Electronic Supplementary Information

Mechanism of Co(III)-catalyzed annulations of N-chlorobenzamides with styrene and origin of cyclopentadienyl ligand-controlled enantioselectivity

Han Gao,[a] Wujie Wang,[b] Xiangying Lv,[a] Gang Lu,*[a,b] and Yuliang Li*[b]

[a] School of Chemistry and Chemical Engineering, Key Laboratory of Colloid and Interface Chemistry, Ministry of Education, Shandong University, Jinan, Shandong 250100, China

[b] Department of Interventional Medicine, The Second Hospital of Shandong University, Jinan, Shandong 250033, China

Corresponding Author: ganglu@sdu.edu.cn; lyl.pro@sdu.edu.cn

Table of Contents

Less Favorable Pathways for Singlet Co Complexes and the Minor Product

As shown in Fig. S1, the singlet catalyst-substrate complex (**int1^{S}**) is 11.5 kcal/mol less stable than the triplet complex (**int1^{T}**). The same trend is observed for the subsequent transition states of C–H activation (**TS1^{S}** vs **TS1^{T}**) and the stability of the formed five-membered aza-cobaltacycle intermediates (**int2^{S}** vs **int2^{T}**). Fig. S2 shows the singlet energy profile for the generation of **2a** from the seven-membered aza-cobaltacycle (**int3^{S}**). All these singlet intermediates and transition states are higher in energy than those in triplet states (Fig. 2 in the main text).

For the minor product **2b**, the triplet energy profile from the seven-membered aza-cobaltacycle (**int4^{T}**) is shown in Fig. S3. The energetics are lower than that of the styrene insertion (**TS3^{S}**, Fig. 1 in the main text), which indicates the irreversibility of the styrene insertion step, thus determining the enantioselectivity.

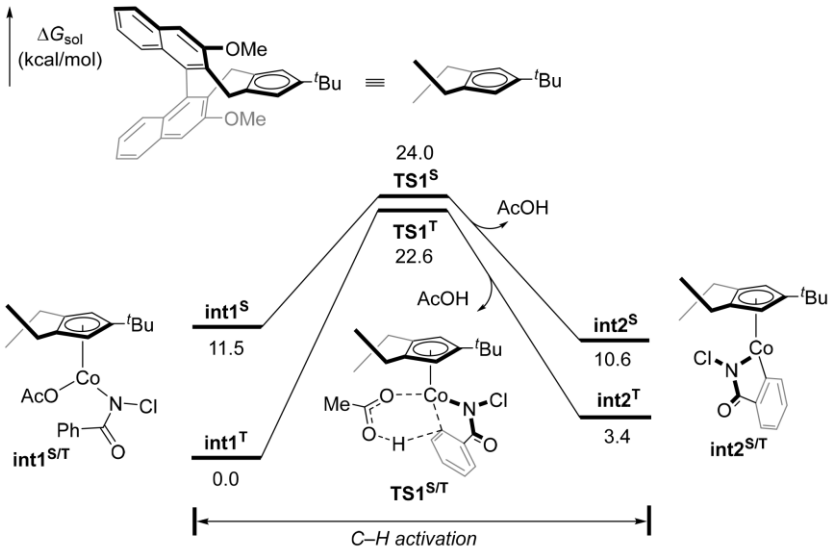

Fig. S1 Comparison of singlet and triplet energy profiles for C–H activation with **L3**.

