Electronic Supplementary Information

How electron-deficient Cp ligand facilitates Rh-catalyzed annulations with alkynes

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Comparison of the Barriers of Alkyne Insertion with Cp^X-Rhodacycles Using Different Levels of Theories

The barriers of alkyne insertion with Cp^X-Rh(III) were calculated using a few popular modern density functionals and basis sets (Table S1). The trend of Cp^E-promoted reactivity of alkyne insertion, i.e., the relative free energies ($\Delta\Delta G^{\ddagger}_{sol}$) of **TS2b** vs **TS2a** and **TS5b** vs **TS5a**, is minimally affected by the choice of density functionals and basis sets. Thus, a more commonly used combination of computational methods, M06 for single-point calculations and B3LYP for geometry optimization, was chosen in the present study. Due to the better efficiency in EDA calculations, the basis set of def2-TZVP for single-point energy calculation is thus chosen in this study.

Table S1. Comparison of barriers (in kcal/mol) of alkyne insertions (TS2a vsTS2b; TS5a vs TS5b)

Method for Single Point Energy Calculation	Method for Geometry Optimization	$\Delta\Delta G^{\ddagger}_{sol}$ (TS2b w/ Cp^E – TS2a w/ Cp*)	$\Delta\Delta G^{\ddagger}_{sol}$ (TS5b w/ Cp^E – TS5a w/ Cp*)
M06/def2-TZVP	B3LYP/LANL2DZ–6-31G(d)	–7.4	–3.3
M06-D3/def2-TZVP		–8.0	–4.6
B3LYP-D3/def2-TZVP		–7.1	–4.1
B97D3/def2-TZVP		–7.1	–3.4
ωB97xD/def2-TZVP		–6.6	–4.0
M06/SDD–6-311+G(d,p)		–7.9	–4.2
M06-D3/SDD–6-311+G(d,p)		–9.2	–5.1
B3LYP-D3/SDD–6-311+G(d,p)		–8.4	–4.5
B97D3/SDD–6-311+G(d,p)		–7.7	–3.9
ωB97xD/SDD–6-311+G(d,p)		–7.6	–4.4

Less Favorable Pathways for C–H Activations

To compare with the cationic pathway for acetanilide **1a** (Fig. 1) and the neutral pathway for 2-phenyl-2-propanol **1b** (Fig. 4), we computed the neutral and cationic pathways for **1a** (Fig. S1) and **1b** (Fig. S2), respectively. The neutral N-directing transition states for C–H metalations (**TS8a** with $\Delta G^{\ddagger}$ = 24.3 kcal/mol and **TS8b** with $\Delta G^{\ddagger}$ = 19.9 kcal/mol, Fig. S1) are less favorable than the cationic O(carbonyl)-directing transition states (**TS1a** with $\Delta G^{\ddagger}$ = 20.4 kcal/mol and **TS1b** with $\Delta G^{\ddagger}$ = 16.5 kcal/mol, Fig. 1). The cationic OH-directing transition states for C–H metalations (**TS9a** with $\Delta G^{\ddagger}$ = 25.3 kcal/mol and **TS9b** with $\Delta G^{\ddagger}$ = 22.9 kcal/mol, Fig. S2) are less favorable than the neutral O-directing transition states (**TS4a** with $\Delta G^{\ddagger}$ = 23.3 kcal/mol and **TS4b** with $\Delta G^{\ddagger}$ = 21.8 kcal/mol, Fig. 4). Therefore, the ligand effects (Cp* vs Cp^{E}) on the rate-determining alkyne insertion step are discussed based on the more favorable cationic pathway for substrate **1a** and neutral pathway for substrate **1b**.

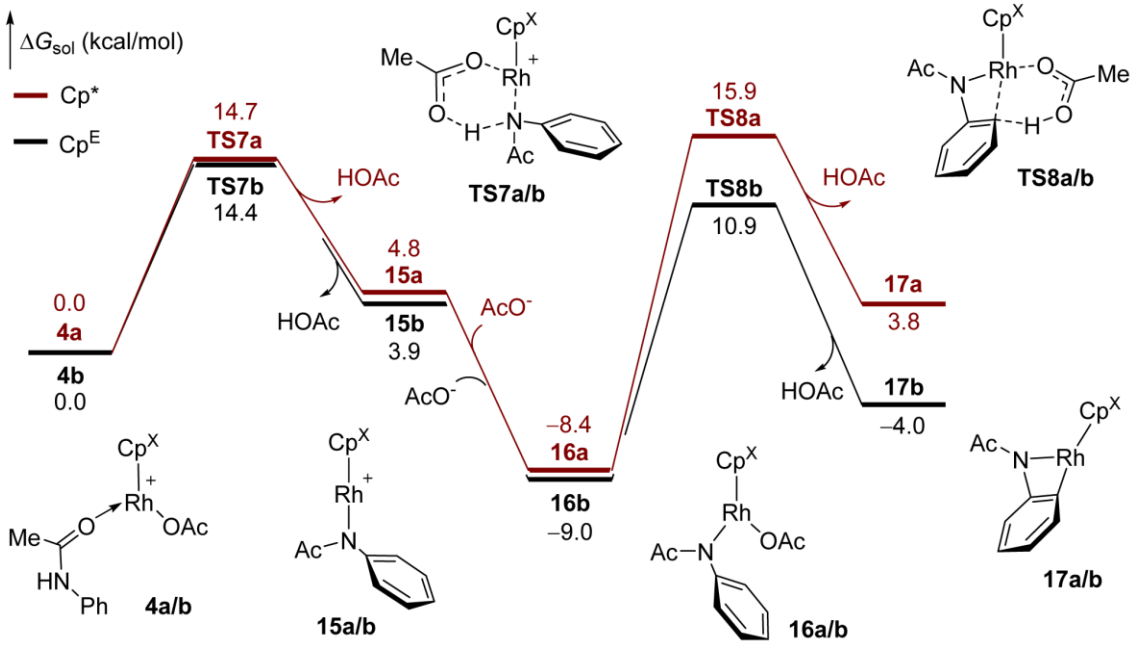

Fig. S1. Energy profile of the neutral N-directing C–H activation.

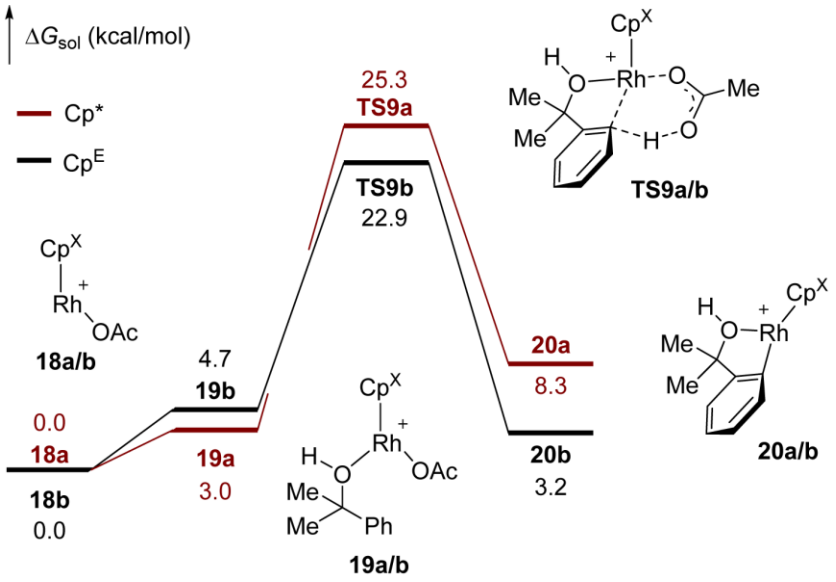

Fig. S2. Energy profile of the cationic OH-directing C–H activation.

Comparable π)(π Pauli Repulsion in TS5a and TS5b

As discussed in the manuscript, the difference of Pauli repulsion between **TS5a** and **TS5b** is mostly derived from the d)(π closed-shell repulsion. Because alkyne insertion involves four atoms (Rh, phenyl carbon and two alkyne carbon atoms), except for the d)(π repulsion, we further considered whether the repulsion between phenyl π orbital and alkyne π orbital contributes to the difference of Pauli repulsion. We thus computed the orbital coefficients on the phenyl carbon atom. As shown in Fig. S3, the coefficients are identical in these two transition states, which indicates that there are comparable π)(π Pauli repulsion. Thus, only the d)(π Pauli repulsion contributes to the total difference of Pauli repulsion.

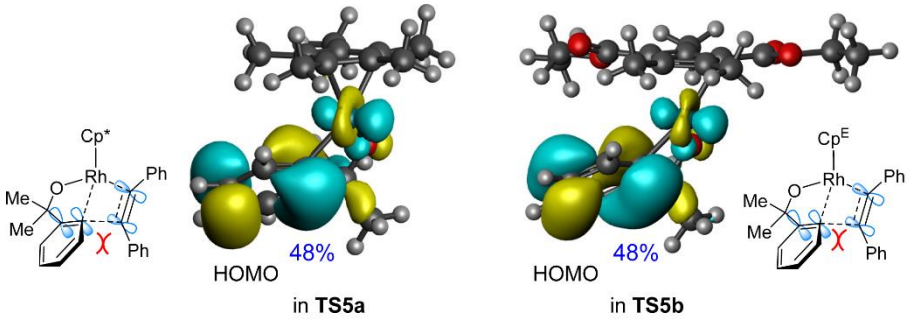

Fig. S3. The π)(π Pauli repulsion in **TS5a** and **TS5b**.

Energy Terms of EDA along IRC

Table S2. EDA energy terms of alkyne insertion with Cp* (TS2a) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS2a** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.68	31.6	151.0	-100.6	-20.2	-48.8	-28.6
2.60	33.3	161.2	-105.9	-22.1	-51.6	-29.6
2.50	35.3	175.9	-113.2	-24.7	-55.4	-31.0
2.38	38.0	198.0	-123.8	-28.9	-61.4	-33.1
2.23	42.1	235.0	-140.8	-36.5	-72.3	-36.5
2.05(TS)	49.5	297.4	-169.1	-51.5	-92.7	-41.7
1.86	60.5	395.9	-213.3	-81.0	-123.3	-49.1
1.69	73.1	528.2	-271.7	-134.2	-152.2	-58.1
1.60	80.8	623.4	-313.1	-182.3	-163.9	-64.3
1.57	85.0	665.7	-330.4	-208.7	-166.7	-67.4

Table S3. EDA energy terms of alkyne insertion with Cp^E (TS2b) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS2b** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.69	32.9	154.6	-102.7	-22.5	-52.6	-30.0
2.61	34.8	165.6	-108.6	-24.5	-55.7	-31.0
2.51	37.1	181.4	-116.7	-27.5	-60.1	-32.5
2.38	40.2	205.0	-128.1	-32.1	-66.8	-34.7
2.22	45.0	243.7	-145.8	-40.4	-78.5	-38.2
2.04(TS)	52.9	310.0	-175.6	-56.6	-100.6	-43.7
1.84	64.6	417.5	-223.7	-89.1	-133.7	-51.6
1.67	77.6	559.3	-286.0	-146.2	-164.1	-61.2
1.59	85.2	653.9	-326.7	-193.9	-175.9	-67.5
1.56	89.7	696.1	-343.5	-220.0	-179.1	-70.8

Table S4. EDA energy terms of alkyne insertion with Cp* (TS5a) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS5a** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{pol}	ΔE_{ct}	ΔE_{disp}
2.62	41.0	195.5	-122.5	-27.9	-63.8	-30.2
2.54	42.7	203.2	-125.6	-29.4	-65.1	-31.2
2.44	44.1	216.4	-131.2	-32.2	-67.7	-32.7
2.32	46.6	239.4	-141.2	-37.2	-73.1	-34.9
2.17	51.1	279.4	-158.9	-46.8	-84.4	-38.5
2.00(TS)	60.5	345.5	-188.0	-64.8	-104.8	-43.9
1.82	70.1	445.9	-231.7	-98.9	-133.1	-51.3
1.68	82.0	566.8	-283.4	-151.6	-157.4	-59.6
1.61	89.1	644.2	-315.3	-192.7	-167.2	-64.9
1.58	93.4	682.7	-329.8	-217.6	-170.6	-67.7

Table S5. EDA energy terms of alkyne insertion with Cp^E (TS5b) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS5b** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.62	40.6	192.7	-121.0	-29.1	-64.2	-31.3
2.55	41.4	200.1	-123.9	-30.7	-65.6	-32.3
2.45	42.7	212.4	-129.0	-33.3	-68.2	-33.7
2.33	45.3	234.0	-138.3	-38.1	-73.6	-35.8
2.18	50.1	271.9	-154.7	-47.0	-84.9	-39.2
2.00(TS)	58.4	335.8	-182.6	-64.1	-106.0	-44.3
1.82	70.4	434.7	-225.4	-96.9	-135.9	-51.4
1.67	83.0	552.1	-275.5	-146.9	-161.3	-59.3
1.61	90.1	623.2	-304.7	-184.4	-171.3	-64.1
1.58	94.7	658.7	-318.0	-207.2	-174.8	-66.8

Cartesian Coordinates (Å) and Energies of the Optimized Structures

1a
B3LYP SCF energy: -440.25674321 a.u.
B3LYP enthalpy: -440.090764 a.u.
B3LYP free energy: -440.137004 a.u.
M06 SCF energy in solution: -440.13375371 a.u.
M06 enthalpy in solution: -439.967774 a.u.
M06 free energy in solution: -440.014014 a.u.
Three lowest frequencies (cm-1): 17.6535 57.4933 91.1361

Cartesian coordinates

ATOM	X	Y	Z
C	-1.244010	-1.334491	-0.000369
C	-0.304431	-0.290548	-0.000277
C	-0.750817	1.040339	0.000128
C	-2.121918	1.300168	0.000473
C	-3.057627	0.264642	0.000405
C	-2.608427	-1.057521	-0.000020
H	-0.901305	-2.367922	-0.000733
H	-0.027157	1.842865	0.000130
H	-2.457906	2.333842	0.000797
H	-4.121595	0.483242	0.000672
H	-3.319653	-1.879186	-0.000096
N	1.061131	-0.651170	-0.000601
H	1.235388	-1.646432	-0.000219
C	2.174841	0.161572	-0.000534
O	2.134616	1.383469	-0.000830
C	3.501302	-0.588654	0.001023
H	4.070049	-0.291847	0.887804
H	3.404338	-1.679107	-0.007788
H	4.079518	-0.278047	-0.874688

1b
B3LYP SCF energy: -425.39550544 a.u.
B3LYP enthalpy: -425.195407 a.u.
B3LYP free energy: -425.240491 a.u.
M06 SCF energy in solution: -425.26158765 a.u.
M06 enthalpy in solution: -425.061489 a.u.
M06 free energy in solution: -425.106573 a.u.
Three lowest frequencies (cm-1): 45.2649 132.1377 222.8367

Cartesian coordinates

ATOM	X	Y	Z
C	0.773069	-1.195866	-0.000077
C	0.073032	0.019981	-0.000078
C	0.806967	1.212145	0.000005
C	2.203809	1.187934	0.000027
C	2.890476	-0.026170	-0.000003
C	2.167476	-1.220978	-0.000040

H	0.229200	-2.137348	-0.000082
H	0.276535	2.156608	0.000036
H	2.755151	2.124964	0.000068
H	3.977178	-0.043448	0.000023
H	2.688413	-2.175095	-0.000040
C	-1.457016	0.030889	-0.000002
O	-1.861677	1.407355	0.000338
H	-2.831331	1.417960	0.000663
C	-2.004937	-0.647300	-1.270193
H	-1.695972	-1.695250	-1.340776
H	-3.103132	-0.623661	-1.269919
H	-1.646545	-0.119310	-2.158963
C	-2.004739	-0.647915	1.269953
H	-1.646359	-0.120270	2.158929
H	-3.102943	-0.624456	1.269769
H	-1.695596	-1.695850	1.340037

2

B3LYP SCF energy: -539.45079265 a.u.
B3LYP enthalpy: -539.246874 a.u.
B3LYP free energy: -539.297932 a.u.
M06 SCF energy in solution: -539.23212605 a.u.
M06 enthalpy in solution: -539.028207 a.u.
M06 free energy in solution: -539.079265 a.u.
Three lowest frequencies (cm-1): 27.8119 47.4369 52.8172

Cartesian coordinates

ATOM	X	Y	Z
C	0.608260	0.000005	0.000135
C	-0.608261	0.000049	0.000159
C	2.033178	0.000005	0.000065
C	2.750900	1.213630	-0.000284
C	2.750888	-1.213628	0.000320
C	4.143254	1.208755	-0.000365
H	2.203155	2.151007	-0.000493
C	4.143243	-1.208769	0.000249
H	2.203133	-2.150999	0.000581
C	4.844675	-0.000010	-0.000094
H	4.683580	2.151619	-0.000638
H	4.683558	-2.151638	0.000459
H	5.931217	-0.000016	-0.000156
C	-2.033178	0.000026	0.000063
C	-2.750869	-1.213617	-0.000275
C	-2.750919	1.213640	0.000328
C	-4.143224	-1.208780	-0.000366
H	-2.203102	-2.150982	-0.000474
C	-4.143273	1.208743	0.000248
H	-2.203190	2.151027	0.000599
C	-4.844676	-0.000033	-0.000104

H	-4.683522	-2.151659	-0.000638
H	-4.683611	2.151599	0.000459
H	-5.931217	-0.000055	-0.000166

3a

B3LYP SCF energy: -978.55921678 a.u.
B3LYP enthalpy: -978.209187 a.u.
B3LYP free energy: -978.277706 a.u.
M06 SCF energy in solution: -978.21650706 a.u.
M06 enthalpy in solution: -977.866477 a.u.
M06 free energy in solution: -977.934996 a.u.
Three lowest frequencies (cm-1): 33.2966 42.9513 49.0753

Cartesian coordinates

ATOM	X	Y	Z
C	-3.743922	-0.033149	-0.214514
C	-2.349369	-0.038403	-0.108444
C	-1.605059	1.161531	-0.062989
C	-2.264469	2.396176	-0.154192
C	-3.650410	2.408655	-0.262193
C	-4.377690	1.206276	-0.286198
H	-4.301476	-0.957462	-0.257399
H	-1.696924	3.321705	-0.144779
H	-4.177005	3.356327	-0.335308
H	-5.460040	1.237548	-0.377043
N	-1.435467	-1.112119	0.002615
C	-1.861939	-2.432374	0.285899
O	-2.990171	-2.782312	-0.009813
C	-0.925563	-3.373692	1.020265
H	-1.559747	-4.112763	1.514194
H	-0.265301	-3.897720	0.323480
H	-0.297018	-2.864818	1.753698
C	-0.124726	-0.564898	0.061625
C	-0.202888	0.808282	0.031967
C	1.100689	-1.388998	-0.002691
C	1.310166	-2.283952	-1.067005
C	2.106329	-1.247937	0.967100
C	2.487092	-3.027603	-1.148596
H	0.549364	-2.385173	-1.836771
C	3.283994	-1.990661	0.881939
H	1.957684	-0.553049	1.788023
C	3.477053	-2.885269	-0.172641
H	2.634464	-3.712503	-1.979383
H	4.050420	-1.871588	1.642966
H	4.393987	-3.464605	-0.236977
C	0.914506	1.777494	0.011717
C	1.966331	1.672179	-0.914108
C	0.924685	2.856377	0.913454
C	2.997803	2.610235	-0.931385

H	1.967184	0.854486	-1.628069
C	1.956601	3.795321	0.894253
H	0.123071	2.947504	1.641230
C	2.997796	3.675560	-0.028025
H	3.800356	2.512174	-1.657811
H	1.947464	4.619126	1.603271
H	3.801105	4.407244	-0.044560

3b

B3LYP SCF energy: -963.70130948 a.u.

B3LYP enthalpy: -963.316486 a.u.

B3LYP free energy: -963.385325 a.u.

M06 SCF energy in solution: -963.34365866 a.u.

M06 enthalpy in solution: -962.958835 a.u.

M06 free energy in solution: -963.027674 a.u.

Three lowest frequencies (cm-1): 34.7298 38.3465 48.4180

Cartesian coordinates

ATOM	X	Y	Z
C	-2.280286	1.855341	-0.442351
C	-1.710664	0.603123	-0.148878
C	-2.566458	-0.515013	-0.026714
C	-3.943560	-0.357677	-0.188206
C	-4.496023	0.894218	-0.469553
C	-3.657369	2.001030	-0.596722
H	-1.633832	2.718577	-0.557705
H	-4.601906	-1.215501	-0.087808
H	-5.571112	0.999269	-0.586703
H	-4.072464	2.980004	-0.821617
C	-1.938904	-1.848463	0.354407
C	0.237747	-0.853816	-0.080102
C	-0.252713	0.416566	-0.029743
C	1.656096	-1.289291	-0.083979
C	2.644632	-0.651054	0.684248
C	2.020886	-2.417033	-0.842196
C	3.959769	-1.113863	0.674874
H	2.382345	0.200516	1.301003
C	3.338371	-2.870013	-0.857098
H	1.261260	-2.933461	-1.418809
C	4.315257	-2.219722	-0.099785
H	4.707261	-0.610270	1.282220
H	3.601458	-3.736223	-1.458714
H	5.341887	-2.576217	-0.107033
C	0.624644	1.624048	0.007660
C	1.464357	1.942732	-1.071326
C	0.598865	2.493258	1.111578
C	2.268952	3.082443	-1.039956
H	1.485669	1.285540	-1.935797
C	1.402482	3.633810	1.144334

H	-0.055290	2.266735	1.949724
C	2.242606	3.930950	0.068700
H	2.914297	3.309171	-1.884691
H	1.372888	4.289749	2.010663
H	2.868445	4.819131	0.093153
O	-0.599998	-1.930610	-0.205336
C	-1.829786	-1.979865	1.884741
H	-2.826656	-1.955987	2.337574
H	-1.341575	-2.924133	2.149728
H	-1.246051	-1.154788	2.304044
C	-2.652230	-3.062331	-0.245777
H	-2.061673	-3.961323	-0.044356
H	-3.642635	-3.200748	0.197415
H	-2.762369	-2.951430	-1.328543

4a

B3LYP SCF energy: -1168.21710038 a.u.
B3LYP enthalpy: -1167.753125 a.u.
B3LYP free energy: -1167.846322 a.u.
M06 SCF energy in solution: -1169.03579786 a.u.
M06 enthalpy in solution: -1168.571822 a.u.
M06 free energy in solution: -1168.665019 a.u.
Three lowest frequencies (cm-1): 15.1214 17.3344 28.4654

Cartesian coordinates

ATOM	X	Y	Z
C	-3.174363	-0.205989	-0.595610
C	-2.338474	-1.049301	-1.425309
C	-1.604758	-1.936628	-0.566417
C	-2.034759	-1.691066	0.802820
C	-3.009619	-0.642199	0.780952
Rh	-1.116182	0.134621	-0.035117
O	-0.320129	1.671604	-1.343919
O	-0.966867	2.195690	0.675532
C	-0.443097	2.556723	-0.434282
C	0.040416	3.961703	-0.648198
H	-0.453313	4.646703	0.044043
H	1.121936	4.002668	-0.471695
H	-0.139124	4.267645	-1.681956
C	5.115439	-0.503098	0.831569
C	3.842225	-0.041579	0.477554
C	3.488960	0.104299	-0.869460
C	4.421049	-0.230375	-1.852423
C	5.690943	-0.697359	-1.507889
C	6.036973	-0.828677	-0.161705
H	5.383403	-0.611959	1.880170
H	2.511510	0.479298	-1.143563
H	4.150265	-0.114380	-2.897851
H	6.407937	-0.951801	-2.282415

H	7.023086	-1.185676	0.119275
N	2.960458	0.316371	1.544522
H	3.416547	0.563913	2.413564
C	1.614846	0.292762	1.568232
O	0.964129	-0.101104	0.570137
C	0.942257	0.753462	2.837303
H	0.301590	-0.051374	3.212511
H	1.648101	1.038165	3.621670
H	0.297848	1.605329	2.598863
C	-0.620389	-2.983484	-0.985815
H	-1.104178	-3.968708	-1.010657
H	-0.216744	-2.783821	-1.980820
H	0.220300	-3.040407	-0.288917
C	-1.575470	-2.466667	1.998541
H	-1.711269	-1.906150	2.926833
H	-2.156071	-3.394593	2.085255
H	-0.521820	-2.746397	1.914118
C	-4.151402	0.820786	-1.079771
H	-5.125480	0.352737	-1.274540
H	-4.302934	1.610208	-0.339203
H	-3.814743	1.287836	-2.008679
C	-3.736370	-0.066063	1.954245
H	-4.750173	-0.485368	2.001905
H	-3.236902	-0.294983	2.898136
H	-3.830395	1.020349	1.870969
C	-2.233795	-0.963734	-2.914010
H	-3.051474	-1.536387	-3.371926
H	-2.313021	0.069052	-3.262656
H	-1.290632	-1.375070	-3.279786

