194
C	2.868670	-1.596833	2.300271
C	-0.103245	-2.749078	0.102071
H	0.370157	-3.089262	-0.826709
H	-0.613961	-1.806202	-0.137328
H	-0.868250	-3.480292	0.375736
C	1.768485	-4.662509	4.331170
H	2.765307	-4.888673	4.724835
H	1.328557	-5.593231	3.958246
H	1.153552	-4.328836	5.177889
C	4.050859	-0.655181	2.421403
H	3.772642	0.334602	2.794745
H	4.559012	-0.495397	1.467228
H	4.780306	-1.075222	3.120596
C	2.091985	-1.005266	-1.656395
C	2.908749	-2.144749	-1.872439
C	3.052785	-2.633200	-3.179138
H	3.676324	-3.511282	-3.333052
C	2.447126	-2.038093	-4.285402
C	1.671450	-0.899448	-4.059365
H	1.190533	-0.402910	-4.899314
C	1.476395	-0.391212	-2.774091
C	3.683094	-2.882610	-0.799227
H	3.037092	-3.513060	-0.180639
H	4.209800	-2.207967	-0.119452
H	4.430643	-3.531463	-1.265854
C	2.605156	-2.614114	-5.671559
H	2.617013	-1.827617	-6.433822
H	1.771589	-3.286716	-5.913387
H	3.529726	-3.193478	-5.762902
C	0.575379	0.809744	-2.621653
H	0.301589	1.241205	-3.589623
H	1.012997	1.625624	-2.032855
H	-0.431074	0.472835	-2.253271
C	2.901657	1.208801	0.265778
C	4.015405	1.524769	-0.564756
C	4.702359	2.730766	-0.356261
H	5.547250	2.954896	-1.003587
C	4.369809	3.636664	0.646830
C	3.319071	3.285184	1.491881

H	3.056117	3.945284	2.315962
C	2.581956	2.109883	1.322425
C	4.597496	0.649195	-1.657858
H	3.963886	0.592936	-2.546834
H	4.771722	-0.374480	-1.321782
H	5.563628	1.057455	-1.969192
C	5.115464	4.937975	0.815139
H	6.126932	4.878244	0.399779
H	5.195657	5.220846	1.870499
H	4.598028	5.757671	0.298960
C	1.473597	1.878563	2.324481
H	1.663225	2.461259	3.232082
H	1.368981	0.832116	2.621432
H	0.510360	2.195028	1.914473
Zn	-5.094947	-1.731915	-0.567034
C	-6.794044	-0.833544	-1.274043
H	-6.615465	-0.363763	-2.250716
H	-7.623471	-1.542682	-1.397616
H	-7.138070	-0.041109	-0.594894
C	-4.010659	-3.330121	0.139307
H	-4.632484	-4.215638	0.326993
H	-3.234059	-3.624215	-0.580518
H	-3.503494	-3.076500	1.080858

30-TS

B3LYP SCF energy: -2627.71787041 a.u.
B3LYP enthalpy: -2626.959470 a.u.
B3LYP free energy: -2627.087048 a.u.
M06 SCF energy in solution: -2627.98800894 a.u.
M06 enthalpy in solution: -2627.229609 a.u.
M06 free energy in solution: -2627.357187 a.u.
Three lowest frequencies (cm-1): -291.3001 20.4745 23.8520
Imaginary frequency: -291.3001 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-4.208271	0.092161	-0.049494
C	-5.166805	-2.408862	-0.855575
C	-3.501472	-0.631785	-1.050790
C	-5.376911	-0.421639	0.521281
C	-5.857726	-1.664441	0.108384
C	-3.997835	-1.905104	-1.414060
H	-5.890982	0.118131	1.312149