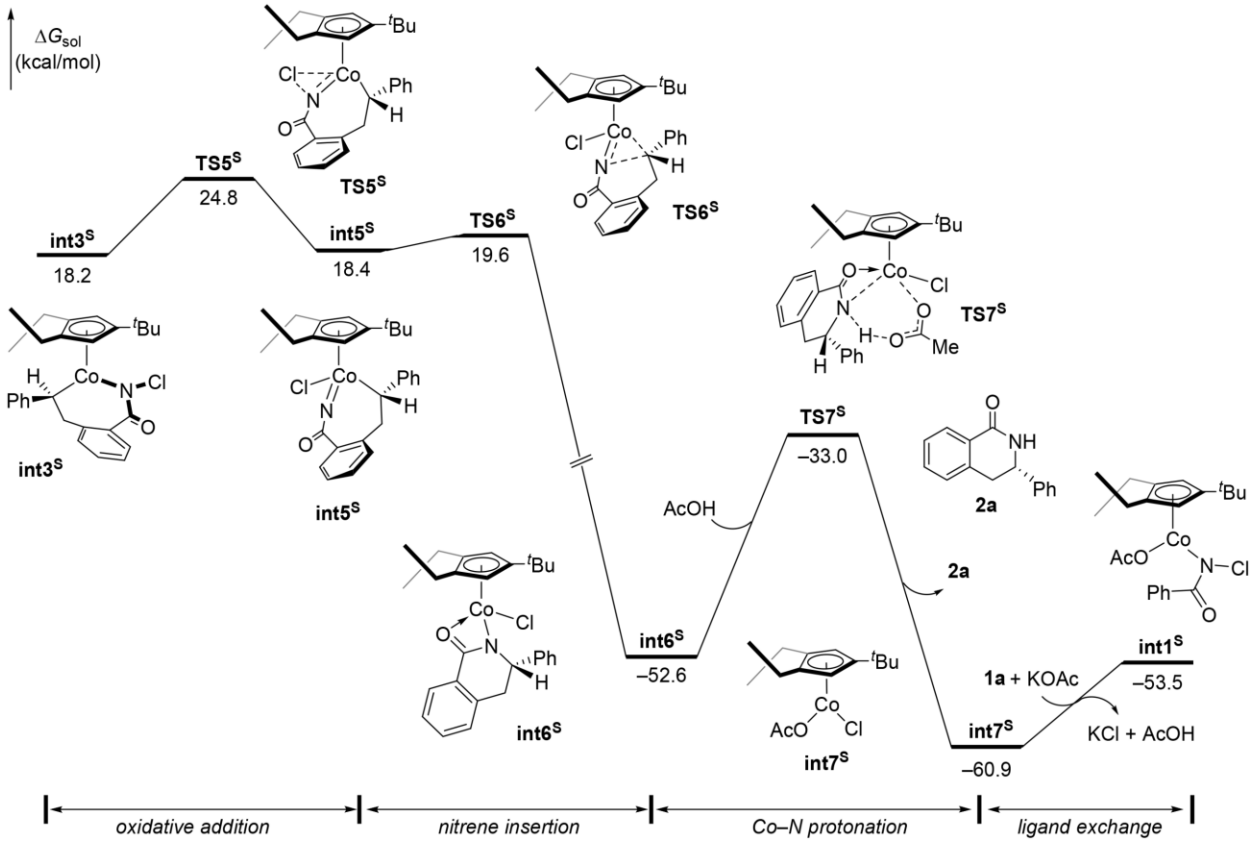

Fig. S2 Less favorable singlet energy profile with **L3** for the major product **2a**.