4b

B3LYP SCF energy: -1623.95207821 a.u.
B3LYP enthalpy: -1623.392509 a.u.
B3LYP free energy: -1623.507103 a.u.
M06 SCF energy in solution: -1624.72025186 a.u.
M06 enthalpy in solution: -1624.160683 a.u.
M06 free energy in solution: -1624.275277 a.u.
Three lowest frequencies (cm-1): 7.5652 14.6138 15.1095

Cartesian coordinates

ATOM	X	Y	Z
C	0.466719	1.393059	1.465382
C	1.490333	0.500373	1.926965
C	2.449543	0.333679	0.849685
C	2.067518	1.201106	-0.256300
C	0.836035	1.826996	0.127582
C	-0.745802	1.832058	2.225209
H	-1.004759	1.117506	3.008911
H	-0.559769	2.806317	2.692213

H	-1.607302	1.941759	1.562720
C	1.527464	-0.189931	3.250936
H	1.774965	-1.247432	3.140832
H	2.320660	0.254453	3.863725
H	0.577916	-0.090186	3.779642
C	2.801215	1.409162	-1.542181
H	3.750627	1.918764	-1.337241
H	3.047755	0.452499	-2.006689
H	2.209280	2.010298	-2.232081
Rh	0.538823	-0.353291	0.099775
C	3.692309	-0.492063	0.988026
O	4.063941	-0.932448	2.055418
O	4.324171	-0.664334	-0.176473
C	5.559187	-1.444566	-0.125092
H	6.246246	-0.944923	0.563467
H	5.320157	-2.427882	0.289211
C	6.106817	-1.526253	-1.535233
H	7.033836	-2.108821	-1.530340
H	5.396972	-2.018961	-2.207238
H	6.332486	-0.531069	-1.930957
C	0.097791	2.823609	-0.713834
O	-0.060465	2.717816	-1.914799
O	-0.325804	3.846763	0.027875
C	-1.024159	4.921764	-0.679838
H	-1.908590	4.490605	-1.157611
H	-0.360009	5.292426	-1.465067
C	-1.372442	5.986890	0.338986
H	-0.471765	6.390194	0.811612
H	-1.892944	6.809396	-0.162314
H	-2.031002	5.590783	1.118184
C	-3.959847	-1.668221	0.713155
C	-4.360538	-1.107879	-0.506211
C	-5.717091	-0.874811	-0.765985
C	-6.674597	-1.192970	0.194311
C	-6.284160	-1.742801	1.416953
C	-4.931086	-1.978064	1.666341
H	-2.915047	-1.866643	0.909432
H	-6.023113	-0.442172	-1.716117
H	-7.724007	-1.009687	-0.015350
H	-7.029238	-1.990743	2.166621
H	-4.621340	-2.416389	2.610597
N	-3.444448	-0.791368	-1.555746
C	-2.128945	-0.520283	-1.495391
O	-1.537495	-0.517548	-0.381415
C	-1.425589	-0.226962	-2.792635
H	-2.101730	-0.233430	-3.651397
H	-0.938321	0.751336	-2.723010
H	-0.640892	-0.974982	-2.941953
C	0.586120	-4.250316	-0.919445
H	-0.455013	-4.553229	-1.082433
H	1.151567	-4.426047	-1.836668

H	0.984440	-4.856062	-0.101408
C	0.625350	-2.798188	-0.548885
O	0.362158	-2.412800	0.640663
O	0.895053	-1.890853	-1.406254
H	-3.863326	-0.715099	-2.474052

5a

B3LYP SCF energy: -939.10142232 a.u.
B3LYP enthalpy: -938.706851 a.u.
B3LYP free energy: -938.783780 a.u.
M06 SCF energy in solution: -939.94637093 a.u.
M06 enthalpy in solution: -939.551800 a.u.
M06 free energy in solution: -939.628729 a.u.
Three lowest frequencies (cm-1): 21.8155 26.3284 68.2046

Cartesian coordinates

ATOM	X	Y	Z
C	1.628959	-1.464663	0.654568
C	1.850109	-1.301115	-0.739640
C	2.422064	0.045313	-0.957753
C	2.523128	0.697308	0.285574
C	1.950083	-0.188560	1.284285
C	1.277497	-2.719219	1.395981
H	0.966607	-3.519328	0.720863
H	2.158408	-3.080010	1.942537
H	0.477640	-2.556902	2.123907
C	1.720618	-2.342299	-1.807594
H	1.363949	-1.913845	-2.748387
H	2.700414	-2.798677	-2.004060
H	1.034118	-3.141128	-1.518952
C	3.032026	2.081092	0.556169
H	4.032556	2.042648	1.005329
H	3.101717	2.673120	-0.359180
H	2.379275	2.618491	1.251097
Rh	0.302173	0.137708	-0.095339
C	-4.024437	-0.405386	-0.013885
C	-2.736573	0.162824	-0.019578
C	-1.568616	-0.637961	-0.037771
C	-1.785185	-2.034653	-0.062361
C	-3.051540	-2.605721	-0.068661
C	-4.183355	-1.781475	-0.038202
H	-4.900845	0.239906	0.004558
H	-0.928223	-2.696928	-0.086044
H	-3.163375	-3.685599	-0.096464
H	-5.180511	-2.210523	-0.036620
N	-2.722393	1.580079	-0.006989
H	-3.637754	2.010725	0.047547
C	-1.688824	2.426920	-0.088320
O	-0.490747	2.050119	-0.171804

C	-1.981061	3.904802	-0.085030
H	-1.598235	4.346240	-1.010828
H	-3.046546	4.131507	0.002508
H	-1.447111	4.374089	0.747185
C	2.827363	0.571461	-2.297706
H	3.780282	0.119830	-2.605542
H	2.088822	0.322283	-3.066159
H	2.958970	1.655494	-2.288530
C	1.885604	0.084597	2.751910
H	1.088537	-0.485715	3.235447
H	2.836076	-0.210046	3.219908
H	1.733019	1.146437	2.961588

5b

B3LYP SCF energy: -1394.84037011 a.u.
B3LYP enthalpy: -1394.350077 a.u.
B3LYP free energy: -1394.448226 a.u.
M06 SCF energy in solution: -1395.63637780 a.u.
M06 enthalpy in solution: -1395.146085 a.u.
M06 free energy in solution: -1395.244234 a.u.
Three lowest frequencies (cm-1): 14.2700 19.0464 25.7955

Cartesian coordinates

ATOM	X	Y	Z
C	-1.456180	-0.651056	-1.425431
C	-0.085968	-1.125462	-1.677721
C	0.418636	-1.652471	-0.450625
C	-0.585168	-1.423542	0.587124
C	-1.762954	-0.885083	-0.064913
C	-2.328688	-0.052796	-2.480976
H	-1.735683	0.484947	-3.225039
H	-2.868176	-0.855236	-3.002399
H	-3.075836	0.617235	-2.056613
C	0.532557	-1.185274	-3.039624
H	1.587687	-1.445786	-2.984531
H	0.017430	-1.952459	-3.634190
H	0.419762	-0.234889	-3.569891
C	-0.482683	-1.799616	2.029036
H	-0.721821	-2.866422	2.135680
H	0.534798	-1.664477	2.398491
H	-1.188672	-1.222247	2.624500
Rh	0.086500	0.522749	-0.192865
C	1.691326	-2.428375	-0.328257
O	2.583308	-2.393328	-1.155761
O	1.708723	-3.193621	0.764987
C	2.895772	-4.027421	0.951004
H	3.000730	-4.664701	0.068887
H	3.766875	-3.367980	0.998966
C	2.699105	-4.825143	2.223691

H	3.573075	-5.463902	2.387801
H	2.589854	-4.167793	3.091959
H	1.815598	-5.467343	2.155415
C	-3.016314	-0.507936	0.658489
O	-3.057129	-0.207886	1.834391
O	-4.083752	-0.574290	-0.148084
C	-5.372456	-0.261972	0.464728
H	-5.332122	0.765718	0.837348
H	-5.508426	-0.926829	1.321930
C	-6.440307	-0.455011	-0.592848
H	-6.450128	-1.486034	-0.959489
H	-7.422197	-0.236745	-0.160355
H	-6.285335	0.217556	-1.442490
C	3.362209	3.346198	0.234116
C	2.093802	2.739095	0.281871
C	1.884636	1.427737	-0.215351
C	3.011831	0.779192	-0.767919
C	4.263050	1.379995	-0.826036
C	4.440766	2.672705	-0.316551
H	3.494211	4.352990	0.625716
H	2.909668	-0.225588	-1.160148
H	5.100504	0.844633	-1.263208
H	5.414410	3.151742	-0.351193
N	1.078942	3.541066	0.855254
H	1.393809	4.435067	1.213303
C	-0.233800	3.301549	0.955284
O	-0.768955	2.238464	0.545625
C	-1.109246	4.352008	1.583871
H	-1.640101	3.910391	2.433028
H	-0.550000	5.226577	1.925410
H	-1.862122	4.671736	0.856216

6a

B3LYP SCF energy: -1478.56131790 a.u.
B3LYP enthalpy: -1477.960877 a.u.
B3LYP free energy: -1478.067285 a.u.
M06 SCF energy in solution: -1479.18778979 a.u.
M06 enthalpy in solution: -1478.587349 a.u.
M06 free energy in solution: -1478.693757 a.u.
Three lowest frequencies (cm-1): 14.3318 19.8336 28.6508

Cartesian coordinates

ATOM	X	Y	Z
C	-0.857073	-2.662402	-0.975458
C	-1.261885	-1.584257	-1.829639
C	-0.084643	-1.152149	-2.604588
C	1.025532	-1.869676	-2.147817
C	0.568213	-2.759844	-1.068323
C	-1.748795	-3.581169	-0.198026

H	-2.704325	-3.117411	0.053204
H	-1.964754	-4.472567	-0.802238
H	-1.282922	-3.914285	0.732543
C	-2.674187	-1.210221	-2.162032
H	-2.777469	-0.146228	-2.385947
H	-3.009295	-1.769348	-3.046778
H	-3.362620	-1.447850	-1.347032
C	2.446341	-1.797287	-2.617211
H	3.122069	-1.542474	-1.792916
H	2.767540	-2.766500	-3.018789
H	2.576900	-1.054071	-3.407398
Rh	0.148210	-0.733856	-0.276089
C	-0.454709	-0.732415	4.060490
C	0.133511	-0.657661	2.786379
C	-0.638796	-0.773301	1.615336
C	-2.019288	-0.948018	1.796037
C	-2.614367	-1.025945	3.057472
C	-1.824217	-0.919949	4.201543
H	0.172114	-0.647089	4.946821
H	-2.660343	-1.000934	0.922486
H	-3.689149	-1.161113	3.141157
H	-2.264584	-0.978628	5.191964
N	1.545330	-0.457169	2.798640
H	1.942039	-0.332003	3.721194
C	2.425615	-0.482580	1.789290
O	2.107771	-0.633931	0.586695
C	3.884686	-0.300707	2.128886
H	4.236965	0.630452	1.673098
H	4.075186	-0.267245	3.204779
H	4.459262	-1.121925	1.690501
C	-0.814586	1.615297	-0.319498
C	0.424458	1.580460	-0.385678
C	-2.196257	1.985858	-0.343312
C	-2.948831	2.064063	0.846372
C	-2.791914	2.382235	-1.561034
C	-4.266908	2.512377	0.810052
H	-2.490694	1.780212	1.786175
C	-4.109555	2.829933	-1.585072
H	-2.204456	2.363264	-2.474005
C	-4.851194	2.891451	-0.401514
H	-4.837459	2.574743	1.731984
H	-4.555504	3.140952	-2.525107
H	-5.878062	3.244334	-0.422635
C	1.742041	2.176584	-0.339727
C	2.037717	3.089827	0.690946
C	2.720002	1.895557	-1.308312
C	3.285304	3.709738	0.741362
H	1.281091	3.314933	1.436396
C	3.961953	2.524466	-1.256039
H	2.497472	1.188103	-2.099509
C	4.249959	3.430087	-0.230729

H	3.499965	4.420437	1.534304
H	4.706651	2.309325	-2.016905
H	5.218570	3.919951	-0.193414
C	1.437377	-3.771516	-0.386455
H	0.991507	-4.124891	0.546729
H	1.584426	-4.643987	-1.037612
H	2.424336	-3.357908	-0.161638
C	-0.140515	-0.140954	-3.708313
H	-0.722169	-0.531870	-4.553213
H	-0.625231	0.784087	-3.380105
H	0.854071	0.115363	-4.080459

6b

B3LYP SCF energy: -1934.30369730 a.u.
B3LYP enthalpy: -1933.607261 a.u.
B3LYP free energy: -1933.733690 a.u.
M06 SCF energy in solution: -1934.87931632 a.u.
M06 enthalpy in solution: -1934.182880 a.u.
M06 free energy in solution: -1934.309309 a.u.
Three lowest frequencies (cm-1): 13.6295 17.2588 20.5554

Cartesian coordinates

ATOM	X	Y	Z
C	-1.460454	0.101784	-1.991758
C	-0.078064	0.187931	-2.337033
C	0.562126	-1.091308	-1.984661
C	-0.401895	-1.922510	-1.376535
C	-1.643546	-1.137085	-1.290298
C	-2.511135	1.093393	-2.386001
H	-2.071248	2.063260	-2.626929
H	-3.028898	0.727299	-3.281298
H	-3.262316	1.228688	-1.607689
C	0.485116	1.264992	-3.215575
H	1.564614	1.182027	-3.302659
H	0.049157	1.166703	-4.219316
H	0.234118	2.263690	-2.847501
C	-0.253529	-3.313622	-0.842353
H	-0.003873	-3.282018	0.225080
H	-1.197046	-3.856118	-0.929388
H	0.535928	-3.846522	-1.368499
Rh	-0.242375	0.018851	-0.023924
C	2.009974	-1.352640	-2.218683
O	2.811294	-0.488043	-2.525575
O	2.348372	-2.642873	-2.056438
C	3.748240	-2.971934	-2.299312
H	4.011198	-2.625227	-3.302214
H	4.358893	-2.418481	-1.579868
C	3.897433	-4.473002	-2.151063
H	4.939730	-4.754533	-2.333680

H	3.627324	-4.802710	-1.142539
H	3.269104	-5.004822	-2.872373
C	-2.915517	-1.684746	-0.730015
O	-2.961874	-2.460878	0.207227
O	-3.989755	-1.237479	-1.391417
C	-5.284251	-1.720767	-0.925194
H	-5.415720	-1.395366	0.111289
H	-5.263734	-2.813911	-0.936134
C	-6.344052	-1.152839	-1.847690
H	-6.183659	-1.480178	-2.879524
H	-7.330755	-1.503174	-1.527334
H	-6.345656	-0.058566	-1.823990
C	-2.954090	1.987635	2.766399
C	-2.104904	1.048628	2.157033
C	-1.429246	1.352253	0.962011
C	-1.645202	2.624364	0.415803
C	-2.490090	3.562604	1.014659
C	-3.149381	3.241654	2.200787
H	-3.462404	1.726949	3.693176
H	-1.137095	2.901003	-0.502085
H	-2.627773	4.536707	0.553764
H	-3.808352	3.956781	2.683097
N	-2.015300	-0.204489	2.825554
H	-2.656531	-0.320591	3.599779
C	-1.216660	-1.246922	2.569082
O	-0.356644	-1.258432	1.655479
C	-1.369535	-2.480310	3.418828
H	-0.378180	-2.854197	3.686448
H	-1.948965	-2.302950	4.328805
H	-1.873145	-3.244642	2.816631
C	1.632909	1.648448	0.358725
C	1.742281	0.582725	0.988643
C	1.881874	2.892799	-0.297892
C	1.348274	4.100664	0.199266
C	2.775679	2.924144	-1.391492
C	1.692967	5.310010	-0.398008
H	0.680826	4.078338	1.053450
C	3.115468	4.141247	-1.974787
H	3.197697	1.993479	-1.756495
C	2.572922	5.333046	-1.484387
H	1.284719	6.237980	-0.008714
H	3.809548	4.161373	-2.809739
H	2.842920	6.280158	-1.942441
C	2.361751	-0.283669	1.966648
C	2.646587	0.230937	3.245413
C	2.724169	-1.606495	1.658369
C	3.291360	-0.563836	4.191103
H	2.369346	1.253448	3.482412
C	3.371875	-2.392264	2.608472
H	2.497797	-2.010487	0.676898
C	3.655715	-1.875409	3.875899

H	3.514927	-0.156056	5.172604
H	3.657598	-3.410536	2.360488
H	4.161720	-2.491434	4.613554

7a

B3LYP SCF energy: -1478.59172468 a.u.
B3LYP enthalpy: -1477.990596 a.u.
B3LYP free energy: -1478.094365 a.u.
M06 SCF energy in solution: -1479.22135962 a.u.
M06 enthalpy in solution: -1478.620231 a.u.
M06 free energy in solution: -1478.724000 a.u.
Three lowest frequencies (cm-1): 14.8178 24.1458 36.8811

Cartesian coordinates

ATOM	X	Y	Z
C	2.593545	0.373648	-1.570786
C	2.291134	1.629862	-0.954557
C	2.688758	1.513681	0.428683
C	3.447793	0.256688	0.588782
C	3.387306	-0.434725	-0.620789
C	2.429885	0.046438	-3.024110
H	1.573007	0.565267	-3.461436
H	3.325188	0.359054	-3.579216
H	2.303862	-1.027091	-3.185725
C	1.744530	2.849818	-1.626652
H	1.163935	3.470082	-0.941028
H	2.575707	3.457540	-2.009543
H	1.100805	2.595131	-2.471851
C	4.100699	-0.161491	1.870518
H	3.386354	-0.138964	2.700610
H	4.513070	-1.171076	1.806987
H	4.921339	0.520899	2.125695
Rh	1.161768	0.028739	0.066083
C	0.281317	-3.825588	0.404482
C	-0.356088	-2.597911	0.604018
C	-0.635461	-1.730398	-0.479255
C	-0.201456	-2.137303	-1.761170
C	0.421273	-3.367794	-1.966091
C	0.652778	-4.218607	-0.881367
H	0.484604	-4.467282	1.257182
H	-0.417158	-1.485689	-2.602391
H	0.708306	-3.671116	-2.968648
H	1.129649	-5.182387	-1.032327
N	-0.759403	-2.244954	1.928388
H	-1.350282	-2.901616	2.422742
C	-0.303477	-1.175785	2.621837
O	0.507082	-0.351935	2.154238
C	-0.825803	-1.000034	4.026601
H	-1.551912	-0.179359	4.031813

H	-1.311712	-1.897078	4.419654
H	0.000391	-0.716769	4.683119
C	-0.777068	0.638557	-0.197730
C	-1.496709	-0.493511	-0.333215
C	-1.225394	2.035250	-0.188822
C	-1.835650	2.593489	-1.329000
C	-1.036785	2.856742	0.940252
C	-2.244717	3.926680	-1.337328
H	-1.995424	1.968867	-2.203326
C	-1.455354	4.187604	0.931151
H	-0.575690	2.436429	1.829924
C	-2.055987	4.729022	-0.209228
H	-2.715698	4.338801	-2.225428
H	-1.316445	4.802590	1.816281
H	-2.377677	5.766308	-0.216564
C	-2.973107	-0.678403	-0.354048
C	-3.547366	-1.783458	-1.009521
C	-3.833918	0.219180	0.307449
C	-4.928955	-1.975812	-1.019135
H	-2.913393	-2.495378	-1.530014
C	-5.212819	0.023549	0.298140
H	-3.420036	1.069748	0.837242
C	-5.768893	-1.072598	-0.366984
H	-5.347573	-2.832148	-1.540561
H	-5.856150	0.728388	0.817625
H	-6.844742	-1.221278	-0.373720
C	2.615180	2.589302	1.465879
H	3.549165	3.168644	1.470699
H	1.791868	3.279787	1.270889
H	2.482290	2.167282	2.466091
C	3.982883	-1.768492	-0.953179
H	4.757210	-1.660593	-1.723714
H	4.444995	-2.235719	-0.080512
H	3.229323	-2.459984	-1.345862

7b
B3LYP SCF energy: -1934.32700557 a.u.
B3LYP enthalpy: -1933.630189 a.u.
B3LYP free energy: -1933.755313 a.u.
M06 SCF energy in solution: -1934.91476744 a.u.
M06 enthalpy in solution: -1934.217951 a.u.
M06 free energy in solution: -1934.343075 a.u.
Three lowest frequencies (cm-1): 9.0129 20.4373 20.7386

Cartesian coordinates

ATOM	X	Y	Z
C	2.109697	0.456233	-1.567471
C	1.138203	1.502769	-1.717291
C	1.087833	2.198829	-0.458629

C	2.152040	1.673850	0.422507
C	2.774322	0.620243	-0.270312
C	2.530563	-0.483610	-2.654784
H	1.722297	-0.661469	-3.368029
H	3.373633	-0.042015	-3.201255
H	2.874890	-1.436484	-2.253698
C	0.377207	1.838841	-2.961794
H	-0.643219	2.151368	-2.739194
H	0.866717	2.678723	-3.469131
H	0.348544	0.991358	-3.650832
C	2.493536	2.197057	1.780878
H	1.621974	2.145751	2.438987
H	3.309367	1.624300	2.219382
H	2.775175	3.254046	1.709601
Rh	0.470354	0.146896	-0.051595
C	0.299499	3.452281	-0.255538
O	-0.099344	4.129626	-1.179866
O	0.117062	3.750678	1.039417
C	-0.576535	5.003901	1.306510
H	-0.007713	5.815317	0.843108
H	-1.555478	4.962439	0.820770
C	-0.681127	5.158894	2.810533
H	-1.198168	6.094926	3.046038
H	-1.247739	4.333707	3.254163
H	0.309596	5.190700	3.274672
C	3.884175	-0.206540	0.282039
O	4.053130	-0.428729	1.465724
O	4.699060	-0.652267	-0.689538
C	5.851448	-1.428137	-0.252222
H	5.488557	-2.317793	0.271725
H	6.416456	-0.825819	0.464402
C	6.665633	-1.773238	-1.483431
H	7.007269	-0.868185	-1.994974
H	7.546851	-2.352062	-1.187831
H	6.083762	-2.373991	-2.189952
C	1.198709	-3.350290	1.602776
C	0.107286	-2.510298	1.385367
C	-0.326008	-2.190759	0.071244
C	0.434398	-2.709627	-1.002848
C	1.520548	-3.559097	-0.787519
C	1.889348	-3.892491	0.516731
H	1.516052	-3.567235	2.618556
H	0.109937	-2.478168	-2.012562
H	2.060986	-3.974439	-1.632594
H	2.727776	-4.558804	0.695676
N	-0.587835	-1.981894	2.511035
H	-0.856488	-2.632813	3.238169
C	-0.738927	-0.661200	2.772467
O	-0.323153	0.236730	2.015225
C	-1.452939	-0.293368	4.049167
H	-2.439759	0.109942	3.796752

H	-1.584475	-1.140750	4.727052
H	-0.891505	0.494682	4.557255
C	-1.489988	-0.203724	-0.515241
C	-1.648853	-1.507330	-0.220239
C	-2.439954	0.799771	-0.996589
C	-3.059710	0.644437	-2.252760
C	-2.753212	1.935459	-0.224755
C	-3.973312	1.590745	-2.714244
H	-2.827487	-0.229072	-2.855140
C	-3.675505	2.872801	-0.687300
H	-2.272941	2.066635	0.741034
C	-4.286366	2.705992	-1.933107
H	-4.443906	1.455598	-3.683956
H	-3.920077	3.736833	-0.075479
H	-4.999734	3.441272	-2.293361
C	-2.885932	-2.327088	-0.155706
C	-2.824639	-3.723992	-0.313022
C	-4.141765	-1.740174	0.094251
C	-3.977198	-4.505883	-0.236690
H	-1.872005	-4.206601	-0.512344
C	-5.290296	-2.523896	0.170740
H	-4.215952	-0.667975	0.237027
C	-5.215551	-3.909668	0.003665
H	-3.905859	-5.581692	-0.370289
H	-6.248349	-2.050527	0.366797
H	-6.113887	-4.517242	0.061993

8a

B3LYP SCF energy: -1478.15749825 a.u.