H	-6.764262	-2.063841	0.555507
H	-3.455582	-2.486671	-2.151418
H	-5.539484	-3.384081	-1.156551
C	-3.623122	1.370542	0.378587
C	-2.373338	3.721361	1.082910
C	-4.379837	2.432370	0.888895
N	-2.272784	1.477231	0.226916
C	-1.677725	2.630397	0.570122
C	-3.753116	3.619799	1.248305
H	-5.455170	2.323359	0.973088
H	-0.607279	2.677693	0.435440
H	-4.332002	4.452274	1.637709
H	-1.831337	4.625791	1.337600
Rh	-1.370426	-0.333165	-0.521452
C	-3.058838	0.344775	-2.541820
O	-4.065068	0.602158	-3.153992
O	-1.839785	0.556642	-2.625905
P	1.072405	-0.156085	0.088416
C	1.663480	1.591217	0.601137
C	1.535759	2.576629	-0.434812
C	1.921212	3.899532	-0.196976
H	1.805015	4.619149	-1.004485
C	2.442075	4.328255	1.024018
C	2.573787	3.366978	2.015942
H	2.986958	3.657432	2.980485
C	2.214071	2.018280	1.842138
C	0.995759	2.305727	-1.823191
H	1.709634	1.733426	-2.422064
H	0.052128	1.755272	-1.830022
H	0.818781	3.252293	-2.342413
C	2.867253	5.760581	1.239524
H	2.149833	6.462813	0.799722
H	2.964025	5.994490	2.304646
H	3.839376	5.959093	0.769202
C	2.512760	1.178921	3.073171
H	1.876795	1.493186	3.908719
H	2.379819	0.113171	2.939728
H	3.549510	1.350212	3.384378
C	2.498699	-0.519689	-1.119627
C	3.847187	-0.493643	-0.643129
C	4.906596	-0.674288	-1.535963
H	5.919889	-0.657915	-1.139608
C	4.716355	-0.877614	-2.902502
C	3.404659	-0.905872	-3.353215
H	3.213502	-1.068841	-4.411476

C	2.292465	-0.736906	-2.508967
C	4.266607	-0.303574	0.798076
H	4.286782	0.755797	1.069936
H	3.615033	-0.818273	1.503584
H	5.278136	-0.695610	0.942343
C	5.886228	-1.045953	-3.841248
H	6.427966	-0.100161	-3.973551
H	6.606761	-1.776766	-3.455192
H	5.559873	-1.381996	-4.830417
C	0.965440	-0.831069	-3.222940
H	1.075962	-0.469618	-4.251137
H	0.162651	-0.269377	-2.761338
C	1.122380	-1.406637	1.503808
C	1.703950	-2.702350	1.371684
C	1.619249	-3.595039	2.449674
H	2.073663	-4.576070	2.331638
C	0.965239	-3.298711	3.642458
C	0.341163	-2.057681	3.726391
H	-0.217199	-1.801595	4.625141
C	0.383959	-1.122473	2.687450
C	2.385853	-3.263862	0.138548
H	1.828762	-3.042481	-0.771075
H	3.407651	-2.895348	0.011303
H	2.440754	-4.352685	0.231079
C	0.931930	-4.280712	4.788389
H	0.051332	-4.127671	5.421242
H	0.916620	-5.314982	4.428176
H	1.817682	-4.173250	5.429274
C	-0.428808	0.133523	2.943490
H	-0.294321	0.463584	3.979445
H	-0.183131	0.969963	2.292852
H	0.625111	-1.870110	-3.264674
H	-1.531639	-0.962411	0.858639
H	-1.494973	-0.077880	2.804168
Cl	-0.851359	-2.589747	-1.153667

31-TS

B3LYP SCF energy:	-3065.19384922 a.u.
B3LYP enthalpy:	-3064.310204 a.u.
B3LYP free energy:	-3064.461780 a.u.
M06 SCF energy in solution:	-3065.39214244 a.u.
M06 enthalpy in solution:	-3064.508497 a.u.
M06 free energy in solution:	-3064.660073 a.u.

Three lowest frequencies (cm-1): -287.3841 14.2697 21.6609
Imaginary frequency: -287.3841 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.735949	-2.317201	1.424843
C	-2.820539	-4.838144	0.221625
C	-2.209495	-2.469900	0.106505
C	-3.295877	-3.399258	2.109814
C	-3.338928	-4.657862	1.507479
C	-2.263937	-3.760826	-0.463740
H	-3.665876	-3.277942	3.124229
H	-3.774683	-5.496504	2.043795
H	-1.889322	-3.888948	-1.472707
H	-2.857030	-5.817737	-0.247132
C	-2.616394	-0.986000	2.026985
C	-2.333095	1.597009	2.944539
C	-3.468945	-0.508118	3.029281
N	-1.628513	-0.200883	1.513913
C	-1.510640	1.061969	1.958311
C	-3.327603	0.792406	3.497712
H	-4.258960	-1.148105	3.404929
H	-0.732249	1.660020	1.504442
H	-3.993587	1.176570	4.264616
H	-2.192108	2.626245	3.255515
Rh	-0.498008	-1.137526	-0.044804
C	-3.165991	-1.331987	-1.242752
O	-3.750762	-0.458779	-0.592864
O	-3.023522	-1.768978	-2.336578
Al	-4.984381	1.015261	-1.180244
C	-6.442501	0.791939	0.151235
H	-6.081830	0.826660	1.188982
H	-7.218521	1.565136	0.059668
H	-6.950044	-0.174833	0.024482
C	-5.297422	0.637767	-3.096015
H	-5.734890	-0.353524	-3.274729
H	-5.998326	1.374190	-3.515949
H	-4.381477	0.694262	-3.698362
O	-3.942122	2.413829	-0.911705
C	-4.110009	3.429968	0.031422
H	-3.188616	3.581454	0.619212
H	-4.343220	4.393117	-0.456153
H	-4.922481	3.230930	0.750893
P	1.712031	0.278513	0.022930
C	1.046803	2.034480	-0.075132