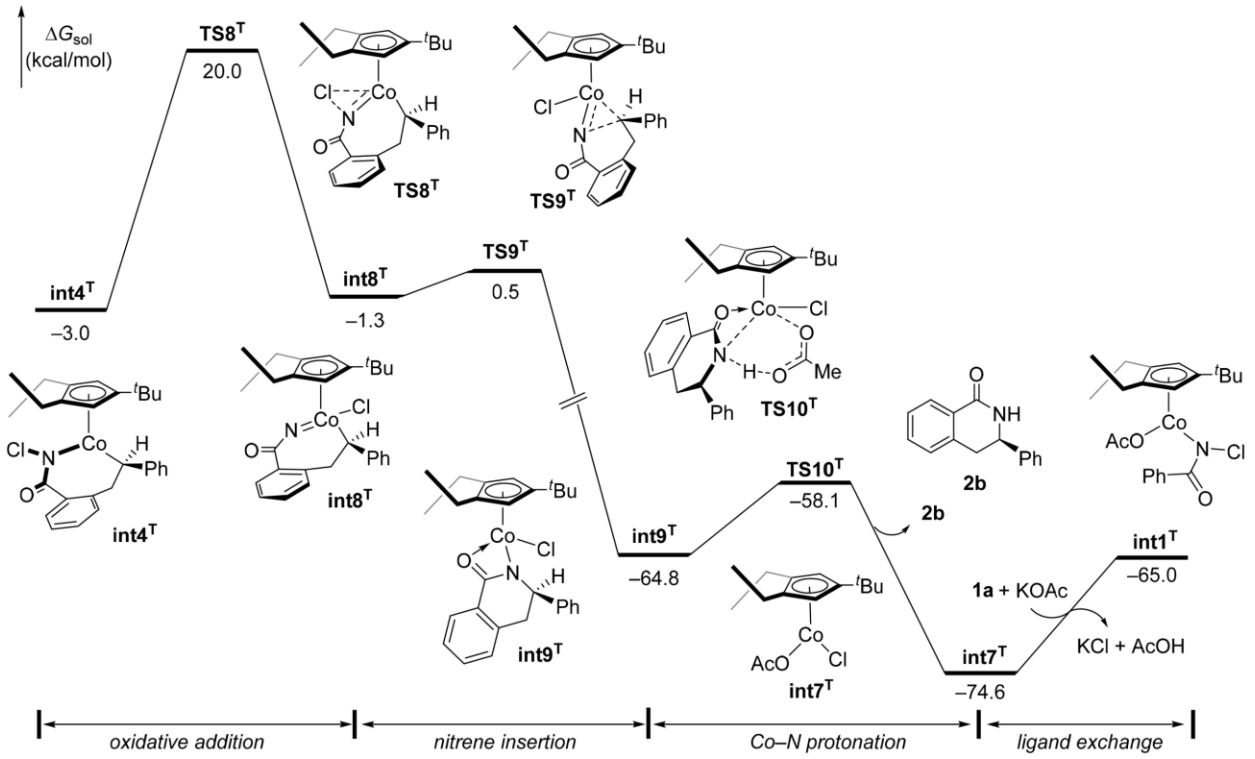

Fig. S3 Triplet energy profile with **L3** for the minor product **2b**.

Conformational Search for the Migratory Insertion Transition States with L1~L3

A series of different conformers for the styrene insertion transition states with **L1**~**L3** ligands are computed. For the transition states with **L3** (Fig. S4), based on the general enantiocontrol model for chiral BINOL-Cp ligands, the enantiomeric products **2a** (major) and **2b** (minor) are generated from **TS2^{S}-1** and **TS3^{S}**, respectively. Styrene approaches the Co center from the ^{t}Bu side in these transition states. However, the barrier difference between **TS2^{S}-1** and **TS3^{S}** is only 0.7 kcal/mol, which cannot account for the excellent enantioselectivity observed experimentally (er of **2a**:**2b** = 99.5:0.5). We thus considered whether styrene can attack the Co–C bond from the binaphthyl side. The computed **TS2^{S}** has a much lower barrier than **TS3^{S}**, and the large barrier difference ($\Delta\Delta G^{\ddagger}$ = 5.7 kcal/mol) is well consistent with the high-level enantiocontrol. Other possible conformers are also considered. For the transition states with **L2** and **L1** (Fig. S5 and S6), the styrene insertion from the binaphthyl side is also the most stable geometry for the generation of enantiomer **2a**. In this styrene insertion into Co–C(aryl) with chiral BINOL-Cp ligands, the enantiocontrol model shows that the orientations of styrene incorporation are different in the two enantiomeric transition states.