B3LYP enthalpy: -1477.570413 a.u.

B3LYP free energy: -1477.674980 a.u.

M06 SCF energy in solution: -1478.75813023 a.u.

M06 enthalpy in solution: -1478.171045 a.u.

M06 free energy in solution: -1478.275612 a.u.

Three lowest frequencies (cm-1): 9.7011 19.2667 27.8598

Cartesian coordinates

ATOM	X	Y	Z
C	3.354161	0.131399	-0.791070
C	3.437000	-1.131925	-0.206106
C	2.399763	-1.998604	-0.801456
C	1.735624	-1.267211	-1.805351
C	2.214722	0.111120	-1.720509
C	4.208518	1.336326	-0.528785
H	4.804754	1.222616	0.380715
H	4.903252	1.511285	-1.361596
H	3.599721	2.238961	-0.415513
C	4.412160	-1.600343	0.831639
H	3.909085	-2.132619	1.646827

H	5.137355	-2.299538	0.392910
H	4.973375	-0.770675	1.268375
C	0.752145	-1.784354	-2.810544
H	1.268796	-2.056377	-3.741429
H	0.232392	-2.672231	-2.443560
H	-0.002039	-1.031526	-3.056356
Rh	1.195025	-0.217878	0.119250
C	0.351575	3.843983	0.117058
C	-0.008260	2.492155	0.296840
C	-1.226300	2.025386	-0.275070
C	-2.031674	2.937799	-0.983566
C	-1.656323	4.263920	-1.162814
C	-0.455410	4.714131	-0.608015
H	1.261931	4.204133	0.576276
H	-2.969729	2.587172	-1.401716
H	-2.295552	4.939969	-1.724280
H	-0.145778	5.748707	-0.734295
N	0.819046	1.597759	1.001837
C	1.484224	2.014978	2.137612
O	1.411699	3.143069	2.624464
C	2.289590	0.954837	2.885433
H	1.726896	0.660145	3.779402
H	2.497542	0.052850	2.300456
H	3.230716	1.398599	3.224752
C	-1.675076	0.627649	-0.097308
C	-0.815938	-0.407466	0.072793
C	-3.163554	0.406366	-0.057528
C	-3.872878	-0.037122	-1.183138
C	-3.878401	0.666032	1.121970
C	-5.255626	-0.228787	-1.130216
H	-3.336497	-0.222298	-2.110383
C	-5.258155	0.468027	1.179581
H	-3.343254	1.024622	1.997148
C	-5.952104	0.019397	0.053132
H	-5.786800	-0.571874	-2.014611
H	-5.792585	0.667632	2.104899
H	-7.027484	-0.131799	0.097097
C	-1.203261	-1.806550	0.377661
C	-1.800873	-2.665755	-0.565628
C	-0.926579	-2.334017	1.657283
C	-2.097861	-3.991551	-0.246726
H	-2.044718	-2.282637	-1.550458
C	-1.225682	-3.658358	1.976291
H	-0.492138	-1.681697	2.411023
C	-1.808045	-4.496815	1.022987
H	-2.567172	-4.629821	-0.991492
H	-1.011248	-4.032985	2.974085
H	-2.044510	-5.528311	1.269838
C	1.866116	1.224449	-2.660401
H	1.869174	2.192741	-2.151167
H	2.594289	1.273185	-3.483192

H	0.873952	1.084944	-3.096758
C	2.236242	-3.455694	-0.483756
H	3.000507	-4.057050	-0.996616
H	2.338958	-3.644217	0.589545
H	1.254710	-3.826656	-0.788530

8b

B3LYP SCF energy: -1933.92413136 a.u.
B3LYP enthalpy: -1933.240781 a.u.
B3LYP free energy: -1933.363509 a.u.
M06 SCF energy in solution: -1934.46230553 a.u.
M06 enthalpy in solution: -1933.778955 a.u.
M06 free energy in solution: -1933.901683 a.u.
Three lowest frequencies (cm-1): 12.6058 17.1845 23.1101

Cartesian coordinates

ATOM	X	Y	Z
C	0.878707	1.081039	1.735827
C	1.846740	0.017110	1.797719
C	2.897266	0.307560	0.841434
C	2.533130	1.491205	0.126074
C	1.304131	1.997070	0.701006
C	-0.274389	1.241140	2.682964
H	-1.117517	1.735323	2.202846
H	-0.604350	0.272045	3.064854
H	0.025900	1.861413	3.537197
C	1.836650	-1.111062	2.785553
H	2.157076	-2.045608	2.325361
H	2.544465	-0.898262	3.596867
H	0.845048	-1.247240	3.223122
C	3.302074	2.129012	-0.994669
H	4.286177	2.446418	-0.631321
H	3.481106	1.407514	-1.795723
H	2.761804	2.987912	-1.386690
Rh	0.806582	-0.082955	-0.190010
C	4.080679	-0.554141	0.658551
O	4.337377	-1.528043	1.345974
O	4.884378	-0.143199	-0.350733
C	6.064619	-0.944467	-0.576426
H	6.661981	-0.961282	0.340988
H	5.757924	-1.973732	-0.788518
C	6.820930	-0.326190	-1.738031
H	7.727697	-0.906741	-1.940984
H	6.207696	-0.317424	-2.645009
H	7.115865	0.703526	-1.511154
C	0.699987	3.302302	0.339231
O	0.926888	3.929240	-0.679321
O	-0.117842	3.768017	1.310914
C	-0.745618	5.042276	1.037712

H	-1.330043	4.952634	0.117825
H	0.036982	5.788736	0.868834
C	-1.612653	5.387967	2.234115
H	-1.015173	5.448813	3.149758
H	-2.095000	6.358516	2.073300
H	-2.395056	4.636204	2.380988
C	-1.403591	-2.596778	0.539607
C	-0.088725	-2.984918	0.178942
C	0.457720	-4.197913	0.606196
C	-0.303806	-5.075984	1.378227
C	-1.607751	-4.724571	1.728662
C	-2.147651	-3.507746	1.310185
H	1.478331	-4.438514	0.322627
H	0.120243	-6.022018	1.703160
H	-2.211754	-5.398325	2.330445
H	-3.167862	-3.261860	1.582690
N	0.668953	-2.079823	-0.583200
C	0.704354	-1.962592	-1.905618
O	0.980385	-0.782121	-2.310451
C	0.447674	-3.080868	-2.877646
H	-0.439836	-2.844135	-3.474809
H	1.295015	-3.161480	-3.566323
H	0.296477	-4.035439	-2.369528
C	-1.241710	-0.219438	-0.318205
C	-1.971773	-1.305908	0.058149
C	-1.842037	1.010929	-0.894536
C	-1.483039	1.423459	-2.194108
C	-2.761215	1.804449	-0.181613
C	-2.042621	2.566100	-2.762999
H	-0.761579	0.833803	-2.751238
C	-3.318234	2.949186	-0.753721
H	-3.057858	1.507420	0.818292
C	-2.964852	3.334738	-2.048459
H	-1.753960	2.858496	-3.769229
H	-4.038700	3.534534	-0.187115
H	-3.402048	4.223742	-2.495447
C	-3.477219	-1.281416	-0.055585
C	-4.098190	-1.584889	-1.275489
C	-4.290661	-0.985897	1.049296
C	-5.488977	-1.582621	-1.392209
H	-3.481926	-1.816055	-2.140156
C	-5.682739	-0.987759	0.937404
H	-3.825484	-0.748435	2.003262
C	-6.286668	-1.285298	-0.285490
H	-5.949588	-1.813472	-2.349383
H	-6.293939	-0.752675	1.805226
H	-7.369709	-1.284308	-0.375522

9a
B3LYP SCF energy: -1478.17008497 a.u.
B3LYP enthalpy: -1477.581797 a.u.
B3LYP free energy: -1477.682795 a.u.
M06 SCF energy in solution: -1478.76597549 a.u.
M06 enthalpy in solution: -1478.177688 a.u.
M06 free energy in solution: -1478.278686 a.u.
Three lowest frequencies (cm-1): 20.0528 27.1134 39.5942

Cartesian coordinates

ATOM	X	Y	Z
C	3.066722	-0.189483	-1.319682
C	2.114883	0.336839	-2.203704
C	1.637529	1.593503	-1.610220
C	2.492050	1.915028	-0.468997
C	3.284007	0.782771	-0.233194
C	3.829325	-1.475726	-1.449748
H	3.378594	-2.142748	-2.189633
H	4.867963	-1.290295	-1.759325
H	3.872111	-2.018066	-0.498489
C	1.687860	-0.218394	-3.531388
H	0.603681	-0.170078	-3.672699
H	2.150250	0.341163	-4.357391
H	1.985250	-1.265387	-3.642355
C	2.530612	3.229225	0.254017
H	3.274484	3.902873	-0.196566
H	1.566102	3.742349	0.208856
H	2.797826	3.109428	1.309116
Rh	1.041724	0.102268	-0.152875
C	-0.513690	-0.237411	2.253912
C	-0.305018	-1.627748	2.144152
C	-0.007031	-2.412129	3.257020
C	0.070638	-1.773516	4.502052
C	-0.152922	-0.399915	4.630402
C	-0.450017	0.376148	3.506543
H	0.147266	-3.475841	3.154131
H	0.296373	-2.368306	5.383067
H	-0.102201	0.068513	5.609670
H	-0.638410	1.441190	3.602086
N	-0.456384	-2.001555	0.773056
C	-0.026466	-3.232782	0.268527
O	0.284645	-4.147854	1.020742
C	0.062436	-3.398826	-1.237181
H	0.421268	-2.495064	-1.735576
H	0.742215	-4.232932	-1.423383
H	-0.915935	-3.647161	-1.659413
C	-0.841410	-0.816492	-0.016823
C	-0.812255	0.320482	0.914242
C	-1.883201	-1.014345	-1.069100
C	-2.886985	-1.986987	-0.907504
C	-1.940937	-0.190461	-2.202014

C	-3.899938	-2.136613	-1.855135
H	-2.875935	-2.624026	-0.027522
C	-2.958316	-0.333139	-3.145994
H	-1.185229	0.575308	-2.326874
C	-3.940164	-1.311627	-2.981582
H	-4.663024	-2.896680	-1.708011
H	-2.980831	0.321163	-4.013833
H	-4.728609	-1.428959	-3.719987
C	-1.636704	1.565877	0.827559
C	-3.003735	1.541847	0.503757
C	-1.068105	2.802629	1.178395
C	-3.760621	2.715204	0.499495
H	-3.483449	0.600065	0.262715
C	-1.825659	3.974518	1.185912
H	-0.018019	2.833552	1.449653
C	-3.177125	3.937321	0.836584
H	-4.815294	2.668621	0.239964
H	-1.358647	4.916351	1.463768
H	-3.769593	4.848422	0.835009
C	0.747093	2.590586	-2.295026
H	1.352732	3.367108	-2.784592
H	0.132836	2.123115	-3.069281
H	0.077808	3.089201	-1.587130
C	4.278128	0.589134	0.874485
H	5.307460	0.706587	0.506637
H	4.129172	1.312912	1.680801
H	4.205856	-0.413825	1.310081

9b

B3LYP SCF energy: -1933.91294128 a.u.
B3LYP enthalpy: -1933.229399 a.u.
B3LYP free energy: -1933.352985 a.u.
M06 SCF energy in solution: -1934.46259955 a.u.
M06 enthalpy in solution: -1933.779057 a.u.
M06 free energy in solution: -1933.902643 a.u.
Three lowest frequencies (cm-1): 12.7022 15.9290 19.9362

Cartesian coordinates

ATOM	X	Y	Z
C	2.763679	-0.513033	-1.348012
C	1.506579	-0.253854	-2.012897
C	1.084774	1.066149	-1.665870
C	2.034642	1.599344	-0.707898
C	3.140430	0.670850	-0.612636
C	3.578393	-1.752634	-1.593658
H	2.933158	-2.591398	-1.867626
H	4.281463	-1.584026	-2.420768
H	4.168116	-2.029372	-0.720838
C	0.874708	-1.194956	-3.000399

H	-0.142621	-0.884558	-3.233334
H	1.453322	-1.205425	-3.935141
H	0.859788	-2.219613	-2.617513
C	2.005448	2.968604	-0.085932
H	2.316707	3.716698	-0.827233
H	0.997805	3.241484	0.228530
H	2.694804	3.018362	0.754613
Rh	1.262659	-0.323219	0.311098
C	-0.185009	1.664524	-2.106451
O	-1.080999	1.076746	-2.700696
O	-0.283454	2.983292	-1.801787
C	-1.517725	3.627863	-2.182213
H	-1.698931	3.448048	-3.246182
H	-2.340983	3.173116	-1.621092
C	-1.374473	5.106909	-1.871673
H	-2.291018	5.635962	-2.155400
H	-1.201947	5.269492	-0.802684
H	-0.537655	5.544295	-2.425798
C	4.374278	0.914263	0.152460
O	4.592640	1.872567	0.877424
O	5.312968	-0.049378	-0.056084
C	6.552301	0.127084	0.658537
H	6.344637	0.155879	1.733405
H	6.987370	1.093485	0.383627
C	7.463072	-1.029951	0.288138
H	7.654373	-1.048479	-0.789824
H	8.423116	-0.928370	0.806456
H	7.018017	-1.988500	0.575278
C	-0.468797	-0.560352	1.700827
C	-0.114936	-1.807130	1.098036
C	1.192343	-2.327121	1.369935
C	1.800261	-1.983599	2.658776
C	1.481436	-0.787587	3.214682
C	0.522213	0.061271	2.511154
H	1.521108	-3.207995	0.839021
H	2.516042	-2.665513	3.108770
H	1.929666	-0.434473	4.138845
H	0.346404	1.069186	2.872319
N	-1.238608	-2.268479	0.363956
C	-1.143670	-3.388938	-0.485511
O	-0.071675	-3.963035	-0.597636
C	-2.360089	-3.874520	-1.243145
H	-2.729075	-3.121390	-1.944242
H	-2.045240	-4.762478	-1.793297
H	-3.186543	-4.129032	-0.575354
C	-2.275851	-1.295419	0.520022
C	-1.834033	-0.252568	1.293126
C	-3.605370	-1.381639	-0.137214
C	-4.640883	-2.149547	0.417992
C	-3.850451	-0.640519	-1.304231
C	-5.896460	-2.188934	-0.188671

H	-4.458725	-2.713144	1.329885
C	-5.108839	-0.684595	-1.908836
H	-3.054545	-0.038915	-1.735933
C	-6.131372	-1.458157	-1.356118
H	-6.690946	-2.785486	0.251603
H	-5.288074	-0.110104	-2.813561
H	-7.109180	-1.488516	-1.829300
C	-2.577263	0.963585	1.683708
C	-3.879200	0.904082	2.208127
C	-1.966423	2.224463	1.557802
C	-4.551222	2.066794	2.584095
H	-4.362502	-0.059628	2.328354
C	-2.638418	3.386304	1.938037
H	-0.967791	2.290986	1.137379
C	-3.934465	3.312546	2.452488
H	-5.557495	1.997167	2.988898
H	-2.147624	4.350392	1.831302
H	-4.457905	4.217028	2.750492

10a

B3LYP SCF energy: -1152.92165286 a.u.
B3LYP enthalpy: -1152.436627 a.u.
B3LYP free energy: -1152.527312 a.u.
M06 SCF energy in solution: -1153.69019929 a.u.
M06 enthalpy in solution: -1153.205173 a.u.
M06 free energy in solution: -1153.295858 a.u.
Three lowest frequencies (cm-1): 17.3697 21.6348 42.5937

Cartesian coordinates

ATOM	X	Y	Z
C	3.501737	-0.112755	2.060566
C	2.605664	0.540227	1.211346
C	2.798513	0.542742	-0.178891
C	3.925171	-0.118223	-0.689819
C	4.821570	-0.776730	0.157116
C	4.612509	-0.780259	1.536968
H	3.334072	-0.095816	3.135234
H	4.112678	-0.127229	-1.759761
H	5.684626	-1.286460	-0.264849
H	5.309828	-1.290333	2.196743
C	1.808320	1.323367	-1.066012
C	-2.466471	-1.373334	-0.502807
C	-1.268951	-1.669764	-1.283485
C	-0.215500	-2.007452	-0.364038
C	-2.135183	-1.471876	0.875818
C	-0.723048	-1.814603	0.966543
Rh	-0.893103	0.107265	-0.057884
O	-1.333954	1.663097	1.513502
C	-1.966011	2.364796	0.661360

O	-2.180431	1.914778	-0.506151
C	-2.428292	3.755933	1.031874
H	-2.663993	3.812707	2.097721
H	-1.612899	4.459232	0.825441
H	-3.293892	4.048686	0.432589
C	-1.240670	-1.786085	-2.777846
H	-1.813443	-0.981629	-3.248982
H	-0.222289	-1.742649	-3.169026
H	-1.683384	-2.740446	-3.095923
C	1.132446	-2.571405	-0.694209
H	1.126647	-3.655291	-0.512707
H	1.397020	-2.414479	-1.741817
H	1.920650	-2.129657	-0.081120
C	0.021598	-2.065761	2.241072
H	-0.347036	-1.422884	3.045591
H	-0.110805	-3.109667	2.559408
H	1.091648	-1.879671	2.122089
C	-3.031785	-1.234195	2.054425
H	-3.205180	-2.169234	2.602816
H	-2.586935	-0.509914	2.743798
H	-4.003767	-0.841793	1.745607
C	-3.795477	-1.016016	-1.095439
H	-4.285486	-1.910558	-1.502907
H	-4.462220	-0.572689	-0.352687
H	-3.682054	-0.292274	-1.907698
C	2.318334	2.787160	-1.161080
H	3.326205	2.832903	-1.590849
H	1.634868	3.371107	-1.786976
H	2.342618	3.235162	-0.163359
C	1.707128	0.753840	-2.496379
H	0.905841	1.284985	-3.019827
H	2.633366	0.888495	-3.066716
H	1.467553	-0.313268	-2.491606
O	0.545157	1.428457	-0.467311
H	1.739624	1.057435	1.611715

10b

B3LYP SCF energy: -1608.66108841 a.u.
B3LYP enthalpy: -1608.080298 a.u.
B3LYP free energy: -1608.190757 a.u.
M06 SCF energy in solution: -1609.38489038 a.u.
M06 enthalpy in solution: -1608.804100 a.u.
M06 free energy in solution: -1608.914559 a.u.
Three lowest frequencies (cm-1): 16.2602 22.8962 25.0307

Cartesian coordinates

ATOM	X	Y	Z
C	2.797025	-3.084085	-1.760243
C	2.209486	-2.579789	-0.597940

C	2.900261	-1.676462	0.225080
C	4.203688	-1.311212	-0.141435
C	4.793365	-1.813743	-1.304689
C	4.090692	-2.699537	-2.122950
H	2.243336	-3.784906	-2.381008
H	4.773101	-0.626891	0.481343
H	5.803946	-1.511573	-1.569412
H	4.548378	-3.091716	-3.027628
C	2.230786	-1.178895	1.520425
C	-1.432679	1.669360	-0.112798
C	0.011611	1.812149	-0.226722
C	0.476713	0.967254	-1.307988
C	-1.846699	0.749418	-1.134430
C	-0.671392	0.283079	-1.839093
Rh	-0.481085	-0.280398	0.294513
O	-1.360337	-2.289006	0.242050
C	-1.909032	-2.121109	1.383874
O	-1.844196	-0.987984	1.944964
C	-2.591397	-3.282748	2.061993
H	-3.368110	-2.926492	2.742890
H	-3.013733	-3.967120	1.321894
H	-1.844373	-3.830772	2.648133
C	1.852386	0.890561	-1.895610
H	2.630152	1.016848	-1.146210
H	2.015806	-0.065129	-2.395862
H	1.970732	1.693770	-2.635078
C	-0.654138	-0.718222	-2.951471
H	-1.393264	-1.501466	-2.779480
H	-0.917332	-0.227284	-3.896671
H	0.333559	-1.172220	-3.054634
C	-2.322733	2.376794	0.865049
H	-3.066514	2.970992	0.322175
H	-2.866928	1.648493	1.470939
H	-1.737752	3.023056	1.516537
C	-3.222199	0.292104	-1.461888
O	-3.516928	-0.249931	-2.509957
C	0.796699	2.803903	0.559533
O	0.462898	3.270601	1.630374
O	1.923834	3.169807	-0.086100
O	-4.108867	0.558938	-0.485454
C	2.752631	4.142516	0.599331
H	2.154874	5.040869	0.780704
H	3.039299	3.730722	1.571725
C	3.953911	4.421444	-0.283910
H	4.600131	5.162892	0.198298
H	4.540308	3.512253	-0.450802
H	3.643285	4.816855	-1.256378
C	-5.472133	0.141174	-0.740717
H	-5.475223	-0.936263	-0.931245
H	-5.827453	0.640698	-1.647730
C	-6.296378	0.509039	0.478480

H	-7.336339	0.199631	0.327416
H	-5.913447	0.009165	1.373820
H	-6.281277	1.589779	0.652589
O	0.830091	-1.240130	1.433085
C	2.577705	-2.183264	2.652820
H	3.662066	-2.254142	2.797869
H	2.110840	-1.856680	3.588132
H	2.193027	-3.175166	2.398603
C	2.713642	0.221400	1.949563
H	2.098266	0.557955	2.789492
H	3.759814	0.213903	2.275986
H	2.622401	0.950130	1.139595
H	1.204383	-2.877392	-0.316334

11a

B3LYP SCF energy: -923.82198973 a.u.
B3LYP enthalpy: -923.406515 a.u.
B3LYP free energy: -923.483203 a.u.
M06 SCF energy in solution: -924.60618286 a.u.
M06 enthalpy in solution: -924.190708 a.u.
M06 free energy in solution: -924.267396 a.u.
Three lowest frequencies (cm-1): 14.7271 30.5875 78.1306

Cartesian coordinates

ATOM	X	Y	Z
C	1.755415	2.128164	0.000031
C	1.462483	0.753744	0.000031
C	2.545324	-0.158386	0.000008
C	3.866315	0.308774	-0.000013
C	4.132960	1.676707	-0.000011
C	3.072741	2.588870	0.000004
H	0.951324	2.857522	0.000052
H	4.693570	-0.398749	-0.000034
H	5.160861	2.031504	-0.000030
H	3.274781	3.658018	0.000005
C	2.180141	-1.625917	0.000003
C	-1.876781	1.482027	0.000213
C	-2.036851	0.643064	-1.149094
C	-2.500027	-0.678482	-0.700371
C	-2.037006	0.642646	1.149204
C	-2.500136	-0.678732	0.699962
Rh	-0.347782	-0.159449	0.000019
C	-1.972968	1.080114	-2.581766
H	-2.967896	1.386745	-2.935976
H	-1.294533	1.927143	-2.712896
H	-1.626073	0.270881	-3.230882
C	-1.663011	2.966164	0.000499
H	-1.110631	3.298078	-0.883067
H	-2.628925	3.490321	0.000600

H	-1.110620	3.297742	0.884184
C	-1.973274	1.079182	2.582038
H	-2.968256	1.385616	2.936267
H	-1.626385	0.269735	3.230890
H	-1.294911	1.926212	2.713536
C	-2.857972	-1.808939	1.617917
H	-2.142378	-1.894794	2.442044
H	-3.852193	-1.655245	2.059860
H	-2.870154	-2.766961	1.091999
C	-2.857733	-1.808357	-1.618782
H	-2.870108	-2.766556	-1.093192
H	-3.851844	-1.654437	-2.060895
H	-2.141962	-1.893983	-2.442778
O	0.765752	-1.752717	-0.000001
C	2.701793	-2.336263	-1.266746
H	3.796396	-2.312540	-1.320505
H	2.374280	-3.381600	-1.264226
H	2.300085	-1.846215	-2.159795
C	2.701769	-2.336249	1.266771
H	2.374207	-3.381570	1.264279
H	3.796374	-2.312564	1.320509
H	2.300093	-1.846150	2.159806

11b

B3LYP SCF energy: -1379.56746777 a.u.
B3LYP enthalpy: -1379.056335 a.u.
B3LYP free energy: -1379.156287 a.u.
M06 SCF energy in solution: -1380.30541257 a.u.
M06 enthalpy in solution: -1379.794280 a.u.
M06 free energy in solution: -1379.894232 a.u.
Three lowest frequencies (cm-1): 13.1168 18.4663 19.5213

Cartesian coordinates

ATOM	X	Y	Z
C	-2.903275	-0.824012	-0.332385
C	-1.620082	-1.371556	-0.175331
C	-1.458385	-2.772459	-0.268891
C	-2.567224	-3.590468	-0.522401
C	-3.834300	-3.031844	-0.679480
C	-4.002289	-1.645957	-0.584001
H	-3.052132	0.249486	-0.261961
H	-2.442305	-4.669095	-0.594692
H	-4.690277	-3.673060	-0.874697
H	-4.990584	-1.208803	-0.708200
C	-0.053690	-3.289500	-0.071084
C	0.988718	0.998709	1.722357
C	1.843069	1.141108	0.585971
C	1.030056	1.551432	-0.534932
C	-0.354905	1.423374	1.348567

C	-0.309244	1.811807	-0.033975
Rh	0.104452	-0.385471	0.163585
C	1.391294	0.547642	3.092396
H	2.206445	-0.173172	3.045585
H	1.755547	1.407812	3.670439
H	0.546255	0.110972	3.629673
C	-1.492888	1.565775	2.317289
H	-1.621651	2.619702	2.594273
H	-2.434594	1.222673	1.889983
H	-1.299504	0.998156	3.230096
C	1.504562	1.788814	-1.937341
H	0.661265	1.929523	-2.609252
H	2.122313	2.696876	-1.960516
H	2.135247	0.966321	-2.275388
C	-1.391953	2.425186	-0.845304
O	-1.324597	2.687126	-2.030920
C	3.289573	0.828292	0.617881
O	3.922328	0.641481	1.641934
O	-2.486311	2.708869	-0.101333
O	3.852736	0.796334	-0.608095
C	-3.583491	3.331632	-0.813783
H	-3.894449	2.667890	-1.626213
H	-3.223410	4.261674	-1.264108
C	-4.697858	3.574257	0.186878
H	-4.363804	4.232336	0.995537
H	-5.546647	4.050821	-0.315513
H	-5.044263	2.633452	0.626966
C	5.268273	0.498167	-0.640562
H	5.431788	-0.473415	-0.164532
H	5.799433	1.251360	-0.049818
C	5.701409	0.501393	-2.094711
H	6.772297	0.280279	-2.161453
H	5.157678	-0.257137	-2.667048
H	5.522834	1.477990	-2.556449
O	0.818650	-2.182136	0.125731
C	0.048695	-4.183999	1.181562
H	-0.572435	-5.081709	1.083416
H	1.089203	-4.491234	1.330628
H	-0.281537	-3.628896	2.065644
C	0.458338	-4.043145	-1.316069
H	1.498222	-4.348543	-1.159749
H	-0.142938	-4.937529	-1.515315
H	0.412827	-3.389814	-2.193094

12a
B3LYP SCF energy: -1463.27249012 a.u.
B3LYP enthalpy: -1462.651483 a.u.
B3LYP free energy: -1462.755588 a.u.
M06 SCF energy in solution: -1463.84582644 a.u.