C	-0.022023	2.226533	-1.001091
C	-0.645217	3.469603	-1.113110
H	-1.476615	3.567570	-1.805402
C	-0.263383	4.561790	-0.332118
C	0.754248	4.356758	0.595304
H	1.052698	5.184857	1.234226
C	1.415264	3.127353	0.760275
C	-0.585896	1.127202	-1.875852
H	0.148519	0.430065	-2.281603
H	-1.353985	0.563341	-1.319545
H	-1.140462	1.552329	-2.717686
C	-0.939673	5.902057	-0.484187
H	-0.622541	6.603513	0.294104
H	-0.704349	6.353305	-1.456486
H	-2.029756	5.801462	-0.433168
C	2.455175	3.111204	1.865096
H	2.289053	2.316037	2.594618
H	3.472853	2.987531	1.488080
H	2.423869	4.064037	2.401724
C	2.749274	-0.147991	-1.478820
C	2.992797	0.681625	-2.608551
C	3.742406	0.168842	-3.676510
H	3.922526	0.816478	-4.531850
C	4.279013	-1.116462	-3.683749
C	4.065764	-1.899344	-2.552665
H	4.484502	-2.902689	-2.514172
C	3.313968	-1.455677	-1.460540
C	2.573315	2.130656	-2.775750
H	1.523247	2.235225	-3.063590
H	2.714225	2.730888	-1.875297
H	3.168786	2.587002	-3.572106
C	5.046623	-1.642175	-4.872175
H	4.379949	-2.174267	-5.563708
H	5.520915	-0.831544	-5.435802
H	5.826249	-2.348385	-4.566333
C	3.218637	-2.425924	-0.299767
H	3.298441	-3.450556	-0.673356
H	4.031575	-2.263164	0.418297
C	3.004150	0.156715	1.395983
C	4.358932	0.536248	1.171367
C	5.326127	0.246167	2.142355
H	6.353243	0.548274	1.947647
C	5.026487	-0.389431	3.344939
C	3.686795	-0.686768	3.584679
H	3.406437	-1.134812	4.535342

C	2.676622	-0.425482	2.651013
C	4.880723	1.302987	-0.028678
H	5.223168	0.636087	-0.825678
H	4.139999	1.973523	-0.463232
H	5.736397	1.913063	0.281061
C	6.102115	-0.729679	4.347289
H	6.498594	-1.738420	4.170368
H	6.945229	-0.033736	4.283213
H	5.717384	-0.707879	5.372461
C	1.272817	-0.759913	3.093260
H	1.271062	-1.048364	4.148791
H	0.594512	0.089377	2.984046
H	0.840502	-1.585426	2.520818
H	0.017839	-2.213155	0.885817
H	2.273340	-2.359671	0.238511
Cl	0.313309	-2.377735	-1.892313

32-TS

B3LYP SCF energy: -2207.38516030 a.u.
B3LYP enthalpy: -2206.590746 a.u.
B3LYP free energy: -2206.719186 a.u.
M06 SCF energy in solution: -2207.62293486 a.u.
M06 enthalpy in solution: -2206.828521 a.u.
M06 free energy in solution: -2206.956961 a.u.
Three lowest frequencies (cm-1): -325.8136 16.7336 21.4164
Imaginary frequency: -325.8136 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-4.190515	-0.162464	-0.125355
C	-5.068848	-2.542017	-1.317214
C	-3.425797	-0.728657	-1.183626
C	-5.347942	-0.799234	0.338410
C	-5.787668	-1.981490	-0.257813
C	-3.900266	-1.925858	-1.757772
H	-5.898327	-0.395022	1.183774
H	-6.688505	-2.466645	0.108961
H	-3.343887	-2.375761	-2.574888
H	-5.415097	-3.459782	-1.785762
C	-3.730303	1.112255	0.461393
C	-2.763373	3.487529	1.471737
C	-4.606295	2.006526	1.095753
N	-2.410708	1.398372	0.325575