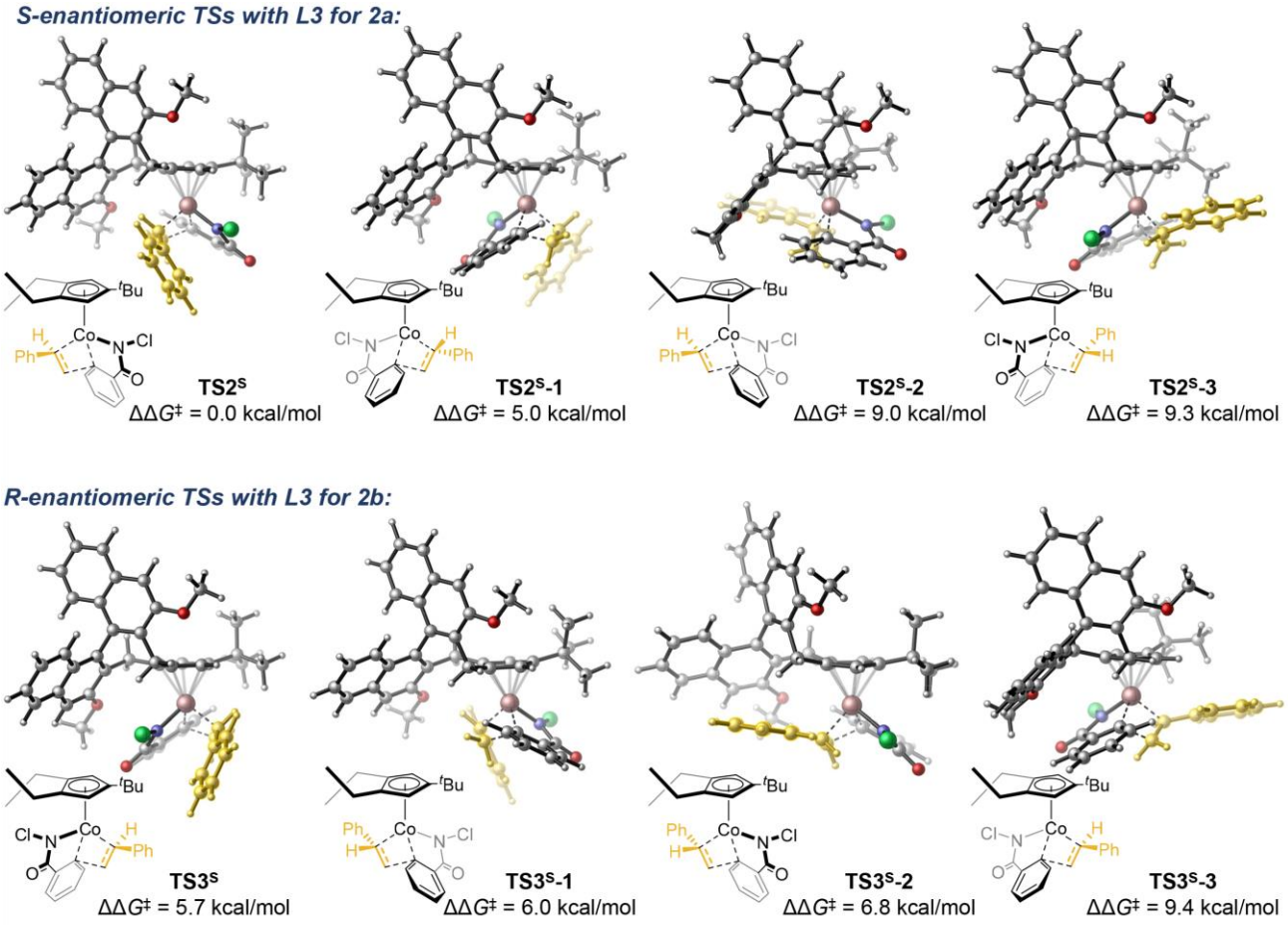

Fig. S4 Conformers of styrene insertion transition states with **L3**.