M06 enthalpy in solution: -1463.224819 a.u.
M06 free energy in solution: -1463.328924 a.u.
Three lowest frequencies (cm-1): 17.2945 21.2115 28.7758

Cartesian coordinates

ATOM	X	Y	Z
C	-2.940679	-0.532824	-0.088422
C	-1.697148	-0.841682	0.471213
C	-1.643689	-1.446614	1.740702
C	-2.836303	-1.742868	2.414064
C	-4.075767	-1.454031	1.838836
C	-4.127668	-0.845188	0.584785
H	-2.997699	-0.026794	-1.047534
H	-2.798231	-2.207580	3.397451
H	-4.992476	-1.697908	2.370294
H	-5.086247	-0.601030	0.131925
C	-0.262814	-1.699477	2.322334
C	-0.488348	-1.297154	-2.537975
C	0.458478	-0.246327	-2.726477
C	1.741251	-0.679762	-2.195838
C	0.162854	-2.334949	-1.779485
C	1.562673	-1.961262	-1.628427
Rh	0.117951	-0.566991	-0.429155
C	0.238876	1.015927	-3.507830
H	0.503955	0.873467	-4.565171
H	-0.804630	1.341703	-3.469684
H	0.859162	1.832653	-3.125877
C	-1.858567	-1.375978	-3.141900
H	-2.293516	-0.384483	-3.300131
H	-1.809036	-1.871345	-4.121959
H	-2.547578	-1.947648	-2.515694
C	-0.405238	-3.678224	-1.427589
H	-0.179574	-4.419604	-2.207433
H	0.016658	-4.042503	-0.486538
H	-1.491245	-3.634598	-1.309633
C	2.571008	-2.799458	-0.905465
H	2.628077	-3.806134	-1.337838
H	3.570275	-2.358040	-0.944140
H	2.274328	-2.893744	0.147791
C	3.022529	0.094103	-2.311655
H	3.778261	-0.269053	-1.611142
H	3.437239	0.012744	-3.326177
H	2.874795	1.158512	-2.103511
C	0.999651	1.264631	0.464979
C	-0.161316	1.635932	0.183031
C	2.360791	1.464989	0.909078
C	3.091331	0.459094	1.567286
C	2.968821	2.714952	0.672304
C	4.400000	0.707870	1.978069
H	2.600537	-0.492342	1.746636
C	4.277065	2.951595	1.088495

H	2.404705	3.493007	0.165813
C	4.998303	1.948584	1.741574
H	4.956348	-0.072836	2.490686
H	4.733503	3.920155	0.901686
H	6.018947	2.134476	2.065469
C	-1.307365	2.501866	0.067573
C	-1.364286	3.452478	-0.971412
C	-2.357338	2.455597	1.004804
C	-2.440000	4.332885	-1.066586
H	-0.554762	3.498060	-1.693311
C	-3.427416	3.342191	0.903541
H	-2.323733	1.723481	1.803232
C	-3.475509	4.280706	-0.130056
H	-2.467449	5.063216	-1.871002
H	-4.228712	3.296779	1.635971
H	-4.313500	4.968498	-0.204578
O	0.703499	-1.501067	1.305471
C	-0.002021	-0.719939	3.491722
H	-0.725956	-0.856557	4.304839
H	1.004556	-0.879770	3.896019
H	-0.070093	0.314257	3.139972
C	-0.105813	-3.151651	2.821666
H	0.927534	-3.313663	3.148555
H	-0.769811	-3.370795	3.666643
H	-0.328499	-3.857521	2.014941

12b

B3LYP SCF energy: -1919.01959840 a.u.
B3LYP enthalpy: -1918.302791 a.u.
B3LYP free energy: -1918.427807 a.u.
M06 SCF energy in solution: -1919.55014171 a.u.
M06 enthalpy in solution: -1918.833334 a.u.
M06 free energy in solution: -1918.958350 a.u.
Three lowest frequencies (cm-1): 14.9933 18.2909 21.8570

Cartesian coordinates

ATOM	X	Y	Z
C	2.820675	1.372329	-0.304698
C	1.936678	0.656468	0.504933
C	2.277145	0.367146	1.837320
C	3.507250	0.812573	2.338275
C	4.397596	1.518489	1.526035
C	4.055696	1.794937	0.202129
H	2.558560	1.617300	-1.328463
H	3.776243	0.600880	3.371149
H	5.352372	1.850133	1.926631
H	4.740132	2.344787	-0.439578
C	1.253798	-0.403408	2.651856
C	0.525394	-0.510415	-2.416181

C	1.140698	-1.575982	-1.651902
C	0.105344	-2.347792	-1.010606
C	-0.883173	-0.595677	-2.205452
C	-1.148345	-1.734534	-1.353405
Rh	0.173622	-0.151489	-0.120744
C	1.197610	0.415310	-3.392222
H	2.270125	0.464179	-3.214327
H	1.062721	0.041004	-4.416080
H	0.777332	1.424956	-3.349286
C	-1.893535	0.295251	-2.868460
H	-2.498927	-0.281482	-3.576740
H	-2.585874	0.730634	-2.144470
H	-1.400436	1.099725	-3.419162
C	0.289484	-3.537497	-0.122638
H	0.325415	-3.187856	0.919148
H	-0.557028	-4.216681	-0.218084
H	1.226653	-4.049168	-0.340666
C	-2.464691	-2.259828	-0.929950
O	-2.637889	-3.258628	-0.254563
C	2.601836	-1.850790	-1.682866
O	3.338117	-1.474328	-2.577320
O	-3.493557	-1.513608	-1.398735
O	3.040024	-2.556049	-0.622085
C	-4.814483	-1.964924	-1.021822
H	-4.867874	-2.020565	0.068819
H	-4.966678	-2.974317	-1.418156
C	-5.814304	-0.972840	-1.586826
H	-5.732942	-0.906739	-2.676974
H	-6.832358	-1.292341	-1.337682
H	-5.653815	0.023106	-1.161979
C	4.466006	-2.806283	-0.588506
H	4.983756	-1.842642	-0.598142
H	4.749750	-3.348813	-1.495946
C	4.763387	-3.599716	0.669644
H	5.836721	-3.813181	0.724706
H	4.477940	-3.035496	1.562761
H	4.223051	-4.552043	0.672616
C	-1.385528	1.134209	0.698745
C	-0.614073	1.962372	0.158658
C	-2.611267	0.755815	1.368856
C	-2.732361	-0.432737	2.109138
C	-3.719526	1.621736	1.263978
C	-3.941548	-0.741857	2.731764
H	-1.863821	-1.076729	2.195130
C	-4.920918	1.303494	1.892454
H	-3.625643	2.540639	0.692325
C	-5.036693	0.119570	2.627796
H	-4.025456	-1.661838	3.303915
H	-5.766553	1.981296	1.810355
H	-5.974606	-0.126524	3.118643
C	-0.094572	3.219390	-0.316683

C	0.910210	3.911353	0.385799
C	-0.633335	3.795847	-1.484703
C	1.355341	5.150558	-0.069917
H	1.332228	3.470498	1.281517
C	-0.179599	5.034028	-1.934014
H	-1.413686	3.268564	-2.024569
C	0.816351	5.714538	-1.228837
H	2.128893	5.676319	0.482801
H	-0.606148	5.469094	-2.833798
H	1.169199	6.680288	-1.580216
O	0.277988	-0.922381	1.762591
C	1.883485	-1.616082	3.367465
H	2.618026	-1.311086	4.122572
H	1.096740	-2.190284	3.868976
H	2.374780	-2.266124	2.637459
C	0.588663	0.529553	3.689627
H	-0.179386	-0.018982	4.246758
H	1.321501	0.922322	4.405393
H	0.110454	1.376504	3.188312

13a

B3LYP SCF energy: -1463.29476990 a.u.
B3LYP enthalpy: -1462.672192 a.u.
B3LYP free energy: -1462.771943 a.u.
M06 SCF energy in solution: -1463.86843675 a.u.
M06 enthalpy in solution: -1463.245859 a.u.
M06 free energy in solution: -1463.345610 a.u.
Three lowest frequencies (cm-1): 25.3483 29.3166 35.4566

Cartesian coordinates

ATOM	X	Y	Z
C	0.526752	-2.391662	1.626503
C	0.612878	-1.709978	0.385169
C	-0.178099	-2.172540	-0.717799
C	-0.990691	-3.312952	-0.497501
C	-1.042802	-3.969796	0.722687
C	-0.278749	-3.502773	1.803242
H	1.142508	-2.028745	2.445196
H	-1.582684	-3.701697	-1.316890
H	-1.667847	-4.852384	0.834103
H	-0.307253	-4.013794	2.762034
C	-0.135352	-1.496458	-2.126187
C	-2.638947	0.220142	1.689924
C	-2.098263	1.508706	1.451860
C	-2.368296	1.831580	0.062338
C	-3.403961	-0.196064	0.508098
C	-3.257238	0.792882	-0.472047
Rh	-1.073369	0.099016	-0.004836
C	-1.447381	2.414973	2.452530

H	-2.191937	3.092464	2.894216
H	-0.987570	1.852229	3.270401
H	-0.671892	3.031788	1.991944
C	-2.621214	-0.540673	2.982841
H	-1.837232	-0.179070	3.653773
H	-3.582067	-0.437594	3.506798
H	-2.452654	-1.610050	2.817636
C	-4.191686	-1.470185	0.428053
H	-5.039334	-1.452786	1.126818
H	-4.592741	-1.633519	-0.575957
H	-3.576608	-2.340659	0.685196
C	-3.775432	0.792296	-1.877903
H	-4.459480	-0.041903	-2.057166
H	-4.312295	1.722207	-2.102340
H	-2.937798	0.700693	-2.581548
C	-2.099695	3.145942	-0.607337
H	-1.994943	3.023024	-1.689184
H	-2.926606	3.848893	-0.427847
H	-1.180281	3.605447	-0.237015
C	0.902900	0.613128	0.155068
C	1.576665	-0.542450	0.303605
C	1.362479	1.989897	-0.062981
C	1.382615	2.508821	-1.373505
C	1.752574	2.832220	0.996268
C	1.798500	3.817982	-1.610891
H	1.056657	1.863608	-2.183315
C	2.162195	4.145270	0.752715
H	1.751160	2.443379	2.011247
C	2.188885	4.643390	-0.551694
H	1.817613	4.197672	-2.629648
H	2.466188	4.776573	1.584186
H	2.511495	5.663740	-0.741280
C	3.034914	-0.817072	0.386215
C	3.997115	0.197228	0.569380
C	3.508047	-2.140115	0.268024
C	5.356696	-0.100204	0.628185
H	3.680681	1.227314	0.668930
C	4.869400	-2.436043	0.328105
H	2.801059	-2.950021	0.119547
C	5.805284	-1.417844	0.509918
H	6.070885	0.707032	0.771634
H	5.196547	-3.468216	0.229408
H	6.866709	-1.645805	0.559469
O	-0.517767	-0.145782	-1.970151
C	1.272902	-1.600711	-2.753090
H	1.557212	-2.646099	-2.929868
H	1.264109	-1.080423	-3.717804
H	2.033474	-1.134558	-2.126421
C	-1.135580	-2.137890	-3.112224
H	-1.104142	-1.553657	-4.036886
H	-0.893076	-3.178794	-3.360976

H -2.158622 -2.090067 -2.724960

13b
B3LYP SCF energy: -1919.04055902 a.u.
B3LYP enthalpy: -1918.322324 a.u.
B3LYP free energy: -1918.443663 a.u.
M06 SCF energy in solution: -1919.57043953 a.u.
M06 enthalpy in solution: -1918.852205 a.u.
M06 free energy in solution: -1918.973544 a.u.
Three lowest frequencies (cm-1): 13.2690 17.8219 26.9542

Cartesian coordinates

ATOM	X	Y	Z
C	0.022552	2.646657	-1.895139
C	-0.207061	2.189511	-0.566656
C	0.853846	2.295209	0.397455
C	2.075099	2.873435	-0.043421
C	2.258360	3.330360	-1.335425
C	1.220847	3.214891	-2.278025
H	-0.794749	2.561146	-2.606190
H	2.888899	2.978853	0.662931
H	3.207593	3.775169	-1.620508
H	1.359487	3.571647	-3.294901
C	0.685892	1.847838	1.883700
C	1.725152	-0.968070	-1.910125
C	2.608016	-1.015223	-0.739430
C	2.000220	-1.824653	0.251983
C	0.603418	-1.795695	-1.665773
C	0.722717	-2.277413	-0.297350
Rh	0.475913	-0.086232	-0.105440
C	2.031341	-0.261749	-3.196265
H	2.315462	0.777964	-3.022167
H	2.884192	-0.737745	-3.693162
H	1.175319	-0.286237	-3.875008
C	-0.469753	-2.144195	-2.656974
H	-0.251482	-3.107427	-3.134891
H	-1.442747	-2.238608	-2.174425
H	-0.541701	-1.386068	-3.441306
C	2.495125	-2.144975	1.629265
H	2.016068	-1.463843	2.344992
H	2.213201	-3.159879	1.913195
H	3.573535	-2.013192	1.693584
C	-0.109985	-3.306519	0.378814
O	-0.079540	-3.552798	1.569298
C	3.891688	-0.287789	-0.695602
O	4.400450	0.258702	-1.660160
O	-0.882339	-3.988280	-0.494495
O	4.474868	-0.277165	0.528916
C	-1.701385	-5.035218	0.078645

H	-2.332203	-4.598732	0.856859
H	-1.043092	-5.772450	0.550118
C	-2.521367	-5.638477	-1.046085
H	-1.876188	-6.042549	-1.833224
H	-3.139643	-6.454598	-0.655845
H	-3.183096	-4.887156	-1.488532
C	5.759037	0.381309	0.602719
H	5.634369	1.430533	0.316033
H	6.435523	-0.079495	-0.124182
C	6.267067	0.237673	2.025644
H	7.240832	0.730602	2.121953
H	5.575742	0.698147	2.738773
H	6.388073	-0.816620	2.295030
C	-1.518163	0.339893	-0.022441
C	-1.592783	1.663102	-0.245254
C	-2.515933	-0.663825	0.357322
C	-2.534561	-1.161821	1.674755
C	-3.463588	-1.150784	-0.564546
C	-3.498663	-2.091218	2.062358
H	-1.783513	-0.803839	2.371310
C	-4.422003	-2.085923	-0.171383
H	-3.459598	-0.768385	-1.581779
C	-4.447472	-2.554649	1.145332
H	-3.507629	-2.456542	3.085891
H	-5.156400	-2.439269	-0.891072
H	-5.201422	-3.274162	1.454137
C	-2.741553	2.604028	-0.210023
C	-2.526832	3.984964	-0.394586
C	-4.065508	2.183419	0.033630
C	-3.579921	4.898263	-0.350788
H	-1.521814	4.354536	-0.569820
C	-5.115097	3.097547	0.078314
H	-4.277359	1.134368	0.192614
C	-4.883483	4.461347	-0.117089
H	-3.375329	5.955887	-0.497188
H	-6.123493	2.738501	0.268520
H	-5.705905	5.170814	-0.083989
O	0.351400	0.473208	1.853013
C	1.994670	1.979364	2.690559
H	2.316441	3.020341	2.820738
H	1.809825	1.557124	3.683003
H	2.803661	1.403236	2.230650
C	-0.405724	2.664998	2.604999
H	-0.515099	2.276759	3.623970
H	-0.133213	3.726187	2.668778
H	-1.372613	2.582392	2.108650

14a
B3LYP SCF energy: -1463.31646560 a.u.

B3LYP enthalpy: -1462.693606 a.u.
B3LYP free energy: -1462.794773 a.u.
M06 SCF energy in solution: -1463.89463645 a.u.
M06 enthalpy in solution: -1463.271777 a.u.
M06 free energy in solution: -1463.372944 a.u.
Three lowest frequencies (cm-1): 22.2567 31.4147 35.3185

Cartesian coordinates

ATOM	X	Y	Z
C	-0.837592	-2.956379	-1.203994
C	-0.847660	-2.078992	-0.098387
C	-0.786140	-2.648389	1.194670
C	-0.705247	-4.036324	1.348978
C	-0.682368	-4.885175	0.243964
C	-0.751957	-4.333452	-1.038219
H	-0.904789	-2.544772	-2.205097
H	-0.668357	-4.464775	2.346463
H	-0.618322	-5.960882	0.382238
H	-0.746409	-4.979494	-1.912601
C	-0.870691	-1.714491	2.385923
C	2.004898	1.448830	-1.408625
C	2.494540	1.883563	-0.106306
C	3.251084	0.818091	0.419053
C	2.654789	0.179180	-1.744641
C	3.354107	-0.234703	-0.601357
Rh	1.092681	0.045302	-0.001251
C	2.207096	3.212477	0.528624
H	2.831387	4.006828	0.094131
H	1.160315	3.505515	0.394929
H	2.403264	3.191549	1.604709
C	1.313137	2.355726	-2.385226
H	0.627948	3.040254	-1.876947
H	2.050603	2.968323	-2.924951
H	0.738115	1.800978	-3.130219
C	2.618730	-0.511198	-3.077083
H	3.475794	-0.216356	-3.700708
H	2.650801	-1.600270	-2.970649
H	1.715437	-0.262481	-3.642008
C	4.158892	-1.492643	-0.442542
H	3.855698	-2.258257	-1.162749
H	5.231395	-1.301466	-0.594091
H	4.048479	-1.920089	0.559955
C	3.937013	0.763464	1.753646
H	3.823595	-0.218592	2.226246
H	5.016339	0.948818	1.653232
H	3.535774	1.510007	2.444930
C	-0.753696	0.255927	0.871036
C	-0.953215	-0.598822	-0.292715
C	-1.315188	1.597226	1.177396
C	-1.464879	2.004676	2.516575
C	-1.653897	2.525709	0.171181

C	-1.952142	3.271942	2.836779
H	-1.185319	1.320883	3.308714
C	-2.144806	3.788870	0.495793
H	-1.532239	2.258188	-0.870719
C	-2.301786	4.172353	1.830390
H	-2.058417	3.553352	3.881707
H	-2.404165	4.478881	-0.303446
H	-2.683849	5.158698	2.079375
C	-1.871625	-0.190207	-1.414146
C	-3.245530	-0.028274	-1.163010
C	-1.427087	-0.038462	-2.734701
C	-4.134856	0.292534	-2.187971
H	-3.617525	-0.146722	-0.149152
C	-2.314778	0.275516	-3.767420
H	-0.372123	-0.173994	-2.945409
C	-3.672672	0.447586	-3.497120
H	-5.190947	0.419568	-1.963725
H	-1.942156	0.386519	-4.782819
H	-4.364534	0.696839	-4.297311
O	-0.273933	-0.433075	2.012974
C	-2.333681	-1.493115	2.809669
H	-2.785936	-2.448279	3.096693
H	-2.393009	-0.808473	3.662217
H	-2.923294	-1.077412	1.987546
C	-0.024349	-2.160580	3.581347
H	-0.027108	-1.372634	4.341051
H	-0.425713	-3.071101	4.035780
H	1.009405	-2.347938	3.275810

14b
B3LYP SCF energy: -1919.07023533 a.u.
B3LYP enthalpy: -1918.351256 a.u.
B3LYP free energy: -1918.474191 a.u.
M06 SCF energy in solution: -1919.60311312 a.u.
M06 enthalpy in solution: -1918.884134 a.u.
M06 free energy in solution: -1919.007069 a.u.
Three lowest frequencies (cm-1): 13.1468 15.6133 17.3877

Cartesian coordinates

ATOM	X	Y	Z
C	0.101896	1.622850	-1.007388
C	1.067730	0.528100	-1.217007
C	0.553751	-0.604865	-1.787283
C	-0.865700	-0.596337	-2.125470
C	-1.520919	0.620141	-2.490584
C	-1.000945	1.804093	-1.899554
H	0.423604	2.488285	-0.440000
H	-1.332027	-1.526890	-2.433560
H	-2.410204	0.628982	-3.112131