C	-1.955659	2.558666	0.819004
C	-4.120024	3.202638	1.610759
H	-5.663039	1.772315	1.154627
H	-0.898408	2.749918	0.688819
H	-4.791216	3.903859	2.099027
H	-2.330884	4.408738	1.848462
Rh	-1.277791	-0.430427	-0.688850
C	-2.977840	0.525644	-2.575674
O	-4.014927	0.961714	-2.994912
O	-1.761108	0.616962	-2.744817
P	1.061749	-0.219596	0.039104
C	1.475426	1.494858	0.781549
C	1.317279	2.578245	-0.146696
C	1.585833	3.890462	0.253927
H	1.456230	4.685349	-0.477368
C	2.002181	4.217834	1.544942
C	2.157209	3.164539	2.433882
H	2.493295	3.375125	3.447863
C	1.923444	1.819843	2.091325
C	0.867705	2.426049	-1.584832
H	1.649723	1.975735	-2.203214
H	-0.030484	1.814605	-1.697262
H	0.643572	3.409660	-2.008243
C	2.289175	5.646457	1.939777
H	2.456906	5.738314	3.017603
H	3.184261	6.026096	1.430286
H	1.461042	6.311958	1.667931
C	2.239764	0.871697	3.236305
H	1.544036	1.035492	4.067065
H	2.206659	-0.179915	2.980519
H	3.243688	1.089229	3.618593
C	2.584770	-0.312055	-1.111324
C	3.902949	-0.186505	-0.571945
C	5.008345	-0.148144	-1.426111
H	5.997536	-0.059529	-0.980974
C	4.894145	-0.222111	-2.814326
C	3.612663	-0.360936	-3.328675
H	3.480455	-0.435365	-4.406010
C	2.461954	-0.415097	-2.522706
C	4.241612	-0.116459	0.900531
H	4.149126	0.904602	1.281592
H	3.609101	-0.759469	1.511801
H	5.278375	-0.431120	1.056256
C	6.109373	-0.148954	-3.706646
H	5.860572	-0.398946	-4.742788

H	6.543824	0.859248	-3.703055
H	6.894165	-0.837183	-3.370660
C	1.179805	-0.617829	-3.296763
H	1.248686	-0.116637	-4.267920
H	0.290118	-0.251657	-2.797727
C	1.190300	-1.633885	1.294595
C	1.898796	-2.843761	1.037406
C	1.834245	-3.886538	1.975579
H	2.385431	-4.799083	1.759829
C	1.096611	-3.813114	3.152277
C	0.366225	-2.646271	3.363624
H	-0.253836	-2.560591	4.254474
C	0.375028	-1.576872	2.463638
C	2.732332	-3.168405	-0.190687
H	2.266255	-2.856211	-1.124664
H	3.723195	-2.705648	-0.160291
H	2.879297	-4.251359	-0.244119
C	1.085894	-4.943166	4.153014
H	1.388480	-5.888928	3.691748
H	1.778921	-4.746216	4.982148
H	0.090805	-5.081347	4.590573
C	-0.552781	-0.436640	2.843276
H	-0.470917	-0.231383	3.916597
H	-0.373054	0.492479	2.307419
H	1.021346	-1.684510	-3.496224
C	-0.841987	-2.295966	-1.489168
H	-1.470095	-3.045917	-1.000313
H	0.198451	-2.608256	-1.382043
H	-1.087567	-2.255433	-2.556414
H	-1.442226	-1.249987	0.591413
H	-1.591035	-0.720571	2.640807