H	-1.462185	2.774009	-2.054533
C	1.473046	-1.774122	-2.070700
C	-3.041976	1.294702	1.499144
C	-3.884587	0.344449	0.849305
C	-3.168710	-0.908083	0.765498
C	-1.841991	0.613796	1.932810
C	-1.949869	-0.770581	1.546809
Rh	-1.731523	0.498405	-0.328618
C	-3.371779	2.729679	1.795337
H	-3.928696	3.185453	0.976690
H	-4.012580	2.796758	2.684750
H	-2.469337	3.315128	1.991432
C	-0.785384	1.247162	2.795907
H	-0.995844	1.051249	3.856005
H	0.203589	0.842390	2.585522
H	-0.764693	2.331362	2.658332
C	-3.695120	-2.195097	0.190171
H	-2.896948	-2.930435	0.114333
H	-4.475928	-2.601373	0.847077
H	-4.157972	-2.029632	-0.783261
C	-0.963417	-1.849717	1.750359
O	-1.014178	-2.963327	1.247071
C	-5.213087	0.686862	0.318368
O	-5.767855	1.763921	0.475064
O	0.048787	-1.490217	2.578433
O	-5.805065	-0.332209	-0.357924
C	1.103015	-2.467799	2.734857
H	1.540268	-2.671997	1.752379
H	0.668125	-3.399496	3.109675
C	2.124792	-1.889750	3.696915
H	1.665783	-1.652901	4.662573
H	2.925882	-2.617968	3.864629
H	2.576164	-0.978268	3.291524
C	-7.128470	-0.056875	-0.860453
H	-7.076320	0.781440	-1.563326
H	-7.767537	0.254664	-0.027848
C	-7.639279	-1.322696	-1.524903
H	-8.647921	-1.154473	-1.918487
H	-6.991583	-1.620035	-2.356431
H	-7.682453	-2.150492	-0.809646
C	3.135732	-0.610433	-0.704361
C	2.470483	0.583171	-0.803018
C	4.490941	-0.870001	-0.168018
C	5.212433	-1.978599	-0.652188
C	5.077965	-0.087498	0.844471
C	6.483219	-2.275709	-0.164786
H	4.764307	-2.604179	-1.415356
C	6.347593	-0.390158	1.331995
H	4.537126	0.753403	1.259885
C	7.059542	-1.481184	0.828143
H	7.023471	-3.131601	-0.560979

H	6.778362	0.226148	2.116711
H	8.049802	-1.713449	1.210851
C	3.116496	1.900265	-0.520148
C	2.766820	2.667236	0.605121
C	4.082854	2.415025	-1.398584
C	3.365957	3.905451	0.843806
H	2.034265	2.278681	1.308293
C	4.686017	3.650537	-1.159252
H	4.362326	1.834762	-2.273517
C	4.328533	4.401567	-0.037952
H	3.084671	4.479214	1.723184
H	5.434327	4.027242	-1.851735
H	4.796077	5.364720	0.148037
O	2.523941	-1.783257	-1.058475
C	0.799918	-3.140335	-1.913887
H	0.079808	-3.314813	-2.719690
H	1.562561	-3.923637	-1.969268
H	0.283856	-3.217804	-0.952340
C	2.129914	-1.637164	-3.456369
H	2.811818	-2.475235	-3.641893
H	1.361925	-1.633705	-4.237714
H	2.693118	-0.701519	-3.528352

15a

B3LYP SCF energy: -939.08995901 a.u.
B3LYP enthalpy: -938.697084 a.u.
B3LYP free energy: -938.776349 a.u.
M06 SCF energy in solution: -939.94081178 a.u.
M06 enthalpy in solution: -939.547937 a.u.
M06 free energy in solution: -939.627202 a.u.
Three lowest frequencies (cm-1): 12.9758 31.9993 45.9156

Cartesian coordinates

ATOM	X	Y	Z
C	1.185883	-1.457014	0.903209
C	1.591924	-1.638353	-0.449053
C	2.635942	-0.651031	-0.753580
C	2.862113	0.136549	0.405824
C	1.935004	-0.315885	1.429980
C	0.188745	-2.283667	1.653196
H	-0.657588	-2.564263	1.019841
H	0.663181	-3.206314	2.012162
H	-0.204920	-1.752223	2.522383
C	1.114556	-2.702460	-1.386048
H	1.066238	-2.345586	-2.418746
H	1.811993	-3.551084	-1.366021
H	0.128394	-3.077698	-1.102735
C	3.846989	1.254207	0.562374
H	3.446590	2.060307	1.183050

H	4.760152	0.883282	1.045806
H	4.129875	1.682865	-0.401546
Rh	0.722842	0.373971	-0.201389
C	-3.466584	0.588589	0.784477
C	-2.498689	0.148618	-0.132560
C	-2.737785	-1.007729	-0.891041
C	-3.937668	-1.702695	-0.747562
C	-4.906634	-1.254740	0.154490
C	-4.667046	-0.109103	0.916844
H	-4.120939	-2.589108	-1.347872
H	-5.841501	-1.795805	0.263338
H	-5.413277	0.240753	1.624079
N	-1.265289	0.822439	-0.270350
C	-1.053645	2.127098	-0.476267
O	0.191673	2.451921	-0.419742
C	-2.089211	3.163109	-0.779005
H	-2.256272	3.780230	0.112249
H	-1.705411	3.823028	-1.562356
H	-3.038677	2.720327	-1.084363
C	1.858089	0.213156	2.823403
H	0.875793	0.044098	3.270586
H	2.602223	-0.301072	3.448522
H	2.077855	1.282997	2.861471
C	3.331956	-0.530202	-2.070527
H	2.650902	-0.713559	-2.906774
H	3.783001	0.455297	-2.204555
H	4.134904	-1.277571	-2.134285
H	-1.988877	-1.334710	-1.607462
H	-3.271544	1.464006	1.397188

15b

B3LYP SCF energy: -1394.82292564 a.u.
B3LYP enthalpy: -1394.334552 a.u.
B3LYP free energy: -1394.434760 a.u.
M06 SCF energy in solution: -1395.62694427 a.u.
M06 enthalpy in solution: -1395.138571 a.u.
M06 free energy in solution: -1395.238779 a.u.
Three lowest frequencies (cm-1): 14.8718 20.3195 23.6144

Cartesian coordinates

ATOM	X	Y	Z
C	0.078897	1.237029	1.405476
C	1.431655	0.746940	1.697770
C	2.204810	0.852767	0.495609
C	1.361240	1.366481	-0.555339
C	0.050785	1.615249	0.023039
C	-1.031942	1.346308	2.396855
H	-0.916896	0.623021	3.206730
H	-1.022566	2.352956	2.835445

H	-2.004784	1.206005	1.923890
C	1.909281	0.271449	3.028458
H	2.688086	-0.484804	2.927104
H	2.356610	1.117787	3.567080
H	1.089279	-0.122742	3.632735
C	1.751448	1.647443	-1.966972
H	2.212166	2.646089	-2.003165
H	2.495850	0.933977	-2.319693
H	0.876812	1.655957	-2.616988
Rh	0.470658	-0.533746	0.191103
C	3.654476	0.473362	0.430730
O	4.370020	0.528370	1.408052
O	4.035449	0.083181	-0.787148
C	5.443509	-0.297760	-0.928887
H	6.054342	0.562369	-0.641542
H	5.641705	-1.108906	-0.223518
C	5.661653	-0.713475	-2.368706
H	6.706434	-1.011973	-2.502932
H	5.027141	-1.564586	-2.635218
H	5.453761	0.111742	-3.057170
C	-1.108870	2.178710	-0.744479
O	-1.290800	1.969656	-1.926817
O	-1.881469	2.937459	0.032777
C	-3.048480	3.547320	-0.611055
H	-3.682530	2.738094	-0.983991
H	-2.693369	4.126612	-1.467154
C	-3.744631	4.405140	0.424758
H	-3.082011	5.193176	0.795334
H	-4.619031	4.881166	-0.030778
H	-4.087508	3.805227	1.273561
C	-3.369455	-2.419744	0.594615
C	-2.472221	-1.766133	-0.265925
C	-2.959407	-1.013216	-1.345309
C	-4.332962	-0.937695	-1.571159
C	-5.226401	-1.603444	-0.726825
C	-4.740863	-2.342780	0.354597
H	-2.991967	-2.974008	1.449220
H	-2.262273	-0.502981	-2.002739
H	-4.704719	-0.366039	-2.416549
H	-6.295076	-1.545683	-0.909754
H	-5.430023	-2.856462	1.018332
N	-1.079950	-1.826114	-0.032414
C	-0.313379	-2.904147	0.147906
O	0.896187	-2.601866	0.484224
C	-0.713023	-4.332461	-0.031485
H	-0.804006	-4.808890	0.952291
H	-1.660707	-4.430588	-0.563151
H	0.083507	-4.853606	-0.570860

16a
B3LYP SCF energy: -1167.77870199 a.u.
B3LYP enthalpy: -1167.328620 a.u.
B3LYP free energy: -1167.417862 a.u.
M06 SCF energy in solution: -1168.56684277 a.u.
M06 enthalpy in solution: -1168.116761 a.u.
M06 free energy in solution: -1168.206003 a.u.
Three lowest frequencies (cm-1): 21.1877 41.0315 48.6257

Cartesian coordinates

ATOM	X	Y	Z
C	0.464829	-2.049543	-0.302968
C	1.718141	-1.683397	-0.963022
C	2.584253	-1.122342	0.005111
C	1.883980	-1.134513	1.289187
C	0.612124	-1.772433	1.101287
C	-0.680046	-2.767054	-0.951065
H	-0.798135	-2.468191	-1.995884
H	-0.510703	-3.852940	-0.928213
H	-1.624363	-2.556854	-0.443435
C	1.975079	-1.851769	-2.428978
H	2.882733	-1.332421	-2.744578
H	2.088070	-2.915504	-2.676181
H	1.141896	-1.458282	-3.019510
C	2.499442	-0.713520	2.588611
H	1.747316	-0.571477	3.367590
H	3.202273	-1.482573	2.938303
H	3.057471	0.221763	2.483337
Rh	0.701474	0.114799	-0.070135
C	-3.262357	-0.334324	0.781963
C	-2.274628	0.324394	0.018548
C	-2.430144	0.350725	-1.379253
C	-3.515803	-0.277297	-1.992286
C	-4.479766	-0.938130	-1.229023
C	-4.346458	-0.954954	0.162558
H	-3.611637	-0.237687	-3.075112
H	-5.328346	-1.420485	-1.707093
H	-5.097353	-1.449320	0.774754
N	-1.126356	0.911637	0.615882
C	-1.299781	1.674088	1.749463
O	-2.408783	1.998516	2.181425
C	-0.048659	2.124468	2.493375
H	0.761253	2.414417	1.822981
H	-0.326371	2.963012	3.136219
H	0.311583	1.313795	3.140260
C	-0.386895	-2.103128	2.165733
H	-1.409768	-1.995557	1.796937
H	-0.251887	-3.142641	2.494063
H	-0.276190	-1.457801	3.040661
C	3.969761	-0.585752	-0.195991
H	4.227332	-0.519179	-1.255786

H	4.069565	0.415964	0.234492
H	4.710452	-1.234958	0.289282
H	-3.192346	-0.317982	1.862829
C	1.187131	3.649806	-2.032584
H	1.196380	3.527154	-3.118287
H	0.309510	4.249364	-1.762908
H	2.080906	4.182473	-1.699014
C	1.083646	2.310502	-1.350476
O	1.567587	2.139579	-0.184914
O	0.481788	1.340751	-1.911315
H	-1.689299	0.872772	-1.973536

16b
B3LYP SCF energy: -1623.51452273 a.u.
B3LYP enthalpy: -1622.968523 a.u.
B3LYP free energy: -1623.077624 a.u.
M06 SCF energy in solution: -1624.25414725 a.u.
M06 enthalpy in solution: -1623.708148 a.u.
M06 free energy in solution: -1623.817249 a.u.
Three lowest frequencies (cm-1): 17.1515 22.2107 27.1222

Cartesian coordinates

ATOM	X	Y	Z
C	0.161347	-2.331652	-0.816722
C	-1.223193	-2.309170	-0.546915
C	-1.744667	-1.009895	-0.995413
C	-0.680100	-0.272740	-1.628803
C	0.512527	-1.050052	-1.438649
C	1.121445	-3.445149	-0.522525
H	0.614053	-4.294989	-0.061791
H	1.594287	-3.789765	-1.449390
H	1.919335	-3.107510	0.142732
C	-2.023669	-3.392226	0.112283
H	-2.613687	-2.993471	0.940220
H	-2.731836	-3.828975	-0.599348
H	-1.373942	-4.183159	0.493775
C	-0.750040	1.038385	-2.346968
H	-0.847650	0.845596	-3.423005
H	-1.604483	1.625337	-2.018525
H	0.171030	1.604255	-2.206338
Rh	-0.249243	-0.569554	0.573388
C	-3.204219	-0.700738	-0.958928
O	-4.044691	-1.510493	-0.619257
O	-3.500301	0.548366	-1.358518
C	-4.909769	0.900863	-1.341116
H	-5.446017	0.208238	-1.996741
H	-5.286289	0.760690	-0.323772
C	-5.025664	2.340494	-1.803205
H	-6.079254	2.640151	-1.803695

H	-4.478122	3.013346	-1.135788
H	-4.634328	2.461849	-2.818435
C	1.839860	-0.668835	-2.005284
O	1.970863	0.062395	-2.965586
O	2.859062	-1.245610	-1.349294
C	4.187980	-0.896643	-1.818712
H	4.296563	0.188918	-1.750250
H	4.271534	-1.184246	-2.871475
C	5.183754	-1.628006	-0.939717
H	5.051611	-2.712880	-1.008497
H	6.203395	-1.385557	-1.258366
H	5.068502	-1.329199	0.106887
C	2.500552	1.454999	1.015503
C	1.273003	2.009078	0.612895
C	1.299055	3.115225	-0.262286
C	2.507077	3.639400	-0.714716
C	3.722470	3.076976	-0.313054
C	3.708616	1.983972	0.554886
H	0.364213	3.579446	-0.552838
H	2.499090	4.496656	-1.383378
H	4.663579	3.493488	-0.662575
H	4.644823	1.546469	0.895400
N	0.043962	1.449459	1.062304
C	-0.923129	2.311444	1.538146
O	-0.697598	3.503002	1.756820
C	-2.314838	1.749530	1.791004
H	-2.790042	1.483390	0.840697
H	-2.294962	0.857608	2.419656
H	-2.905669	2.531524	2.272653
C	0.425450	-1.269495	4.486402
H	1.324437	-1.868257	4.651068
H	0.582232	-0.281944	4.936479
H	-0.439085	-1.733183	4.967215
C	0.176010	-1.092513	3.015864
O	1.136378	-1.071206	2.179786
O	-1.005046	-0.923070	2.565775
H	2.496402	0.613326	1.697192

17a
B3LYP SCF energy: -938.64676783 a.u.
B3LYP enthalpy: -938.266622 a.u.
B3LYP free energy: -938.343769 a.u.
M06 SCF energy in solution: -939.45919728 a.u.
M06 enthalpy in solution: -939.079051 a.u.
M06 free energy in solution: -939.156198 a.u.
Three lowest frequencies (cm-1): 22.7965 31.2955 70.4410

Cartesian coordinates

ATOM	X	Y	Z

C	1.760930	-1.593548	0.260923
C	2.055592	-0.941528	-0.970519
C	2.463156	0.447760	-0.686538
C	2.313375	0.668995	0.683231
C	1.780683	-0.570828	1.278458
C	1.470569	-3.050449	0.469592
H	1.041730	-3.506181	-0.427007
H	2.390964	-3.597340	0.715613
H	0.761924	-3.203695	1.287855
C	2.127257	-1.576553	-2.325865
H	1.758232	-0.900678	-3.103462
H	3.167040	-1.831074	-2.576060
H	1.537023	-2.495012	-2.372220
C	2.608465	1.917593	1.457652
H	1.819832	2.131581	2.185863
H	3.549189	1.813638	2.015717
H	2.702867	2.788619	0.804469
Rh	0.225101	-0.053168	-0.108431
C	-3.736648	0.100071	-0.107068
C	-2.347538	0.142787	-0.082168
C	-1.567722	-1.026556	-0.030653
C	-2.159848	-2.276157	0.000558
C	-3.570703	-2.344412	-0.017863
C	-4.331468	-1.178627	-0.069421
H	-1.574927	-3.193136	0.041007
H	-4.064308	-3.313052	0.012220
H	-5.416713	-1.251332	-0.079723
N	-1.391731	1.203539	-0.111142
C	-1.725518	2.528175	-0.078288
O	-2.888349	2.938775	-0.062969
C	-0.553131	3.500473	-0.042964
H	-0.898910	4.485003	-0.365833
H	-0.172122	3.590440	0.982338
H	0.272503	3.168475	-0.680153
C	1.554826	-0.781042	2.743964
H	0.864027	-1.607652	2.927021
H	2.504717	-1.015342	3.246116
H	1.140490	0.113893	3.216689
C	2.935502	1.413769	-1.730699
H	2.284656	1.400479	-2.611432
H	2.963118	2.438549	-1.351604
H	3.947824	1.155818	-2.070863
H	-4.326466	1.006051	-0.149378

17b

B3LYP SCF energy: -1394.39065058 a.u.

B3LYP enthalpy: -1393.914818 a.u.

B3LYP free energy: -1394.013760 a.u.

M06 SCF energy in solution: -1395.15586390 a.u.

M06 enthalpy in solution: -1394.680031 a.u.
M06 free energy in solution: -1394.778973 a.u.
Three lowest frequencies (cm-1): 14.6490 20.7494 29.2253

Cartesian coordinates

ATOM	X	Y	Z
C	0.676089	1.176299	-1.428549
C	-0.671048	0.699951	-1.716143
C	-1.563429	1.196059	-0.682273
C	-0.768555	1.849411	0.299133
C	0.615127	1.856621	-0.170618
C	1.827369	1.059014	-2.382136
H	1.812409	0.096224	-2.898491
H	1.754714	1.848302	-3.143399
H	2.780899	1.163982	-1.869898
C	-1.065218	0.000590	-2.979552
H	-1.875829	-0.707077	-2.810277
H	-1.436103	0.738948	-3.703047
H	-0.213390	-0.519188	-3.423509
C	-1.217897	2.452295	1.593722
H	-1.239164	3.544763	1.495694
H	-2.207183	2.097528	1.871015
H	-0.499555	2.237927	2.387652
Rh	0.107028	-0.331688	0.039842
C	-3.026844	0.971150	-0.730109
O	-3.614677	0.614599	-1.735677
O	-3.655836	1.204093	0.440827
C	-5.094528	1.019644	0.429894
H	-5.526025	1.692568	-0.317565
H	-5.310646	-0.006656	0.119582
C	-5.603270	1.313102	1.828402
H	-6.690328	1.181791	1.858717
H	-5.155650	0.632667	2.559990
H	-5.374020	2.341945	2.124583
C	1.700365	2.565263	0.557319
O	1.499243	3.380712	1.437571
O	2.937179	2.227523	0.138390
C	4.030428	2.906639	0.807428
H	3.970006	2.689623	1.877969
H	3.901578	3.985682	0.678224
C	5.325570	2.407342	0.196018
H	5.366514	2.625394	-0.876209
H	6.174173	2.904043	0.678788
H	5.436535	1.327383	0.336804
C	1.735411	-1.548978	0.130180
C	1.003807	-2.718661	0.385790
C	1.630563	-3.933702	0.633281
C	3.041194	-3.931508	0.599175
C	3.773560	-2.773504	0.345870
C	3.115939	-1.545762	0.106436
H	1.062469	-4.832024	0.835743

H	3.569119	-4.865941	0.774326
H	4.859987	-2.814372	0.324867
H	3.687360	-0.642224	-0.090533
N	-0.353234	-2.284598	0.342942
C	-1.432674	-3.130722	0.358204
O	-1.317400	-4.347232	0.508478
C	-2.793894	-2.473323	0.194769
H	-2.885007	-1.577677	0.818155
H	-2.957033	-2.171552	-0.847115
H	-3.565918	-3.194810	0.470288

18a

B3LYP SCF energy: -727.91469317 a.u.
B3LYP enthalpy: -727.619773 a.u.
B3LYP free energy: -727.689422 a.u.
M06 SCF energy in solution: -728.87749932 a.u.
M06 enthalpy in solution: -728.582579 a.u.
M06 free energy in solution: -728.652228 a.u.
Three lowest frequencies (cm-1): 18.5488 33.4139 36.0523

Cartesian coordinates

ATOM	X	Y	Z
C	1.355149	-1.182101	0.544432
C	1.624556	-0.740143	-0.781216
C	1.625941	0.730406	-0.787762
C	1.357726	1.185090	0.533930
C	1.138347	0.005650	1.363258
O	-2.165155	-1.092126	-0.145823
O	-2.164880	1.093802	-0.145822
C	-2.839708	0.001128	-0.192028
C	-4.328719	0.000292	-0.268571
H	-4.731918	-0.051064	0.750880
H	-4.686612	0.921402	-0.733404
H	-4.679370	-0.878373	-0.815018
Rh	-0.362620	-0.000045	-0.167736
C	1.897643	1.578879	-1.987040
H	2.983101	1.680622	-2.124656
H	1.494141	1.133354	-2.900432
H	1.479882	2.582194	-1.879646
C	1.294386	2.603164	1.006281
H	0.530622	2.738854	1.776455
H	2.260901	2.892176	1.439946
H	1.075054	3.292941	0.188522
C	1.288221	-2.595465	1.030097
H	1.069388	-3.292669	0.218539
H	2.253212	-2.882034	1.468756
H	0.522458	-2.722370	1.799792
C	0.860928	0.012476	2.828325
H	0.305318	-0.874133	3.142781

H	1.817310	0.014394	3.371670
H	0.306363	0.902577	3.134659
C	1.894405	-1.599752	-1.973030
H	1.479028	-1.168491	-2.888050
H	2.979509	-1.693144	-2.118812
H	1.486547	-2.605368	-1.850775

18b

B3LYP SCF energy: -1183.64354991 a.u.
B3LYP enthalpy: -1183.253351 a.u.
B3LYP free energy: -1183.344786 a.u.
M06 SCF energy in solution: -1184.55904245 a.u.
M06 enthalpy in solution: -1184.168844 a.u.
M06 free energy in solution: -1184.260279 a.u.
Three lowest frequencies (cm-1): 17.9559 18.5443 23.5005

Cartesian coordinates

ATOM	X	Y	Z
C	0.229905	-1.286909	-0.858781
C	1.363502	-0.799281	-0.090994
C	0.925336	-0.494923	1.233908
C	-0.519214	-0.774153	1.299333
C	-0.920860	-1.274532	0.011652
O	0.511827	2.774485	-0.170722
O	-1.613862	2.296371	-0.252284
C	-0.695293	3.194988	-0.304241
C	-1.008496	4.632380	-0.537313
H	-0.978344	4.831268	-1.616065
H	-2.011364	4.864900	-0.172329
H	-0.259100	5.263976	-0.054423
Rh	-0.163720	0.789053	-0.161883
C	2.738436	-0.604676	-0.669274
O	2.921213	-0.277743	-1.822285
C	-2.273965	-1.761290	-0.427103
O	-2.391828	-2.590712	-1.302658
C	1.753026	0.006517	2.369521
H	2.159386	-0.854507	2.917712
H	2.598753	0.597685	2.017542
H	1.160296	0.601156	3.067932
C	-1.354117	-0.642983	2.527757
H	-2.403193	-0.491657	2.278536
H	-1.269904	-1.573334	3.108455
H	-1.006437	0.173133	3.165554
C	0.251396	-1.708057	-2.285792
H	1.098314	-1.267589	-2.810945
H	0.342189	-2.803521	-2.315244
H	-0.690181	-1.470877	-2.784859
O	-3.269791	-1.185906	0.243973
O	3.683248	-0.852525	0.234782

C	-4.627062	-1.605080	-0.127639
H	-4.747671	-1.423086	-1.198505
H	-4.703150	-2.681389	0.048618
C	-5.598248	-0.803012	0.712378
H	-6.621627	-1.086396	0.445876
H	-5.459710	-1.000468	1.780110
H	-5.482974	0.270307	0.532684
C	5.072058	-0.712278	-0.224250
H	5.207186	0.318315	-0.563208
H	5.205191	-1.375696	-1.082541
C	5.974042	-1.071601	0.937386
H	7.018288	-0.982380	0.620970
H	5.817922	-0.398513	1.786177
H	5.804417	-2.101138	1.266955

19a

B3LYP SCF energy: TAB -1153.34349762 a.u.
B3LYP enthalpy: TAB -1152.846341 a.u.
B3LYP free energy: TAB -1152.938097 a.u.
M06 SCF energy in solution: TAB -1154.15946845 a.u.
M06 enthalpy in solution: TAB -1153.662312 a.u.
M06 free energy in solution: TAB -1153.754068 a.u.
Three lowest frequencies (cm-1): 14.6897 22.8206 40.2997

Cartesian coordinates

ATOM	X	Y	Z
C	3.256558	0.434443	2.130797
C	2.574334	0.821393	0.976100
C	2.791095	0.161466	-0.245066
C	3.727617	-0.880606	-0.281043
C	4.414020	-1.267223	0.874129
C	4.177165	-0.616326	2.085160
H	3.082090	0.966593	3.062097
H	3.937661	-1.399953	-1.210409
H	5.137871	-2.075600	0.821729
H	4.714723	-0.913244	2.980983
C	2.057900	0.636931	-1.502843
C	-2.483012	-0.946259	1.009561
C	-2.651671	-1.272000	-0.373985
C	-1.475663	-2.029071	-0.820592
C	-1.163527	-1.396805	1.395892
C	-0.572796	-2.122539	0.272214
Rh	-0.933312	0.043330	-0.194221
O	0.046903	3.246815	-0.340433
C	-1.067302	3.075035	0.192617
O	-1.644531	1.915349	0.334558
C	-1.856004	4.249728	0.724238
H	-2.132397	4.077309	1.769105
H	-1.269123	5.164894	0.637331

H	-2.784605	4.354621	0.152532
H	1.878239	1.654173	1.023270
C	-3.853663	-0.970086	-1.208785
H	-3.582335	-0.759782	-2.247127
H	-4.526356	-1.839120	-1.213831
H	-4.409931	-0.115489	-0.817223
C	-1.332925	-2.643840	-2.175970
H	-1.937584	-3.559534	-2.226770
H	-1.689456	-1.973695	-2.963585
H	-0.299305	-2.914618	-2.397457
C	0.709066	-2.889687	0.336382
H	1.484013	-2.353093	0.888966
H	0.529280	-3.843329	0.851446
H	1.099678	-3.119518	-0.656770
C	-0.538337	-1.250712	2.743260
H	-0.691660	-2.174274	3.319480
H	0.539618	-1.081905	2.665847
H	-0.980493	-0.425316	3.305458
C	-3.455811	-0.190032	1.861722
H	-3.267303	-0.362382	2.924074
H	-3.375960	0.886802	1.668165
H	-4.481470	-0.503674	1.645969
C	2.693010	1.931404	-2.039253
H	3.729948	1.738121	-2.330200
H	2.145913	2.293705	-2.915918
H	2.698465	2.716354	-1.277320
C	1.966581	-0.409177	-2.612992
H	1.339302	-0.022906	-3.421403
H	2.952736	-0.630057	-3.030089
H	1.532995	-1.344516	-2.246594
O	0.670040	0.973129	-1.142909
H	0.545375	1.971019	-0.880777

19b
B3LYP SCF energy: TAB -1609.07681621 a.u.
B3LYP enthalpy: TAB -1608.483074 a.u.
B3LYP free energy: TAB -1608.595402 a.u.
M06 SCF energy in solution: TAB -1609.84079094 a.u.
M06 enthalpy in solution: TAB -1609.247049 a.u.
M06 free energy in solution: TAB -1609.359377 a.u.
Three lowest frequencies (cm-1): 15.3562 22.1719 24.9369

Cartesian coordinates

ATOM	X	Y	Z
C	2.575930	-0.364467	-2.867350
C	2.089570	-1.180755	-1.844072
C	2.837538	-1.383353	-0.672513
C	4.089865	-0.763661	-0.561046
C	4.583933	0.036493	-1.594091

C	3.827364	0.244050	-2.748781
H	1.982226	-0.222704	-3.766374
H	4.694694	-0.901138	0.328303
H	5.566093	0.490685	-1.495083
H	4.214924	0.862046	-3.553828
C	2.337418	-2.344292	0.400402
C	-0.805765	1.620272	0.120671
C	-2.031026	1.078733	0.696601
C	-1.749739	0.614906	2.040285
C	0.229196	1.394175	1.084710
C	-0.341808	0.757812	2.267201
Rh	-0.669891	-0.560861	0.499855
O	-1.203559	-1.481385	-1.430687
C	-1.803896	-2.413843	-0.815946
O	-1.842745	-2.339624	0.469387
C	-2.421595	-3.577950	-1.530640
H	-3.355839	-3.867826	-1.042706
H	-2.596703	-3.330030	-2.579242
H	-1.739418	-4.435124	-1.482825
H	1.121957	-1.656338	-1.958551
C	-2.742107	0.036624	2.993676
H	-3.453986	-0.613659	2.480740
H	-2.250940	-0.523211	3.791794
H	-3.323254	0.851802	3.441350
C	0.352788	0.448248	3.557350
H	1.430264	0.383541	3.422413
H	0.147611	1.254087	4.275114
H	-0.017618	-0.481814	3.997103
C	-0.659137	2.247921	-1.227594
H	-0.667950	3.339475	-1.114011
H	0.295967	1.976836	-1.680452
H	-1.478409	1.953955	-1.881529
C	1.667221	1.816437	0.995738
O	2.552118	1.315059	1.659865
C	-3.429925	1.154706	0.153269
O	-4.381857	1.306187	0.888808
O	-3.487383	1.044718	-1.174418
O	1.824812	2.837800	0.155322
C	-4.822138	1.141957	-1.768867
H	-5.439072	0.349231	-1.337008
H	-5.252213	2.103912	-1.477076
C	-4.664450	1.004012	-3.268826
H	-5.650417	1.056010	-3.742048
H	-4.047513	1.809729	-3.678883
H	-4.207460	0.044845	-3.531311
C	3.182255	3.373102	0.030187
H	3.824893	2.565892	-0.329319
H	3.518890	3.666069	1.028333
C	3.122094	4.543419	-0.929461
H	4.122817	4.974992	-1.035204
H	2.781339	4.226439	-1.920094

H	2.451678	5.325372	-0.559666
O	0.864845	-2.148837	0.502301
C	2.527883	-3.799791	-0.056930
H	3.593096	-4.008120	-0.193940
H	2.145056	-4.504034	0.693722
H	2.021672	-3.978888	-1.009776
C	2.939595	-2.119938	1.788147
H	2.421461	-2.748121	2.521997
H	3.994243	-2.410422	1.806951
H	2.860889	-1.072982	2.087997
H	0.479887	-2.902020	0.982303

20a

B3LYP SCF energy: -924.22766979 a.u.

B3LYP enthalpy: -923.799416 a.u.

B3LYP free energy: -923.877818 a.u.

M06 SCF energy in solution: -925.06512978 a.u.

M06 enthalpy in solution: -924.636876 a.u.

M06 free energy in solution: -924.715278 a.u.

Three lowest frequencies (cm-1): 12.3652 26.4067 61.0379

Cartesian coordinates

ATOM	X	Y	Z
C	1.627010	2.154799	-0.012201
C	1.411503	0.765137	0.018567
C	2.543280	-0.090091	0.059334
C	3.832558	0.458949	0.061923
C	4.018870	1.838924	0.030167
C	2.911740	2.691967	-0.001462
H	0.781997	2.834070	-0.036469
H	4.702782	-0.191741	0.086152
H	5.025074	2.247380	0.032097
H	3.052437	3.769006	-0.018292
C	2.375955	-1.596764	0.068711
C	-2.548845	-0.917045	-0.350892
C	-2.549704	-0.329279	0.922648
C	-2.068490	1.063696	0.793980
C	-2.021896	0.070674	-1.289800
C	-1.836405	1.329679	-0.588771
Rh	-0.385992	-0.149561	0.116437
C	-2.955210	-0.952655	2.220936
H	-2.238657	-0.723275	3.016302
H	-3.929260	-0.558626	2.540655
H	-3.044843	-2.038636	2.145338
C	-2.040402	2.052515	1.917171
H	-3.051326	2.446339	2.091557
H	-1.701495	1.594568	2.850607
H	-1.385461	2.898545	1.697623
C	-1.599304	2.658371	-1.239990

H	-0.841774	2.605647	-2.026608
H	-2.532652	3.010100	-1.698993
H	-1.289728	3.416977	-0.517781
C	-1.907328	-0.118647	-2.768094
H	-2.875026	0.102819	-3.240974
H	-1.163863	0.552136	-3.205471
H	-1.644951	-1.147263	-3.029351
C	-2.965536	-2.310211	-0.718848
H	-3.964476	-2.302469	-1.173884
H	-2.285414	-2.759473	-1.449984
H	-3.009641	-2.967238	0.153406
C	2.717901	-2.219308	-1.289993
H	3.777060	-2.068589	-1.517804
H	2.532846	-3.301464	-1.285185
H	2.130064	-1.755241	-2.088061
C	3.109731	-2.285627	1.223407
H	2.893936	-3.360527	1.229302
H	4.192227	-2.168986	1.119296
H	2.806397	-1.857046	2.182546
O	0.927856	-1.802198	0.306721
H	0.677970	-2.719657	0.109772

20b

B3LYP SCF energy: -1379.97416337 a.u.

B3LYP enthalpy: -1379.449914 a.u.

B3LYP free energy: -1379.546998 a.u.

M06 SCF energy in solution: -1380.75870940 a.u.

M06 enthalpy in solution: -1380.234460 a.u.

M06 free energy in solution: -1380.331544 a.u.

Three lowest frequencies (cm-1): 18.3925 21.9240 29.7872

Cartesian coordinates

ATOM	X	Y	Z
C	3.069191	-0.458370	-0.920147
C	1.929657	-1.097344	-0.406921
C	2.034281	-2.397956	0.150664
C	3.278800	-3.037163	0.149999
C	4.401575	-2.402361	-0.383090
C	4.298963	-1.115856	-0.921079
H	2.997570	0.545293	-1.328653
H	3.381875	-4.033384	0.571411
H	5.360265	-2.912650	-0.373384
H	5.174914	-0.626012	-1.336587
C	0.815031	-3.045273	0.780057
C	-0.705378	1.202687	0.602941
C	0.163133	1.792394	-0.410292
C	-0.399558	1.501629	-1.691493
C	-1.892160	0.701611	-0.102461
C	-1.716856	0.877418	-1.480047

Rh	0.071758	-0.394335	-0.571372
C	0.112669	1.903820	-3.038974
H	1.170826	2.157113	-3.001329
H	-0.049317	1.110833	-3.775696
H	-0.441119	2.787288	-3.386614
C	-2.640202	0.473579	-2.585788
H	-3.483076	-0.110632	-2.214187
H	-3.042502	1.369657	-3.076172
H	-2.117251	-0.105809	-3.353677
C	-0.583822	1.300971	2.090733
H	-0.992297	2.264956	2.422081
H	-1.147286	0.502125	2.576935
H	0.458032	1.265765	2.409195
C	-2.941649	-0.131328	0.563352
O	-2.666997	-1.075636	1.295445
C	1.407076	2.594755	-0.196055
O	2.253536	2.762924	-1.052465
O	1.451950	3.121295	1.030756
O	-4.170131	0.263520	0.268334
C	2.619910	3.947481	1.335796
H	3.514348	3.336250	1.187187
H	2.646799	4.769692	0.615662
C	2.476512	4.432099	2.763954
H	3.333136	5.064737	3.018216
H	1.565357	5.024808	2.890970
H	2.452191	3.594122	3.467842
C	-5.278592	-0.497273	0.859738
H	-5.165737	-0.455982	1.946102
H	-5.176048	-1.538573	0.542394
C	-6.567911	0.136732	0.382107
H	-7.415859	-0.406026	0.812259
H	-6.634668	1.182105	0.697821
H	-6.652033	0.092750	-0.708050
O	-0.331163	-2.281627	0.225914
C	0.599143	-4.501747	0.362572
H	1.405824	-5.137114	0.740133
H	-0.342730	-4.877719	0.775500
H	0.567754	-4.590421	-0.726770
C	0.809385	-2.873162	2.303488
H	-0.108926	-3.283432	2.741297
H	1.656572	-3.408279	2.742331
H	0.898906	-1.816863	2.576757
H	-1.077362	-2.187356	0.860553

TS1a
B3LYP SCF energy: -1168.18124331 a.u.
B3LYP enthalpy: -1167.722871 a.u.
B3LYP free energy: -1167.810727 a.u.
M06 SCF energy in solution: -1169.00307941 a.u.

M06 enthalpy in solution: -1168.544707 a.u.
M06 free energy in solution: -1168.632563 a.u.
Three lowest frequencies (cm-1): -1038.5922 26.5948 30.4564
Imaginary frequency: -1038.5922 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.286581	-0.433138	1.257572
C	-2.699349	-0.410251	-0.104758
C	-1.891136	-1.373893	-0.837325
C	-1.062836	-2.076191	0.122994
C	-1.254085	-1.459629	1.396965
C	-2.802501	0.408509	2.383022
H	-3.436594	1.221404	2.023699
H	-3.393467	-0.203197	3.076616
H	-1.978438	0.853319	2.950356
C	-3.725586	0.479224	-0.731952
H	-3.268703	1.115188	-1.497523
H	-4.505304	-0.125365	-1.210537
H	-4.204028	1.129215	0.003088
C	-0.218244	-3.281689	-0.147806
H	-0.791406	-4.184357	0.103181
H	0.070797	-3.352411	-1.197304
H	0.693170	-3.288861	0.455429
Rh	-0.516918	0.101252	0.005878
C	3.609704	-1.212850	0.155407
C	2.560333	-0.291390	0.250170
C	1.561387	-0.197234	-0.751229
C	1.710222	-1.050133	-1.871063
C	2.754649	-1.961978	-1.984175
C	3.699437	-2.049563	-0.955579
H	4.363718	-1.268364	0.937689
H	0.996695	-0.957891	-2.686239
H	2.848024	-2.589659	-2.865355
H	4.522054	-2.755017	-1.026366
N	2.604547	0.605815	1.348068
H	3.508398	0.685594	1.797059
C	1.635568	1.410594	1.842883
O	0.447257	1.401304	1.462363
C	2.049279	2.383262	2.920602
H	1.278574	2.412634	3.694286
H	3.013423	2.139039	3.374782
H	2.115500	3.385056	2.480720
H	1.347736	1.047131	-1.094642
C	-0.314223	3.871519	-2.303400
H	-0.133068	3.748667	-3.377157
H	-1.364450	4.115683	-2.139001
H	0.326047	4.686597	-1.955506
C	0.061523	2.590983	-1.594596
O	-0.876120	1.856645	-1.144883
O	1.291981	2.294908	-1.501152

C	-2.089472	-1.731438	-2.279000
H	-2.927728	-2.433655	-2.382669
H	-2.322674	-0.847735	-2.879361
H	-1.205419	-2.211051	-2.705825
C	-0.630565	-1.876080	2.693711
H	-1.288875	-2.580672	3.219458
H	0.330164	-2.373699	2.539679
H	-0.474739	-1.019282	3.355179

TS1b

B3LYP SCF energy: -1623.91782578 a.u.
B3LYP enthalpy: -1623.364040 a.u.
B3LYP free energy: -1623.474374 a.u.
M06 SCF energy in solution: -1624.69238627 a.u.
M06 enthalpy in solution: -1624.138600 a.u.
M06 free energy in solution: -1624.248934 a.u.
Three lowest frequencies (cm-1): -965.6026 16.3572 21.1209
Imaginary frequency: -965.6026 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.120810	-1.262560	1.589677
C	-0.257647	-1.292615	1.968674
C	-1.046922	-1.423401	0.758705
C	-0.149634	-1.566408	-0.377543
C	1.171356	-1.412935	0.144773
C	2.288894	-1.136850	2.518455
H	1.986153	-0.688733	3.467746
H	2.718371	-2.124894	2.723880
H	3.079135	-0.519982	2.082527
C	-0.773381	-1.154490	3.366193
H	-1.860355	-1.225578	3.392377
H	-0.340091	-1.935603	4.001568
H	-0.489871	-0.180610	3.780176
C	-0.510457	-1.890419	-1.793697
H	-0.703265	-2.967008	-1.875057
H	-1.420866	-1.375328	-2.102958
H	0.303001	-1.623977	-2.469659
Rh	0.063793	0.458030	0.585492
C	-2.536105	-1.564640	0.754874
O	-3.273426	-0.964302	1.510534
O	-2.937727	-2.454287	-0.160496
C	-4.374493	-2.709864	-0.223520
H	-4.706232	-3.023826	0.769761
H	-4.877015	-1.768308	-0.464132
C	-4.603130	-3.776149	-1.275418
H	-5.673749	-3.995037	-1.343473
H	-4.259197	-3.443342	-2.259873
H	-4.080916	-4.702512	-1.017206

C	2.414376	-1.415287	-0.694696
O	2.532237	-0.796700	-1.734871
O	3.350739	-2.195075	-0.152342
C	4.607773	-2.317620	-0.889024
H	5.059768	-1.323114	-0.950878
H	4.373105	-2.647861	-1.904467
C	5.480336	-3.305723	-0.142818
H	5.000823	-4.287415	-0.083292
H	6.431481	-3.420841	-0.672791
H	5.694636	-2.957846	0.872387
C	-0.674527	1.809972	-3.428538
C	-0.168010	1.888755	-2.127309
C	-0.977363	1.597244	-1.001044
C	-2.324573	1.238752	-1.254188
C	-2.839198	1.162155	-2.544226
C	-2.003116	1.441069	-3.632257
H	-0.039442	2.040308	-4.280995
H	-2.977406	1.056551	-0.404225
H	-3.881535	0.906516	-2.709145
H	-2.389987	1.388174	-4.645685
N	1.161809	2.350950	-1.986980
H	1.568160	2.748103	-2.824862
C	1.978050	2.307417	-0.913350
O	1.689759	1.775913	0.182596
C	3.344308	2.925307	-1.070352
H	4.081995	2.120014	-1.159845
H	3.421772	3.576257	-1.944834
H	3.580530	3.499714	-0.171306
H	-0.899869	2.506064	-0.082524
C	-1.061480	3.845881	3.154967
H	-0.767539	4.879996	2.963087
H	-2.139528	3.831765	3.353997
H	-0.540120	3.450925	4.028479
C	-0.787311	2.996061	1.936496
O	-0.456077	1.778510	2.133250
O	-0.926335	3.510632	0.789318

TS2a
B3LYP SCF energy: -1478.54145666 a.u.
B3LYP enthalpy: -1477.942635 a.u.
B3LYP free energy: -1478.045473 a.u.
M06 SCF energy in solution: -1479.17070186 a.u.
M06 enthalpy in solution: -1478.571880 a.u.
M06 free energy in solution: -1478.674718 a.u.
Three lowest frequencies (cm-1): -292.2441 16.1585 28.3674
Imaginary frequency: -292.2441 cm-1

Cartesian coordinates

ATOM	X	Y	Z

C	0.969805	-2.591737	-1.516395
C	0.707970	-1.384005	-2.284620
C	1.843966	-0.484840	-2.122600
C	2.697541	-1.054113	-1.150560
C	2.141188	-2.362925	-0.765751
C	0.152792	-3.846938	-1.558796
H	-0.919079	-3.645055	-1.481634
H	0.321468	-4.375152	-2.506326
H	0.419588	-4.529385	-0.748441
C	-0.360902	-1.238675	-3.327012
H	-0.700126	-0.204347	-3.428283
H	0.026140	-1.555750	-4.305227
H	-1.231535	-1.862181	-3.107171
C	4.024457	-0.541089	-0.678174
H	4.837641	-1.145969	-1.100744
H	4.191138	0.494557	-0.982590
H	4.109449	-0.597137	0.411995
Rh	0.668246	-0.695142	-0.172538
C	-2.290062	-1.930588	2.790689
C	-1.304824	-1.156852	2.157957
C	-1.222442	-1.098268	0.748188
C	-2.183298	-1.836182	0.026883
C	-3.151712	-2.615938	0.650134
C	-3.209995	-2.661416	2.045782
H	-2.321355	-1.968611	3.877609
H	-2.193148	-1.754838	-1.054847
H	-3.870889	-3.167734	0.051873
H	-3.966351	-3.253767	2.551001
N	-0.432692	-0.442164	3.027602
H	-0.812630	-0.247336	3.945240
C	0.893352	-0.234085	2.886672
O	1.522551	-0.486473	1.839274
C	1.632795	0.337804	4.071052
H	2.043231	1.313406	3.790519
H	1.005382	0.456404	4.958217
H	2.475100	-0.317100	4.313660
C	0.088520	1.284433	0.111035
C	-1.113858	0.820321	0.043517
C	0.837675	2.519640	0.253169
C	2.217318	2.518091	0.529940
C	0.169834	3.758222	0.139617
C	2.912304	3.718217	0.676210
H	2.728956	1.570408	0.650241
C	0.870174	4.951947	0.285567
H	-0.895248	3.774347	-0.069585
C	2.243276	4.937610	0.551159
H	3.977048	3.701632	0.891831
H	0.343861	5.897464	0.191047
H	2.785834	5.871757	0.662923
C	-2.440543	1.176267	-0.451317
C	-2.538183	1.847080	-1.687131

C	-3.610444	0.956215	0.298331
C	-3.774752	2.283319	-2.159666
H	-1.636637	2.028451	-2.265013
C	-4.841561	1.402583	-0.174500
H	-3.547749	0.445629	1.253191
C	-4.928643	2.061339	-1.404846
H	-3.836646	2.796389	-3.114949
H	-5.736729	1.238029	0.418033
H	-5.892380	2.402000	-1.771883
C	2.805098	-3.292904	0.202483
H	3.700234	-3.740255	-0.249549
H	3.124476	-2.759322	1.103217
H	2.142167	-4.105803	0.507648
C	2.057084	0.784784	-2.891247
H	2.531468	0.565307	-3.856998
H	1.111745	1.293467	-3.100080
H	2.699365	1.484920	-2.352716

TS2b

B3LYP SCF energy: -1934.28194052 a.u.
B3LYP enthalpy: -1933.587398 a.u.
B3LYP free energy: -1933.712629 a.u.
M06 SCF energy in solution: -1934.86600065 a.u.
M06 enthalpy in solution: -1934.171458 a.u.
M06 free energy in solution: -1934.296689 a.u.
Three lowest frequencies (cm-1): -302.1517 6.4167 14.6272
Imaginary frequency: -302.1517 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.754827	-0.930536	-1.752340
C	-0.362527	-0.793454	-2.135468
C	0.397888	-1.804940	-1.410839
C	-0.468420	-2.433831	-0.480550
C	-1.811779	-1.864413	-0.691933
C	-2.893839	-0.221309	-2.419952
H	-2.533800	0.516299	-3.140039
H	-3.504974	-0.951330	-2.962703
H	-3.550951	0.269450	-1.700288
C	0.110060	0.002879	-3.317348
H	1.197197	0.041056	-3.350614
H	-0.249520	-0.466297	-4.243080
H	-0.275669	1.026719	-3.300063
C	-0.153116	-3.523217	0.498446
H	-0.707425	-4.429349	0.226972
H	0.909994	-3.756670	0.495504
H	-0.485633	-3.248494	1.501690
Rh	-0.376607	-0.181387	0.033891
C	1.860907	-2.016126	-1.628464

O	2.607112	-1.156555	-2.060215
O	2.249334	-3.263741	-1.332554
C	3.664478	-3.557079	-1.527917
H	3.920331	-3.325199	-2.565306
H	4.241500	-2.891406	-0.879246
C	3.876507	-5.020537	-1.195150
H	4.930592	-5.278256	-1.342213
H	3.615264	-5.233193	-0.153472
H	3.273320	-5.663510	-1.843445
C	-3.005025	-2.300290	0.088392
O	-2.942488	-2.986536	1.089240
O	-4.154866	-1.861068	-0.451295
C	-5.373260	-2.263809	0.236362
H	-5.331995	-1.882544	1.261086
H	-5.393133	-3.356180	0.286037
C	-6.546519	-1.701152	-0.541344
H	-6.561869	-2.086397	-1.565712
H	-7.481757	-1.993731	-0.052746
H	-6.509132	-0.607618	-0.579687
C	-2.515878	3.073498	1.979380
C	-1.526362	2.110392	1.733088
C	-1.175902	1.754957	0.409988
C	-1.872633	2.403418	-0.630367
C	-2.870186	3.341496	-0.387315
C	-3.188879	3.688639	0.928607
H	-2.770960	3.324575	3.006808
H	-1.592224	2.190133	-1.655605
H	-3.380734	3.816001	-1.220138
H	-3.952736	4.431051	1.137216
N	-0.918585	1.540077	2.885294
H	-0.980804	2.104386	3.723420
C	-0.538444	0.258449	3.071578
O	-0.470718	-0.581104	2.150190
C	-0.180229	-0.167478	4.472181
H	-0.312018	0.625719	5.212523
H	-0.802158	-1.024501	4.748746
H	0.862864	-0.499775	4.481489
C	1.395363	0.753699	0.545930
C	0.830117	1.815142	0.071868
C	2.597084	0.259774	1.180043
C	2.719748	-1.070663	1.621637
C	3.676472	1.147878	1.383715
C	3.894183	-1.505355	2.234762
H	1.886405	-1.751608	1.496000
C	4.845724	0.704903	1.992704
H	3.590505	2.177729	1.051187
C	4.960590	-0.622350	2.419456
H	3.974368	-2.534330	2.574125
H	5.670888	1.396476	2.135971
H	5.874634	-0.963283	2.896729
C	1.160202	2.973854	-0.747663

C	2.105000	2.803987	-1.781473
C	0.651267	4.258482	-0.482067
C	2.525025	3.900639	-2.531818
H	2.500450	1.812037	-1.979170
C	1.082262	5.348862	-1.232337
H	-0.066563	4.397857	0.318956
C	2.014448	5.172361	-2.260192
H	3.250765	3.761720	-3.327774
H	0.694834	6.339696	-1.014196
H	2.343573	6.026031	-2.845623

TS3a

B3LYP SCF energy: -1478.13318933 a.u.