33-TS

B3LYP SCF energy: -2644.86460093 a.u.
B3LYP enthalpy: -2643.944702 a.u.
B3LYP free energy: -2644.097087 a.u.
M06 SCF energy in solution: -2645.02669494 a.u.
M06 enthalpy in solution: -2644.106796 a.u.
M06 free energy in solution: -2644.259181 a.u.
Three lowest frequencies (cm-1): -262.4232 15.1376 22.6398
Imaginary frequency: -262.4232 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.678813	-2.606487	-0.845080
C	2.666041	-4.855705	0.819371
C	2.063318	-2.502998	0.438365
C	3.256851	-3.809623	-1.273169
C	3.248298	-4.933183	-0.448471
C	2.093242	-3.660186	1.246561
H	3.687920	-3.884617	-2.267742
H	3.696231	-5.861405	-0.793001
H	1.678328	-3.606700	2.247435
H	2.663740	-5.724074	1.473295
C	2.661095	-1.424970	-1.724364
C	2.534055	0.855310	-3.269262
C	3.614170	-1.213769	-2.732790
N	1.675177	-0.523776	-1.491829
C	1.628912	0.584734	-2.245970
C	3.550030	-0.066971	-3.515102
H	4.414410	-1.930761	-2.876009
H	0.832619	1.282116	-2.017162
H	4.288181	0.109982	-4.292285
H	2.442985	1.771443	-3.843213
Rh	0.397157	-1.121594	0.387058
C	3.110605	-1.082175	1.638507
O	3.661928	-0.339531	0.836772
O	2.986962	-1.389139	2.775525
Al	4.967693	1.201704	1.167049
C	6.479200	0.602857	0.029984
H	6.171294	0.394575	-1.004004
H	7.284069	1.349770	-0.021881
H	6.933184	-0.319278	0.418839
C	5.101009	1.226105	3.139429
H	5.474596	0.285191	3.564052
H	5.798605	2.015684	3.454938
H	4.142795	1.440623	3.630900
O	4.034887	2.553208	0.534900
C	4.262073	3.257518	-0.652376
H	3.405320	3.167560	-1.340694
H	4.405954	4.332398	-0.447876
H	5.154461	2.912404	-1.200655
P	-1.735808	0.225624	-0.039416
C	-1.054358	1.925773	-0.473662
C	0.045470	2.359832	0.324041
C	0.688332	3.567556	0.049534
H	1.539843	3.847167	0.664021
C	0.297684	4.387720	-1.010712

C	-0.757048	3.944113	-1.803343
H	-1.069705	4.555749	-2.646708
C	-1.443339	2.738413	-1.574816
C	0.615466	1.561506	1.478184
H	-0.132665	1.110753	2.131917
H	1.295229	0.777672	1.101863
H	1.264098	2.192099	2.092812
C	0.996263	5.697967	-1.280546
H	0.704912	6.117268	-2.248939
H	0.751868	6.440360	-0.509777
H	2.084978	5.574297	-1.271905
C	-2.540516	2.431857	-2.576418
H	-2.384746	1.485164	-3.098681
H	-3.530313	2.382090	-2.118056
H	-2.571913	3.223819	-3.330513
C	-2.775597	0.304249	1.527085
C	-2.982500	1.444311	2.353214
C	-3.679011	1.294694	3.561758
H	-3.826404	2.178342	4.178987
C	-4.204958	0.079812	3.993606
C	-4.040697	-1.016052	3.149567
H	-4.462409	-1.976413	3.438940
C	-3.343834	-0.937813	1.938949
C	-2.579648	2.871989	2.031615
H	-1.519686	3.067003	2.217029
H	-2.771679	3.148901	0.993313
H	-3.147891	3.557404	2.667663
C	-4.914125	-0.046679	5.320104
H	-4.214801	-0.344684	6.112662
H	-5.366941	0.902439	5.626030
H	-5.703198	-0.805538	5.282545
C	-3.297477	-2.217560	1.126877
H	-3.454864	-3.078313	1.784061
H	-4.087046	-2.231299	0.366958
C	-3.025717	-0.289311	-1.314982
C	-4.398372	0.072040	-1.195719
C	-5.342895	-0.520414	-2.044792
H	-6.385647	-0.229824	-1.932767
C	-5.002393	-1.443121	-3.030906
C	-3.646239	-1.716953	-3.198219
H	-3.335321	-2.382003	-4.000827
C	-2.657317	-1.158076	-2.380183
C	-4.967731	1.116780	-0.253211
H	-5.288633	0.686736	0.700671
H	-4.263416	1.916669	-0.026309