B3LYP enthalpy: -1477.547218 a.u.

B3LYP free energy: -1477.647651 a.u.

M06 SCF energy in solution: -1478.72749172 a.u.

M06 enthalpy in solution: -1478.141520 a.u.

M06 free energy in solution: -1478.241953 a.u.

Three lowest frequencies (cm-1): -135.0160 21.2108 29.3631

Imaginary frequency: -135.0160 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.088122	0.855794	0.570252
C	3.246891	-0.010282	-0.601527
C	2.569720	0.581647	-1.689293
C	1.902536	1.768120	-1.185344
C	2.334279	1.979995	0.190904
C	3.723952	0.593363	1.905716
H	3.581928	-0.445671	2.221516
H	4.806631	0.780471	1.873615
H	3.300792	1.233585	2.684764
C	4.141616	-1.214788	-0.641004
H	3.912618	-1.869061	-1.487134
H	5.194036	-0.910474	-0.736889
H	4.062008	-1.811214	0.273000
C	1.172101	2.775094	-2.027219
H	1.871716	3.502441	-2.464380
H	0.637572	2.293799	-2.851741
H	0.435166	3.334146	-1.443870
Rh	0.920131	0.122622	-0.073250
C	-1.377276	0.061177	1.845773
C	-0.612963	-1.059930	2.252348
C	-0.762675	-1.570118	3.548570
C	-1.651721	-0.952544	4.435617
C	-2.408888	0.146986	4.039174
C	-2.274991	0.649733	2.740495
H	-0.188356	-2.434733	3.845695
H	-1.747472	-1.345622	5.444704

H	-3.111271	0.611304	4.726282
H	-2.891112	1.483454	2.422271
N	0.242779	-1.539375	1.240657
C	0.681811	-2.847455	1.214234
O	0.523429	-3.643599	2.140230
C	1.377476	-3.318758	-0.053927
H	1.571484	-2.518547	-0.767793
H	2.317344	-3.808567	0.219301
H	0.744834	-4.078766	-0.526810
C	-0.792419	-0.573355	-0.519306
C	-1.194555	0.451590	0.414310
C	-1.498432	-1.505613	-1.361438
C	-2.840798	-1.843659	-1.073339
C	-0.866140	-2.103705	-2.472358
C	-3.522791	-2.756607	-1.870881
H	-3.324343	-1.387961	-0.214593
C	-1.555571	-3.007772	-3.273005
H	0.162061	-1.834999	-2.690553
C	-2.881951	-3.337117	-2.970815
H	-4.551030	-3.018690	-1.638896
H	-1.065751	-3.459012	-4.131232
H	-3.417355	-4.048020	-3.594481
C	-1.852712	1.692859	-0.104839
C	-2.551908	1.733728	-1.324681
C	-1.739338	2.896820	0.619785
C	-3.118751	2.919894	-1.793837
H	-2.662095	0.831070	-1.915958
C	-2.308765	4.080590	0.152607
H	-1.192196	2.897881	1.556789
C	-3.003964	4.100491	-1.059234
H	-3.657174	2.915768	-2.738298
H	-2.205191	4.991096	0.737573
H	-3.448259	5.022377	-1.424250
C	2.571293	0.119559	-3.118598
H	3.371802	0.609010	-3.692226
H	2.732078	-0.960718	-3.197733
H	1.627534	0.355251	-3.620580
C	2.013546	3.185198	1.025679
H	2.747922	3.985815	0.856377
H	1.028460	3.593971	0.781796
H	2.022428	2.951426	2.094640

TS3b

B3LYP SCF energy: -1933.88422138 a.u.
B3LYP enthalpy: -1933.202422 a.u.
B3LYP free energy: -1933.325067 a.u.
M06 SCF energy in solution: -1934.43507299 a.u.
M06 enthalpy in solution: -1933.753274 a.u.
M06 free energy in solution: -1933.875919 a.u.

Three lowest frequencies (cm-1): -139.3032 12.6206 19.1565
Imaginary frequency: -139.3032 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.208878	-2.475164	-1.569477
C	1.155295	-2.439060	-1.098033
C	1.104380	-2.313867	0.323246
C	-0.285888	-2.273480	0.743728
C	-1.089954	-2.462703	-0.439787
C	-0.617962	-2.615067	-3.008039
H	0.139972	-2.203270	-3.679715
H	-0.760365	-3.673123	-3.261508
H	-1.568027	-2.116055	-3.199662
C	2.366702	-2.659498	-1.959541
H	3.121407	-1.881144	-1.833105
H	2.846073	-3.610310	-1.696171
H	2.093092	-2.709785	-3.015711
C	-0.744755	-2.320020	2.173496
H	-0.459591	-3.283233	2.614458
H	-0.259272	-1.549839	2.774513
H	-1.824279	-2.207913	2.238947
Rh	0.045410	-0.382000	-0.489217
C	2.233243	-2.303642	1.277369
O	2.129082	-2.360774	2.488548
O	3.444139	-2.239236	0.658023
C	4.592297	-2.290577	1.534629
H	4.558347	-1.432036	2.213247
H	4.528538	-3.195339	2.147002
C	5.834883	-2.280150	0.662985
H	6.730160	-2.320767	1.293012
H	5.849027	-3.142915	-0.010696
H	5.884280	-1.370192	0.055036
C	-2.553661	-2.590130	-0.578908
O	-3.103324	-3.045472	-1.567432
O	-3.256137	-2.162599	0.502182
C	-4.690786	-2.315509	0.403014
H	-4.922042	-3.372418	0.235774
H	-5.044618	-1.757645	-0.469137
C	-5.302375	-1.798845	1.692374
H	-5.078625	-0.736608	1.836759
H	-6.391244	-1.915155	1.655846
H	-4.927519	-2.355267	2.557944
C	-1.759016	1.954146	-0.447650
C	-1.421867	1.836674	-1.816920
C	-2.286090	2.345366	-2.793140
C	-3.499753	2.920414	-2.401731
C	-3.846387	3.016843	-1.054462
C	-2.972842	2.537946	-0.074038
H	-2.011121	2.278139	-3.835625
H	-4.178007	3.291233	-3.165863

H	-4.786089	3.475899	-0.759726
H	-3.224680	2.644137	0.975265
N	-0.206560	1.159653	-2.022345
C	0.583401	1.401570	-3.133193
O	0.255651	2.163447	-4.040095
C	1.895305	0.642533	-3.211324
H	2.334199	0.446253	-2.231560
H	1.727406	-0.322678	-3.702482
H	2.588102	1.218795	-3.829192
C	0.645870	1.350666	0.038746
C	-0.697392	1.506252	0.492597
C	1.883021	2.075772	0.185103
C	1.866907	3.488684	0.240384
C	3.123710	1.403612	0.216662
C	3.056997	4.203450	0.326538
H	0.913798	4.007179	0.194537
C	4.309034	2.124276	0.322017
H	3.134250	0.319139	0.173724
C	4.277967	3.522010	0.373087
H	3.036853	5.288948	0.356399
H	5.260423	1.601147	0.360195
H	5.206595	4.081577	0.445913
C	-0.964084	1.589982	1.969344
C	-0.186369	2.360460	2.848109
C	-2.050605	0.871221	2.501348
C	-0.488954	2.416297	4.210197
H	0.657250	2.928577	2.473261
C	-2.354157	0.932328	3.860282
H	-2.644620	0.248683	1.839446
C	-1.574459	1.706431	4.722908
H	0.127183	3.022468	4.869140
H	-3.197406	0.365704	4.246694
H	-1.808920	1.751968	5.782900

TS4a

B3LYP SCF energy: -1152.89046827 a.u.
B3LYP enthalpy: -1152.411597 a.u.
B3LYP free energy: -1152.498502 a.u.
M06 SCF energy in solution: -1153.65065724 a.u.
M06 enthalpy in solution: -1153.171786 a.u.
M06 free energy in solution: -1153.258691 a.u.
Three lowest frequencies (cm-1): -1142.2497 20.5853 41.2135
Imaginary frequency: -1142.2497 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.717344	-0.382821	-2.176543
C	-1.442509	0.088456	-0.875542
C	-2.398592	-0.150880	0.148357

C	-3.579516	-0.836496	-0.154319
C	-3.822700	-1.297646	-1.450802
C	-2.893043	-1.070178	-2.470598
H	-1.007924	-0.171810	-2.974091
H	-4.317412	-1.025992	0.620574
H	-4.746150	-1.830084	-1.666836
H	-3.094047	-1.415311	-3.481907
C	-2.054677	0.374973	1.539835
C	2.617735	-0.487882	0.680898
C	1.724384	-1.447545	1.237009
C	1.000480	-2.066511	0.146264
C	2.532094	-0.577619	-0.775322
C	1.572555	-1.569852	-1.099435
Rh	0.531473	0.073361	0.073348
O	-0.901309	2.653917	-1.136012
C	0.208413	2.996364	-0.612757
O	1.010334	2.195826	-0.057062
C	0.564058	4.469795	-0.641726
H	0.261326	4.913869	-1.593501
H	0.009689	4.978057	0.155827
H	1.632818	4.613371	-0.472026
H	-1.039038	1.357669	-0.957542
C	1.448765	-1.664392	2.693615
H	0.609635	-1.023464	2.999532
H	1.181511	-2.706907	2.893948
H	2.320314	-1.415534	3.305954
C	0.027052	-3.202330	0.268784
H	0.543246	-4.171462	0.214402
H	-0.508856	-3.161493	1.220754
H	-0.719404	-3.175347	-0.529950
C	1.255402	-2.096726	-2.467192
H	1.422996	-1.344639	-3.243695
H	1.898741	-2.957796	-2.696026
H	0.217509	-2.429733	-2.540058
C	3.372665	0.227800	-1.720607
H	4.415283	-0.118009	-1.709452
H	3.008901	0.153842	-2.749203
H	3.369052	1.285360	-1.437497
C	3.533319	0.441217	1.420600
H	4.583484	0.145585	1.291392
H	3.422898	1.466164	1.051555
H	3.312605	0.450506	2.490820
C	-2.699054	1.771218	1.728403
H	-3.794697	1.723113	1.689631
H	-2.400675	2.173431	2.703297
H	-2.355149	2.455990	0.948433
C	-2.552052	-0.570775	2.655547
H	-2.187892	-0.195878	3.617514
H	-3.646034	-0.627823	2.706443
H	-2.157506	-1.582049	2.508296
O	-0.651039	0.481019	1.678814

TS4b
B3LYP SCF energy: -1608.63505480 a.u.
B3LYP enthalpy: -1608.060141 a.u.
B3LYP free energy: -1608.167163 a.u.
M06 SCF energy in solution: -1609.34776371 a.u.
M06 enthalpy in solution: -1608.772850 a.u.
M06 free energy in solution: -1608.879872 a.u.
Three lowest frequencies (cm-1): -1022.7390 17.9423 24.0737
Imaginary frequency: -1022.7390 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.270453	0.618065	-2.460650
C	-1.150655	1.110414	-1.142736
C	-2.327372	1.475470	-0.433609
C	-3.572350	1.355334	-1.058380
C	-3.663640	0.873924	-2.367382
C	-2.514094	0.503615	-3.075527
H	-0.367942	0.357373	-3.009034
H	-4.480211	1.633647	-0.530282
H	-4.639307	0.796428	-2.841900
H	-2.593449	0.143535	-4.098064
C	-2.132068	1.999875	0.985027
C	0.433076	-1.805851	-0.345518
C	1.738258	-1.331145	-0.014410
C	1.765913	-0.978619	1.408040
C	-0.374553	-1.687663	0.857452
C	0.479111	-1.236395	1.947644
Rh	0.268346	0.379350	0.332259
O	0.536891	3.133767	-1.261254
C	1.512268	2.977820	-0.467549
O	1.676499	1.965979	0.279022
C	2.541312	4.086529	-0.381198
H	3.475154	3.717370	0.046561
H	2.712972	4.517300	-1.370646
H	2.145769	4.877003	0.267128
H	-0.241193	2.045708	-1.132164
C	2.942562	-0.430807	2.159029
H	3.386525	0.408177	1.617884
H	2.644606	-0.077866	3.148404
H	3.715944	-1.197451	2.276905
C	0.035433	-0.980899	3.355131
H	-0.636228	-0.114367	3.374349
H	-0.519712	-1.836987	3.743896
H	0.888045	-0.776932	4.006934
C	0.027432	-2.435401	-1.645988
H	-0.099718	-3.514558	-1.489372
H	-0.929038	-2.050872	-1.996829

H	0.793593	-2.271159	-2.401818
C	-1.783875	-2.109735	1.050937
O	-2.350891	-2.130480	2.128302
C	2.864712	-1.253264	-0.979963
O	2.751402	-1.223300	-2.192196
O	4.062912	-1.236348	-0.357867
O	-2.383859	-2.475245	-0.100197
C	5.218765	-1.131466	-1.222294
H	5.217544	-1.980045	-1.913423
H	5.128628	-0.218322	-1.819111
C	6.451026	-1.116897	-0.337065
H	7.350558	-1.040232	-0.957575
H	6.432303	-0.263392	0.348254
H	6.519516	-2.034913	0.255571
C	-3.773307	-2.863291	0.009688
H	-4.334545	-2.030729	0.444281
H	-3.848266	-3.711203	0.698004
C	-4.259539	-3.209911	-1.384971
H	-5.312100	-3.511334	-1.345175
H	-4.170855	-2.345774	-2.050951
H	-3.681059	-4.037236	-1.809007
O	-0.880897	1.560541	1.490740
C	-2.142052	3.547747	0.957824
H	-3.114878	3.940565	0.636864
H	-1.929057	3.923156	1.964996
H	-1.373110	3.921587	0.276105
C	-3.222832	1.489355	1.951793
H	-2.996295	1.858347	2.957456
H	-4.223606	1.846177	1.679563
H	-3.231091	0.396091	1.986200

TS5a

B3LYP SCF energy: -1463.24545079 a.u.
B3LYP enthalpy: -1462.626026 a.u.
B3LYP free energy: -1462.728450 a.u.
M06 SCF energy in solution: -1463.81983844 a.u.
M06 enthalpy in solution: -1463.200414 a.u.
M06 free energy in solution: -1463.302838 a.u.
Three lowest frequencies (cm-1): -299.0871 14.6807 21.5343
Imaginary frequency: -299.0871 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.909689	-2.003227	-0.627177
C	-1.088044	-1.326464	0.291427
C	-1.066344	-1.739172	1.645980
C	-1.916293	-2.780919	2.040219
C	-2.740231	-3.437863	1.122253
C	-2.722120	-3.060723	-0.222398

H	-1.933382	-1.672524	-1.662333
H	-1.916439	-3.108595	3.076408
H	-3.384021	-4.247718	1.456049
H	-3.349608	-3.573340	-0.947427
C	-0.052104	-1.082211	2.582405
C	1.408633	-0.915382	-2.413728
C	2.223441	0.167790	-1.937038
C	2.958758	-0.308533	-0.809174
C	1.741579	-2.107548	-1.652990
C	2.673344	-1.735135	-0.658613
Rh	0.791683	-0.462366	-0.237923
C	2.304518	1.542386	-2.535527
H	3.114289	1.595977	-3.276505
H	1.376477	1.815456	-3.047428
H	2.498815	2.304996	-1.776143
C	0.530206	-0.892994	-3.632462
H	0.074524	0.089839	-3.788129
H	1.105682	-1.134675	-4.537687
H	-0.276992	-1.627960	-3.556513
C	1.174845	-3.473248	-1.909874
H	1.517074	-3.866272	-2.876828
H	1.478796	-4.183542	-1.136539
H	0.079339	-3.458974	-1.925998
C	3.278432	-2.586155	0.415158
H	2.929130	-3.620846	0.360662
H	4.373597	-2.595209	0.341782
H	3.002653	-2.185211	1.398587
C	3.987468	0.437145	-0.011127
H	3.943539	0.148502	1.043814
H	5.003040	0.223242	-0.374394
H	3.834236	1.518469	-0.066125
C	-0.135823	1.306016	0.191686
C	-1.215347	0.639000	-0.052040
C	0.411377	2.599206	0.562668
C	1.444936	2.666798	1.517346
C	-0.076356	3.793587	-0.001340
C	1.972463	3.900408	1.894115
H	1.785747	1.737768	1.963762
C	0.462721	5.022854	0.376691
H	-0.879530	3.751675	-0.730579
C	1.488950	5.081123	1.322784
H	2.762670	3.941425	2.639563
H	0.078659	5.937332	-0.068122
H	1.906389	6.041020	1.615380
C	-2.590511	0.904082	-0.489156
C	-2.810202	1.692842	-1.632686
C	-3.701970	0.456190	0.246571
C	-4.105423	2.034187	-2.024497
H	-1.955995	2.027871	-2.214228
C	-4.992457	0.808718	-0.140598
H	-3.542938	-0.161302	1.124379

C	-5.199828	1.595936	-1.277478
H	-4.257499	2.641532	-2.912898
H	-5.840892	0.466818	0.446130
H	-6.209010	1.863286	-1.579229
O	1.024265	-0.579002	1.818528
C	-0.728251	0.048483	3.399591
H	-1.527096	-0.343376	4.042404
H	0.020991	0.531729	4.037282
H	-1.155567	0.808254	2.740950
C	0.551185	-2.108403	3.569428
H	1.363446	-1.620008	4.118001
H	-0.178133	-2.476568	4.301322
H	0.966964	-2.963257	3.026402

TS5b

B3LYP SCF energy: -1918.99504991 a.u.
B3LYP enthalpy: -1918.279719 a.u.
B3LYP free energy: -1918.403435 a.u.
M06 SCF energy in solution: -1919.52646761 a.u.
M06 enthalpy in solution: -1918.811137 a.u.
M06 free energy in solution: -1918.934853 a.u.
Three lowest frequencies (cm-1): -297.1244 10.6604 16.7363
Imaginary frequency: -297.1244 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.252232	1.910588	-0.856099
C	1.512380	1.318746	0.182444
C	2.057609	1.257338	1.488459
C	3.302426	1.856525	1.718678
C	4.022376	2.459723	0.684834
C	3.505342	2.467037	-0.613030
H	1.829568	1.960097	-1.854664
H	3.733611	1.825623	2.715574
H	4.989762	2.910477	0.891191
H	4.066832	2.915420	-1.428365
C	1.303002	0.459431	2.546695
C	0.649571	-1.165681	-2.277682
C	1.425848	-1.947359	-1.334349
C	0.521731	-2.604581	-0.439598
C	-0.735294	-1.366263	-1.994757
C	-0.822486	-2.248770	-0.852557
Rh	0.198705	-0.320002	-0.122042
C	1.196380	-0.397253	-3.446836
H	2.175649	0.023372	-3.223582
H	1.332836	-1.069980	-4.303666
H	0.517554	0.403296	-3.755043
C	-1.873414	-0.803582	-2.798827
H	-2.347239	-1.590835	-3.397035

H	-2.649811	-0.382905	-2.156596
H	-1.522875	-0.027126	-3.483985
C	0.862790	-3.500996	0.710921
H	0.830253	-2.911201	1.637198
H	0.126138	-4.299460	0.803994
H	1.865704	-3.910630	0.600280
C	-2.043411	-2.820123	-0.240143
O	-2.068670	-3.519554	0.756493
C	2.902811	-1.991623	-1.361719
O	3.576576	-1.655588	-2.321456
O	-3.162874	-2.501238	-0.932845
O	3.453650	-2.439096	-0.209976
C	-4.399276	-3.025387	-0.398678
H	-4.486873	-2.720732	0.647454
H	-4.357740	-4.119426	-0.428181
C	-5.532531	-2.474760	-1.244679
H	-5.415228	-2.759065	-2.295705
H	-6.488328	-2.872931	-0.886110
H	-5.570178	-1.382555	-1.180061
C	4.897405	-2.499146	-0.191838
H	5.291406	-1.493058	-0.366181
H	5.236542	-3.135190	-1.015927
C	5.316304	-3.046308	1.160313
H	6.409409	-3.099810	1.214855
H	4.961881	-2.401187	1.970640
H	4.914715	-4.052277	1.320337
C	-1.243782	1.013566	0.418555
C	-0.394984	1.902163	0.021089
C	-2.563145	0.790232	0.981915
C	-2.761727	-0.235931	1.924608
C	-3.650869	1.607462	0.615976
C	-4.021731	-0.433024	2.487707
H	-1.910066	-0.841018	2.217302
C	-4.908368	1.397322	1.179329
H	-3.502430	2.405672	-0.104907
C	-5.098578	0.377131	2.115696
H	-4.160320	-1.221131	3.223081
H	-5.740205	2.033972	0.889213
H	-6.079554	0.218477	2.555915
C	-0.394417	3.258682	-0.532086
C	0.379499	4.289043	0.030397
C	-1.249967	3.560062	-1.607211
C	0.280828	5.589040	-0.458744
H	1.047973	4.062097	0.854174
C	-1.336573	4.861919	-2.101811
H	-1.837382	2.762678	-2.053136
C	-0.573710	5.879655	-1.526925
H	0.873743	6.379343	-0.006494
H	-1.998477	5.078770	-2.935939
H	-0.641660	6.894395	-1.909632
O	0.480536	-0.490803	1.896778

C	2.271177	-0.349702	3.439302
H	2.898285	0.289385	4.072390
H	1.678419	-0.997885	4.092890
H	2.915141	-0.981742	2.819957
C	0.460463	1.400840	3.442290
H	-0.117358	0.800931	4.154160
H	1.099735	2.090028	4.008538
H	-0.240335	1.990358	2.846159

TS6a

B3LYP SCF energy: -1463.26164774 a.u.
B3LYP enthalpy: -1462.640611 a.u.
B3LYP free energy: -1462.738575 a.u.
M06 SCF energy in solution: -1463.83959655 a.u.
M06 enthalpy in solution: -1463.218560 a.u.
M06 free energy in solution: -1463.316524 a.u.
Three lowest frequencies (cm-1): -329.3125 24.2817 27.7734
Imaginary frequency: -329.3125 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.263271	-2.046120	-1.569968
C	-1.845476	-1.429164	-0.377595
C	-1.314746	-2.236965	0.657295
C	-1.291405	-3.627043	0.487045
C	-1.749577	-4.229252	-0.686856
C	-2.223906	-3.431988	-1.727739
H	-2.621709	-1.422523	-2.383939
H	-0.912124	-4.262603	1.280499
H	-1.722958	-5.311208	-0.787522
H	-2.562139	-3.882586	-2.657640
C	-0.847774	-1.582910	1.970581
C	2.262570	-1.574268	-0.888054
C	1.995330	-0.564810	-1.863577
C	2.723133	0.602437	-1.459643
C	3.305086	-1.074482	0.025806
C	3.596463	0.244289	-0.336693
Rh	1.288902	0.144137	0.184055
C	1.122252	-0.701889	-3.075976
H	1.706045	-1.037844	-3.944973
H	0.320146	-1.425896	-2.910031
H	0.654405	0.250502	-3.343656
C	1.833378	-3.008221	-0.969171
H	0.864309	-3.120677	-1.459016
H	2.572951	-3.586600	-1.543059
H	1.758040	-3.466884	0.019672
C	3.951361	-1.890446	1.106388
H	4.681945	-2.594467	0.683443
H	4.478979	-1.259571	1.827526

H	3.216927	-2.482746	1.661232
C	4.594339	1.176717	0.282722
H	4.949689	0.807479	1.248987
H	5.471229	1.301611	-0.368135
H	4.164692	2.172173	0.441573
C	2.821562	1.889513	-2.224032
H	2.923363	2.752618	-1.559605
H	3.699907	1.874602	-2.885156
H	1.939975	2.054956	-2.848445
C	-0.762108	0.578684	0.327460
C	-1.914012	0.047246	-0.178230
C	-0.154136	1.880652	0.476360
C	0.754667	2.117752	1.555754
C	-0.251490	2.870639	-0.557868
C	1.523053	3.308481	1.575429
H	0.705932	1.489667	2.435609
C	0.489927	4.026714	-0.493089
H	-0.943057	2.697543	-1.375730
C	1.399637	4.248471	0.572682
H	2.185512	3.489167	2.418072
H	0.379289	4.779950	-1.268962
H	1.974850	5.169787	0.607596
C	-3.201459	0.776387	-0.265451
C	-3.354660	2.103976	0.204392
C	-4.371650	0.162078	-0.770555
C	-4.569720	2.778215	0.127781
H	-2.515735	2.616741	0.658445
C	-5.587922	0.839666	-0.843914
H	-4.339952	-0.870557	-1.094573
C	-5.701871	2.159364	-0.407720
H	-4.631961	3.796978	0.504131
H	-6.456580	0.320120	-1.242434
H	-6.649383	2.687641	-0.468517
O	-0.099373	-0.373601	1.755414
C	-2.078539	-1.191670	2.822903
H	-2.658535	-2.082857	3.088943
H	-1.744393	-0.702773	3.744947
H	-2.730607	-0.503173	2.281737
C	0.066657	-2.492805	2.808281
H	0.449276	-1.913325	3.653769
H	-0.468081	-3.360733	3.209293
H	0.919985	-2.847378	2.221656

TS6b
B3LYP SCF energy: -1919.01867135 a.u.
B3LYP enthalpy: -1918.302149 a.u.
B3LYP free energy: -1918.424701 a.u.
M06 SCF energy in solution: -1919.54874459 a.u.
M06 enthalpy in solution: -1918.832222 a.u.

M06 free energy in solution: -1918.954774 a.u.
Three lowest frequencies (cm-1): -171.3180 12.9263 15.1848
Imaginary frequency: -171.3180 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.375064	-3.029372	-0.241609
C	-0.613013	-2.155748	0.567768
C	-1.190324	-1.687969	1.783529
C	-2.464440	-2.145714	2.138515
C	-3.194325	-3.022719	1.334411
C	-2.645594	-3.458143	0.128846
H	-0.945267	-3.383156	-1.173357
H	-2.905303	-1.802421	3.067737
H	-4.179346	-3.356892	1.649377
H	-3.196286	-4.135370	-0.519053
C	-0.430032	-0.698116	2.673816
C	-1.653688	0.932922	-1.882281
C	-2.232080	1.532673	-0.704015
C	-1.242087	2.406745	-0.135026
C	-0.380849	1.551321	-2.144677
C	-0.121452	2.469935	-1.072069
Rh	-0.232553	0.391845	-0.151280
C	-2.288878	-0.100333	-2.768433
H	-2.705500	-0.923528	-2.184673
H	-3.117278	0.344278	-3.332181
H	-1.568150	-0.505019	-3.482814
C	0.445343	1.332301	-3.380671
H	0.361851	0.301992	-3.737980
H	0.097536	1.991195	-4.188177
H	1.494063	1.568239	-3.208652
C	-1.409718	3.256563	1.091868
H	-0.566620	3.124957	1.772446
H	-1.431192	4.314377	0.803798
H	-2.336796	3.001827	1.600391
C	1.042526	3.380767	-1.027438
O	1.854171	3.502573	-1.932846
C	-3.529605	1.216000	-0.080455
O	-3.897976	1.572791	1.027789
O	1.126742	4.080422	0.121448
O	-4.323133	0.475096	-0.894436
C	2.260963	4.970149	0.238870
H	2.234185	5.686410	-0.588551
H	3.177829	4.380809	0.140679
C	2.165790	5.652152	1.590901
H	2.187538	4.916635	2.401264
H	3.013096	6.334479	1.720772
H	1.241065	6.232286	1.674398
C	-5.586787	0.065575	-0.329478
H	-6.152497	0.956855	-0.040195
H	-5.393145	-0.515065	0.578110

C	-6.312303	-0.753314	-1.381619
H	-7.284202	-1.078279	-0.993938
H	-6.483794	-0.164428	-2.288734
H	-5.734480	-1.643459	-1.651128
C	1.408155	-0.639151	0.222576
C	0.808415	-1.873829	0.128946
C	2.814548	-0.277302	0.294067
C	3.685157	-1.001643	1.135802
C	3.335771	0.807738	-0.434390
C	5.029226	-0.655743	1.233826
H	3.292653	-1.833712	1.710519
C	4.683869	1.146240	-0.341126
H	2.684096	1.375760	-1.085453
C	5.534604	0.418653	0.494971
H	5.684954	-1.222903	1.889038
H	5.067565	1.979690	-0.923411
H	6.584953	0.686926	0.572665
C	1.547441	-3.003931	-0.515261
C	1.519375	-4.283980	0.070335
C	2.308758	-2.822954	-1.681956
C	2.246629	-5.337009	-0.480474
H	0.927566	-4.446828	0.966289
C	3.031315	-3.879922	-2.236400
H	2.330018	-1.846558	-2.156084
C	3.005746	-5.140326	-1.637485
H	2.221248	-6.313846	-0.004383
H	3.610682	-3.717417	-3.141498
H	3.567260	-5.964007	-2.070084
O	0.314987	0.207055	1.870435
C	-1.369295	0.148817	3.558674
H	-1.848841	-0.436762	4.352304
H	-0.766905	0.927652	4.036724
H	-2.144706	0.630443	2.955455
C	0.565939	-1.464121	3.577151
H	1.177243	-0.746815	4.135485
H	0.037117	-2.106544	4.291522
H	1.234115	-2.091583	2.979780

TS7a
B3LYP SCF energy: -1168.18310202 a.u.
B3LYP enthalpy: -1167.725123 a.u.
B3LYP free energy: -1167.812582 a.u.
M06 SCF energy in solution: -1169.01213920 a.u.
M06 enthalpy in solution: -1168.554160 a.u.
M06 free energy in solution: -1168.641619 a.u.
Three lowest frequencies (cm-1): -644.3082 25.9945 40.8680
Imaginary frequency: -644.3082 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.703472	-2.272543	-0.491199
C	0.716479	-2.344256	-0.652269
C	1.328003	-1.988875	0.626065
C	0.274062	-1.726664	1.568709
C	-0.982292	-1.833121	0.866164
C	-1.741482	-2.597008	-1.516562
H	-1.322125	-2.633682	-2.524047
H	-2.175548	-3.581712	-1.296773
H	-2.559171	-1.869577	-1.511520
C	1.478486	-2.755598	-1.872743
H	2.308873	-2.069438	-2.062900
H	1.895536	-3.761708	-1.736066
H	0.843389	-2.773635	-2.761005
C	0.417242	-1.424977	3.024205
H	-0.245876	-0.611345	3.335123
H	0.136952	-2.314335	3.604917
H	1.443829	-1.165214	3.291757
Rh	0.218340	-0.268470	-0.152083
C	-2.656433	1.538171	0.248194
C	-1.306830	1.589104	-0.198273
C	-1.036727	1.381883	-1.588229
C	-2.087830	1.079693	-2.478267
C	-3.391420	1.011723	-2.020258
C	-3.665203	1.269442	-0.658603
H	-1.864074	0.953816	-3.533381
H	-4.207064	0.808872	-2.707506
H	-4.694864	1.262757	-0.311896
N	-0.164816	1.785865	0.605943
C	-0.224716	1.877551	2.022048
O	-1.177991	1.506338	2.688435
C	1.017691	2.480183	2.639501
H	0.997581	2.322679	3.718716
H	1.932362	2.060586	2.210036
H	1.037255	3.558860	2.440419
C	-2.333953	-1.712574	1.497182
H	-3.108562	-1.501991	0.756816
H	-2.594045	-2.656868	1.994648
H	-2.352726	-0.918174	2.247618
C	2.797531	-2.012013	0.900255
H	3.359908	-1.596692	0.059805
H	3.053546	-1.446707	1.799204
H	3.132783	-3.047295	1.048348
H	-0.066444	1.632911	-1.997652
H	-2.877912	1.720244	1.289520
C	3.748256	1.979531	-1.852624
H	3.596850	2.810086	-2.549431
H	4.493304	2.307582	-1.119820
H	4.114154	1.103273	-2.388481
C	2.453243	1.679778	-1.143803
O	1.969479	0.511608	-1.202059

O	1.899201	2.651748	-0.514018
H	0.921170	2.312683	0.009853

TS7b

B3LYP SCF energy: -1623.91651318 a.u.
B3LYP enthalpy: -1623.362863 a.u.
B3LYP free energy: -1623.470858 a.u.
M06 SCF energy in solution: -1624.69801838 a.u.
M06 enthalpy in solution: -1624.144368 a.u.
M06 free energy in solution: -1624.252363 a.u.
Three lowest frequencies (cm-1): -580.6138 19.7491 23.5036
Imaginary frequency: -580.6138 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.277442	0.886971	-1.657528
C	-0.101243	1.013661	-2.000787
C	-0.810560	1.455496	-0.802463
C	0.145769	1.705945	0.253188
C	1.419033	1.269752	-0.254332
C	2.394428	0.446968	-2.548293
H	2.020174	-0.035622	-3.452821
H	2.997580	1.314576	-2.839105
H	3.050123	-0.254362	-2.026888
C	-0.710305	0.754627	-3.341351
H	-1.601804	0.130097	-3.261137
H	-1.037425	1.705049	-3.779749
H	0.006416	0.288621	-4.020181
C	-0.104916	2.308526	1.596696
H	-0.415198	3.351762	1.463250
H	-0.924865	1.806800	2.116760
H	0.795192	2.274081	2.209881
Rh	0.144574	-0.491818	-0.327714
C	-2.278339	1.760841	-0.796986
O	-2.987674	1.592877	-1.768218
O	-2.686622	2.239830	0.378569
C	-4.103950	2.575091	0.492141
H	-4.319579	3.373109	-0.224138
H	-4.683383	1.694476	0.202270
C	-4.358230	2.990245	1.926787
H	-5.419053	3.230639	2.052030
H	-4.102187	2.182186	2.619123
H	-3.775188	3.877803	2.191566
C	2.687026	1.290857	0.547541
O	2.742538	0.952588	1.713423
O	3.709632	1.746380	-0.174264
C	4.999417	1.849248	0.513169
H	5.278322	0.848204	0.854113
H	4.859795	2.482279	1.393325

C	5.995263	2.429471	-0.469395
H	5.685182	3.423616	-0.805300
H	6.970735	2.522770	0.018911
H	6.112645	1.782928	-1.344586
C	-3.056126	-1.340374	0.379288
C	-1.713940	-1.814830	0.349954
C	-1.240633	-2.468241	-0.837210
C	-2.080868	-2.582608	-1.967359
C	-3.369776	-2.089218	-1.926937
C	-3.853255	-1.494190	-0.738142
H	-3.428484	-0.872265	1.277920
H	-0.333598	-3.058475	-0.804819
H	-1.713301	-3.106329	-2.844626
H	-4.027104	-2.190827	-2.784622
H	-4.882005	-1.148089	-0.702289
N	-0.732527	-1.636947	1.341581
C	-0.957024	-0.920993	2.557144
O	-1.974024	-0.291015	2.787864
C	0.204420	-1.000420	3.521101
H	0.476376	-2.041202	3.726105
H	1.087620	-0.505668	3.098783
H	-0.077012	-0.504774	4.451043
C	3.321987	-3.584544	0.301469
H	3.122368	-4.660013	0.286856
H	3.865856	-3.286779	-0.595410
H	3.932482	-3.379748	1.188197
C	2.023580	-2.832831	0.422228
O	1.216607	-3.205121	1.345554
O	1.784608	-1.883522	-0.383224
H	0.285462	-2.527240	1.374443

TS8a

B3LYP SCF energy: -1167.73969821 a.u.
B3LYP enthalpy: -1167.295733 a.u.
B3LYP free energy: -1167.384641 a.u.
M06 SCF energy in solution: -1168.52232764 a.u.
M06 enthalpy in solution: -1168.078362 a.u.
M06 free energy in solution: -1168.167270 a.u.
Three lowest frequencies (cm-1): -1182.8474 12.2003 40.1792
Imaginary frequency: -1182.8474 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.512661	-1.489405	-1.268322
C	2.448863	-0.508014	-0.842923
C	2.520406	-0.542134	0.616221
C	1.613072	-1.534773	1.072134
C	0.918031	-2.079793	-0.079737
C	1.216902	-1.892304	-2.682514

H	1.362881	-1.063656	-3.381094
H	1.886185	-2.707970	-2.989524
H	0.189501	-2.246592	-2.792103
C	3.294850	0.378002	-1.708265
H	3.259494	1.414766	-1.358252
H	4.344207	0.054172	-1.689270
H	2.960501	0.363796	-2.748979
C	1.406968	-1.983231	2.487677
H	0.360056	-2.228290	2.686184
H	1.999939	-2.887386	2.683231
H	1.716686	-1.221635	3.206933
Rh	0.418966	0.056017	-0.055737
C	-3.480379	-0.584095	0.298013
C	-2.184527	-0.042545	0.193073
C	-1.516492	0.051888	-1.062313
C	-2.119681	-0.517687	-2.200984
C	-3.404857	-1.047493	-2.109991
C	-4.070175	-1.065612	-0.868914
H	-1.620468	-0.471230	-3.167475
H	-3.907049	-1.426555	-2.996547
H	-5.075481	-1.478519	-0.816933
N	-1.284246	0.366574	1.163569
C	-1.576694	0.526412	2.491509
O	-2.697832	0.344939	2.972271
C	-0.429450	1.009324	3.367599
H	0.464445	1.259381	2.791776
H	-0.765799	1.894708	3.917215
H	-0.187683	0.244559	4.114731
C	-0.049230	-3.227206	-0.055587
H	-0.733589	-3.188757	-0.907207
H	0.479596	-4.190104	-0.089015
H	-0.659035	-3.212733	0.852132
C	3.448064	0.300062	1.440057
H	3.440392	1.340607	1.099676
H	3.167193	0.293919	2.496558
H	4.481554	-0.066214	1.367450
H	-1.124103	1.327526	-1.354021
H	-3.976179	-0.634857	1.258010
C	0.355633	4.425260	-0.847488
H	0.309421	4.812690	-1.868850
H	-0.411795	4.943957	-0.261785
H	1.334126	4.622389	-0.406202
C	0.050873	2.941379	-0.841143
O	0.752418	2.188718	-0.107965
O	-0.915558	2.548470	-1.573316

TS8b
B3LYP SCF energy: -1623.48339625 a.u.
B3LYP enthalpy: -1622.943550 a.u.

B3LYP free energy: -1623.052908 a.u.
M06 SCF energy in solution: -1624.21591298 a.u.
M06 enthalpy in solution: -1623.676067 a.u.
M06 free energy in solution: -1623.785425 a.u.
Three lowest frequencies (cm-1): -1124.3128 17.0723 24.4290
Imaginary frequency: -1124.3128 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.508902	-1.591803	1.499020
C	-0.866116	-1.387559	1.788131
C	-1.624937	-1.474256	0.542791
C	-0.701527	-1.711731	-0.529460
C	0.622820	-1.745763	0.051286
C	1.609085	-1.708297	2.514797
H	1.312250	-1.267423	3.469088
H	1.848773	-2.764850	2.690383
H	2.523415	-1.225164	2.173658
C	-1.455145	-1.146165	3.145907
H	-2.120480	-0.280626	3.131826
H	-2.060378	-2.005290	3.453410
H	-0.674289	-0.981585	3.891840
C	-0.997238	-1.955553	-1.980869
H	-0.413108	-1.287197	-2.615445
H	-0.684029	-2.972796	-2.243882
H	-2.057240	-1.842382	-2.191140
Rh	-0.128157	0.311460	0.432979
C	-3.103589	-1.386436	0.520340
O	-3.792528	-1.355503	1.524046
O	-3.632629	-1.354471	-0.724223
C	-5.078121	-1.281059	-0.788217
H	-5.496150	-2.124132	-0.229891
H	-5.402468	-0.360878	-0.292703
C	-5.474875	-1.310952	-2.252368
H	-6.565542	-1.255146	-2.338657
H	-5.044216	-0.463294	-2.794822
H	-5.140218	-2.236432	-2.732298
C	1.842241	-2.042818	-0.747237
O	1.870704	-2.096788	-1.961274
O	2.923683	-2.271322	0.026673
C	4.160771	-2.512543	-0.687405
H	4.381761	-1.632350	-1.298393
H	4.017160	-3.363118	-1.360385
C	5.239875	-2.776458	0.345802
H	4.991329	-3.646850	0.961795
H	6.192546	-2.972856	-0.158060
H	5.372666	-1.911985	1.004468
C	1.727774	1.369781	0.156518
C	1.326304	1.790747	-1.149109
C	2.274508	2.171904	-2.121233
C	3.616172	2.050219	-1.779865

C	4.039991	1.544942	-0.529804
C	3.101712	1.165176	0.421297
H	1.241763	2.191849	1.093491
H	1.954501	2.509539	-3.097618
H	4.369915	2.340352	-2.508619
H	5.102313	1.481318	-0.308903
H	3.426885	0.813015	1.397730
N	-0.036058	1.623640	-1.214793
C	-0.848549	2.050659	-2.241530
O	-0.422906	2.665844	-3.217311
C	-2.327062	1.762974	-2.050802
H	-2.680701	2.212886	-1.115925
H	-2.879859	2.181643	-2.894213
H	-2.521696	0.688137	-1.982085
C	-1.308556	3.806514	2.839595
H	-1.492766	4.688391	2.215398
H	-2.265582	3.373354	3.134544
H	-0.745220	4.132666	3.717600
C	-0.491069	2.812645	2.041986
O	0.750161	3.047205	1.908628
O	-1.100497	1.819411	1.542196

TS9a

B3LYP SCF energy: -1153.31260041 a.u.
B3LYP enthalpy: -1152.820115 a.u.
B3LYP free energy: -1152.908622 a.u.
M06 SCF energy in solution: -1154.12250013 a.u.
M06 enthalpy in solution: -1153.630015 a.u.
M06 free energy in solution: -1153.718522 a.u.
Three lowest frequencies (cm-1): -1103.8720 17.7816 43.9485
Imaginary frequency: -1103.8720 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.610932	-0.441285	-2.183734
C	-1.420531	0.033760	-0.866785
C	-2.412444	-0.276228	0.108306
C	-3.530299	-1.031288	-0.255616
C	-3.684792	-1.489822	-1.567259
C	-2.728547	-1.190178	-2.540640
H	-0.883560	-0.173745	-2.946708
H	-4.298540	-1.267477	0.474447
H	-4.564042	-2.071723	-1.829022
H	-2.863875	-1.527873	-3.564034
C	-2.281040	0.280200	1.523400
C	2.795103	-0.220142	0.194460
C	2.192475	-0.993925	1.219709
C	1.287166	-1.957537	0.589453
C	2.233125	-0.652353	-1.082048

C	1.381971	-1.794922	-0.827092
Rh	0.565092	0.079410	0.097981
O	-1.035622	2.622517	-1.109757
C	0.037050	3.000611	-0.549502
O	0.810762	2.212522	0.089603
C	0.425210	4.456798	-0.652784
H	0.785576	4.652300	-1.669437
H	-0.451264	5.089460	-0.491121
H	1.214141	4.702658	0.059351
H	-1.129366	1.322105	-0.954404
C	2.434298	-0.902338	2.694581
H	1.495459	-0.944916	3.255380
H	3.053577	-1.746099	3.026161
H	2.951844	0.019658	2.967958
C	0.544558	-3.039458	1.311536
H	1.199362	-3.908349	1.462946
H	0.209410	-2.707156	2.297616
H	-0.328400	-3.376146	0.746950
C	0.781357	-2.698778	-1.856891
H	0.665267	-2.202417	-2.821922
H	1.450406	-3.557409	-2.005374
H	-0.193566	-3.084496	-1.551144
C	2.672183	-0.152744	-2.424858
H	3.572912	-0.689105	-2.752915
H	1.902878	-0.303806	-3.186601
H	2.915130	0.912674	-2.393643
C	3.784915	0.890820	0.349361
H	4.727171	0.627326	-0.146857
H	3.410315	1.813492	-0.105269
H	4.002817	1.097632	1.398960
C	-3.032827	1.612366	1.655097
H	-4.104920	1.454354	1.506286
H	-2.895121	2.036551	2.657524
H	-2.696445	2.331090	0.900590
C	-2.696979	-0.708888	2.616268
H	-2.480199	-0.281740	3.599891
H	-3.768596	-0.922207	2.571940
H	-2.153053	-1.652665	2.515935
O	-0.837379	0.534556	1.756788
H	-0.702663	1.479806	1.944524

TS9b
B3LYP SCF energy: -1609.04824767 a.u.
B3LYP enthalpy: -1608.460368 a.u.
B3LYP free energy: -1608.570535 a.u.
M06 SCF energy in solution: -1609.80809352 a.u.
M06 enthalpy in solution: -1609.220214 a.u.
M06 free energy in solution: -1609.330381 a.u.
Three lowest frequencies (cm-1): -1068.4889 13.1447 21.7267

Imaginary frequency: -1068.4889 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.002425	0.654378	2.499402
C	0.141706	1.283936	1.242336
C	1.253338	2.154280	1.042361
C	2.153258	2.374287	2.086963
C	1.979072	1.741622	3.321851
C	0.897872	0.882544	3.535795
H	-0.863226	0.011888	2.663359
H	2.999421	3.041356	1.954196
H	2.689151	1.931027	4.122018
H	0.758018	0.408278	4.502880
C	1.408136	2.885777	-0.286023
C	0.151372	-1.851968	0.023982
C	-1.138377	-1.742833	-0.620176
C	-0.941192	-1.430522	-2.035560
C	1.113880	-1.395275	-0.936124
C	0.440597	-1.176947	-2.221744
Rh	-0.320762	0.263653	-0.642980
O	-2.177897	2.460199	0.824999
C	-2.656808	2.145663	-0.302058
O	-2.062048	1.371918	-1.129998
C	-4.006458	2.689088	-0.706421
H	-4.765929	1.925427	-0.500793
H	-4.246450	3.584197	-0.130877
H	-4.027671	2.898784	-1.778369
H	-1.027236	1.817017	0.962584
C	-2.026268	-1.337543	-3.060195
H	-2.848250	-0.712492	-2.700395
H	-1.654203	-0.922588	-3.998945
H	-2.439114	-2.333451	-3.251221
C	1.120055	-0.787311	-3.496546
H	1.922136	-0.072294	-3.309289
H	1.574276	-1.676757	-3.953649
H	0.414119	-0.367069	-4.215849
C	0.429055	-2.403747	1.386046
H	0.749464	-3.446884	1.266294
H	1.241432	-1.873282	1.881976
H	-0.463804	-2.384941	2.008642
C	2.596197	-1.280729	-0.758002
O	3.280448	-0.479315	-1.363411
C	-2.474668	-2.123457	-0.059942
O	-3.329058	-2.654295	-0.735738
O	-2.610263	-1.810928	1.238075
O	3.065175	-2.175293	0.116828
C	-3.883806	-2.189903	1.850239
H	-4.685903	-1.704386	1.287935
H	-4.002685	-3.271495	1.742407
C	-3.847519	-1.751964	3.299917

H	-4.792448	-2.021811	3.782695
H	-3.036645	-2.246363	3.844628
H	-3.720679	-0.667702	3.384041
C	4.510500	-2.166076	0.337969
H	4.785280	-1.184968	0.736128
H	5.000398	-2.287308	-0.631732
C	4.833803	-3.293871	1.296457
H	5.913462	-3.316854	1.476966
H	4.330266	-3.155440	2.258442
H	4.536681	-4.261697	0.881142
O	0.681944	2.075452	-1.304212
C	0.750598	4.271015	-0.220486
H	1.278561	4.899586	0.502528
H	0.805433	4.770612	-1.195672
H	-0.293908	4.201515	0.101282
C	2.850465	2.961296	-0.792899
H	2.866132	3.444414	-1.774685
H	3.472700	3.556737	-0.118337
H	3.280238	1.961355	-0.889297
H	-0.015399	2.618881	-1.712118