H	-5.847414	1.574763	-0.718782
C	-6.051841	-2.102951	-3.891609
H	-6.345125	-3.076362	-3.476205
H	-6.957930	-1.491848	-3.960050
H	-5.683247	-2.283141	-4.907285
C	-1.230063	-1.478584	-2.751226
H	-1.205296	-2.115243	-3.641022
H	-0.661525	-0.571885	-2.980989
H	-0.689846	-1.989044	-1.950439
H	-0.216365	-2.437083	-0.073014
H	-2.346141	-2.364785	0.613384
C	-0.214945	-1.742907	2.263931
H	-0.956906	-1.068412	2.693534
H	0.684156	-1.727145	2.885867
H	-0.625946	-2.757131	2.259746

AlMe2OMe

B3LYP SCF energy: -437.44603306 a.u.
B3LYP enthalpy: -437.321683 a.u.
B3LYP free energy: -437.368257 a.u.
M06 SCF energy in solution: -437.36244064 a.u.
M06 enthalpy in solution: -437.238091 a.u.
M06 free energy in solution: -437.284665 a.u.
Three lowest frequencies (cm-1): 20.6910 26.5099 93.0634

Cartesian coordinates

ATOM	X	Y	Z
Al	-0.478861	-0.022717	-0.002623
C	-2.017675	1.195028	0.001685
H	-2.510096	1.207846	0.983757
H	-1.718605	2.224149	-0.226590
H	-2.782478	0.895638	-0.726571
C	-0.620699	-1.987454	0.001938
H	-1.013208	-2.351882	-0.957551
H	0.334473	-2.496538	0.175901
H	-1.323262	-2.329722	0.773465
O	1.060970	0.738323	-0.008695
C	2.383322	0.262105	0.005382
H	2.444976	-0.837088	0.023236
H	2.922261	0.614678	-0.884962
H	2.913672	0.643580	0.888948

CH4

B3LYP SCF energy: -40.51766309 a.u.
B3LYP enthalpy: -40.468641 a.u.
B3LYP free energy: -40.489773 a.u.
M06 SCF energy in solution: -40.48728895 a.u.
M06 enthalpy in solution: -40.438267 a.u.
M06 free energy in solution: -40.459399 a.u.
Three lowest frequencies (cm-1): 1374.3645 1374.3645 1374.3645

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	0.000000
H	0.631397	0.631397	0.631397
H	-0.631397	-0.631397	0.631397
H	-0.631397	0.631397	-0.631397
H	0.631397	-0.631397	-0.631397

CO2

B3LYP SCF energy: -188.57757052 a.u.
B3LYP enthalpy: -188.562367 a.u.
B3LYP free energy: -188.586668 a.u.
M06 SCF energy in solution: -188.56077334 a.u.
M06 enthalpy in solution: -188.545570 a.u.
M06 free energy in solution: -188.569871 a.u.
Three lowest frequencies (cm-1): 646.8590 646.8590 1370.4469

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.169583
O	0.000000	0.000000	-1.169583

ZnMe2

B3LYP SCF energy: -145.39018196 a.u.
B3LYP enthalpy: -145.312715 a.u.
B3LYP free energy: -145.347651 a.u.
M06 SCF energy in solution: -306.96894673 a.u.
M06 enthalpy in solution: -306.891480 a.u.
M06 free energy in solution: -306.926416 a.u.
Three lowest frequencies (cm-1): 45.2006 111.0916 111.0927

Cartesian coordinates

ATOM	X	Y	Z
Zn	0.000000	0.000000	0.000000
C	0.000000	0.000000	-2.023610
H	-0.511076	-0.885394	-2.421634
H	-0.511236	0.885301	-2.421634
H	1.022311	0.000092	-2.421634
C	0.000000	0.000000	2.023610
H	0.511236	0.885301	2.421634
H	-1.022311	0.000092	2.421634
H	0.511076	-0.885394	2.421634

RhCl-dimer

B3LYP SCF energy: -3919.73121860 a.u.
B3LYP enthalpy: -3918.604755 a.u.
B3LYP free energy: -3918.783927 a.u.
M06 SCF energy in solution: -3920.76582740 a.u.
M06 enthalpy in solution: -3919.639364 a.u.
M06 free energy in solution: -3919.818536 a.u.
Three lowest frequencies (cm-1): 7.1346 12.5002 18.6486

Cartesian coordinates

ATOM	X	Y	Z
Rh	1.702905	0.580822	-0.418190
P	3.852557	-0.125862	-0.014394
C	4.201701	0.044800	1.834694
C	3.253154	-0.560698	2.710347
C	3.339554	-0.351088	4.090167
H	2.605624	-0.836047	4.730541
C	4.322884	0.450224	4.666404
C	5.267978	1.004249	3.808122
H	6.074116	1.599538	4.231628
C	5.247992	0.817372	2.417105
C	2.127124	-1.454139	2.246125
H	1.736644	-2.033079	3.089931
H	2.420881	-2.159976	1.465422
H	1.304650	-0.863712	1.829038
C	4.361747	0.703701	6.153922
H	4.021167	-0.171222	6.718718
H	3.706325	1.541090	6.428944
H	5.372215	0.956295	6.492536
C	6.419293	1.444768	1.684616

H	6.132575	2.302717	1.071147
H	6.929694	0.735469	1.030129
H	7.154219	1.794837	2.415841
C	4.303006	-1.813293	-0.661090
C	4.916359	-2.848964	0.094292
C	5.065511	-4.116699	-0.484662
H	5.535820	-4.899446	0.107003
C	4.651720	-4.409264	-1.782333
C	4.109257	-3.365954	-2.531237
H	3.813843	-3.550180	-3.561840
C	3.929198	-2.079745	-2.011846
C	5.494208	-2.697761	1.488209
H	4.725129	-2.659347	2.265129
H	6.095735	-1.792272	1.599508
H	6.139420	-3.553993	1.708388
C	4.785845	-5.799195	-2.356058
H	5.001978	-5.771522	-3.429770
H	3.855488	-6.368615	-2.227967
H	5.584069	-6.363035	-1.861484
C	3.408042	-1.029861	-2.969354
H	3.076978	-1.501061	-3.899606
H	4.186405	-0.299441	-3.222653
H	2.563863	-0.468076	-2.551115
C	4.919927	1.130194	-0.899872
C	6.190510	0.904489	-1.484420
C	6.848575	1.976004	-2.105589
H	7.822784	1.791441	-2.553972
C	6.317246	3.264737	-2.158004
C	5.066515	3.472403	-1.571822
H	4.619859	4.464462	-1.598878
C	4.359083	2.430050	-0.969944
C	6.922918	-0.421703	-1.478624
H	6.488567	-1.134275	-2.187261
H	6.909362	-0.908836	-0.500593
H	7.969452	-0.268242	-1.760295
C	7.051692	4.387875	-2.850274
H	8.133050	4.215418	-2.857950
H	6.863064	5.350650	-2.362884
H	6.729135	4.485105	-3.895593
C	2.971045	2.716604	-0.451077
H	2.815578	2.440091	0.603055
H	2.231343	2.223557	-1.157961
H	2.698634	3.772890	-0.536047
Cl	0.571900	-1.544044	-0.772139
Rh	-1.702836	-0.581149	-0.417518

P	-3.852526	0.125814	-0.014517
C	-4.201825	-0.043147	1.834699
C	-3.253356	0.563184	2.709901
C	-3.339932	0.354925	4.089896
H	-2.606056	0.840468	4.729891
C	-4.323378	-0.445807	4.666793
C	-5.268323	-1.000684	3.808933
H	-6.074480	-1.595608	4.232910
C	-5.248158	-0.815169	2.417716
C	-2.127213	1.456093	2.244919
H	-1.736642	2.035705	3.088222
H	-2.420896	2.161299	1.463615
H	-1.304817	0.865218	1.828313
C	-4.362435	-0.697695	6.154576
H	-4.025662	0.179202	6.718616
H	-3.703969	-1.532189	6.431109
H	-5.372190	-0.953751	6.492685
C	-6.419297	-1.443421	1.685693
H	-6.132370	-2.301829	1.072970
H	-6.929806	-0.734780	1.030573
H	-7.154197	-1.793015	2.417171
C	-4.302959	1.812637	-0.662789
C	-4.916405	2.849004	0.091573
C	-5.065615	4.116166	-0.488609
H	-5.536001	4.899456	0.102277
C	-4.651790	4.407502	-1.786552
C	-4.109212	3.363513	-2.534418
H	-3.813720	3.546779	-3.565169
C	-3.929088	2.077815	-2.013772
C	-5.494262	2.699107	1.485627
H	-4.725186	2.661291	2.262578
H	-6.095892	1.793783	1.597740
H	-6.139375	3.555606	1.705058
C	-4.785972	5.796884	-2.361594
H	-5.001154	5.768200	-3.435467
H	-3.855962	6.366795	-2.233164
H	-5.584855	6.360829	-1.868198
C	-3.407807	1.027045	-2.970240
H	-3.076207	1.497415	-3.900716
H	-4.186309	0.296671	-3.223279
H	-2.563969	0.465326	-2.551220
C	-4.919806	-1.131045	-0.898943
C	-6.190363	-0.905893	-1.483769
C	-6.848344	-1.977980	-2.104029
H	-7.822524	-1.793857	-2.552657

C	-6.316969	-3.266745	-2.155262
C	-5.066273	-3.473858	-1.568815
H	-4.619575	-4.465922	-1.594970
C	-4.358913	-2.430942	-0.967826
C	-6.922813	0.420276	-1.479185
H	-6.488412	1.132264	-2.188377
H	-6.909383	0.908229	-0.501560
H	-7.969310	0.266536	-1.760839
C	-7.051337	-4.390511	-2.846598
H	-8.132716	-4.218190	-2.854320
H	-6.862553	-5.352881	-2.358473
H	-6.728857	-4.488521	-3.891868
C	-2.970900	-2.716958	-0.448597
H	-2.815603	-2.439697	0.605356
H	-2.231217	-2.224293	-1.155825
H	-2.698318	-3.773259	-0.532846
Cl	-0.571847	1.543489	-0.773355

Pmes3

B3LYP SCF energy: -1390.10109545 a.u.
B3LYP enthalpy: -1389.544504 a.u.
B3LYP free energy: -1389.638655 a.u.
M06 SCF energy in solution: -1389.55316132 a.u.
M06 enthalpy in solution: -1388.996570 a.u.
M06 free energy in solution: -1389.090721 a.u.
Three lowest frequencies (cm-1): 24.9750 29.6262 31.6548

Cartesian coordinates

ATOM	X	Y	Z
P	-0.002244	0.000378	0.802392
C	0.918744	1.498329	0.204579
C	2.084314	1.801560	0.966915
C	2.805274	2.968994	0.703833
H	3.696762	3.174839	1.293769
C	2.410880	3.879961	-0.278773
C	1.266341	3.576038	-1.013761
H	0.944643	4.264247	-1.792981
C	0.517134	2.408258	-0.806827
C	2.598346	0.889275	2.061418
H	2.884801	-0.096245	1.675463
H	1.837020	0.713941	2.830133
H	3.479340	1.326769	2.541720
C	3.212424	5.131941	-0.547735

H	2.665794	5.825362	-1.194435
H	4.165029	4.898891	-1.042537
H	3.457102	5.658508	0.382702
C	-0.670407	2.197176	-1.721519
H	-1.626668	2.347459	-1.210027
H	-0.695296	1.186516	-2.138177
H	-0.626877	2.902227	-2.557959
C	0.834983	-1.544308	0.200262
C	1.821270	-1.647960	-0.814957
C	2.458505	-2.878705	-1.027359
H	3.208646	-2.942324	-1.813452
C	2.156738	-4.023199	-0.290665
C	1.169706	-3.914557	0.690641
H	0.900850	-4.793241	1.273947
C	0.517655	-2.707712	0.959106
C	2.223543	-0.512980	-1.732542
H	2.835229	0.240013	-1.225017
H	1.357294	0.013669	-2.142120
H	2.806417	-0.902531	-2.573442
C	2.880784	-5.326588	-0.532000
H	2.215712	-6.186765	-0.395994
H	3.718107	-5.452242	0.167963
H	3.294310	-5.373902	-1.545054
C	-0.531401	-2.704629	2.051927
H	-0.590682	-3.688814	2.527422
H	-1.528593	-2.460875	1.666728
H	-0.305252	-1.960989	2.824836
C	-1.759288	0.049470	0.202038
C	-2.342440	-0.749224	-0.815800
C	-3.728304	-0.692666	-1.021076
H	-4.159474	-1.313281	-1.804475
C	-4.568857	0.136156	-0.279116
C	-3.981758	0.929084	0.708746
H	-4.610395	1.588441	1.304342
C	-2.609063	0.896387	0.970342
C	-1.560172	-1.660819	-1.737331
H	-1.213091	-2.569306	-1.234276
H	-0.671362	-1.170958	-2.144037
H	-2.188321	-1.967318	-2.580029
C	-6.052325	0.202370	-0.557266
H	-6.415066	-0.722715	-1.017613
H	-6.293839	1.024385	-1.245400
H	-6.624675	0.372579	0.361038
C	-2.081955	1.793103	2.071549
H	-2.904923	2.329980	2.553970

H	-1.374973	2.540396	1.691765
H	-1.547927	1.219079	2.837576