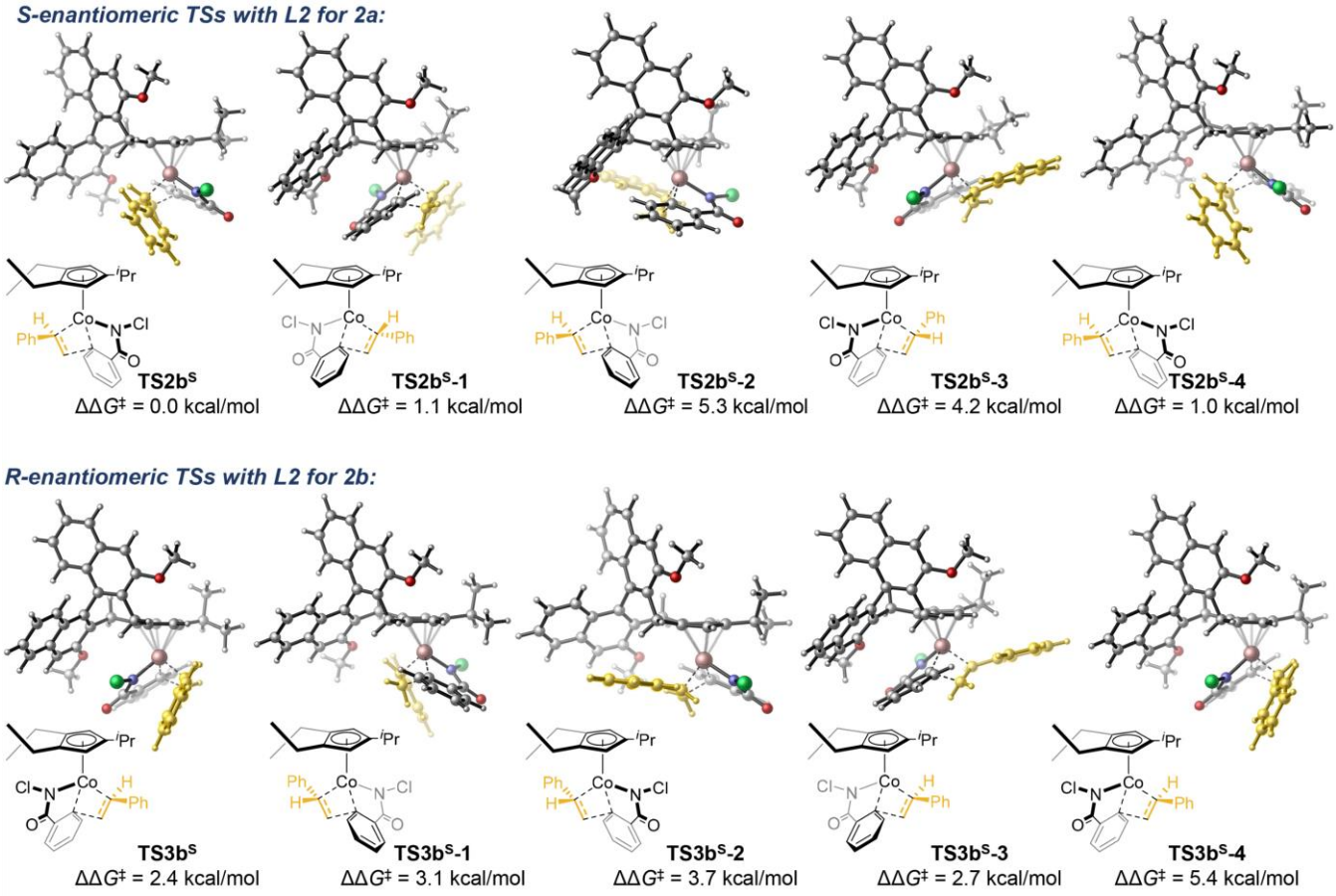

Fig. S5 Conformers of styrene insertion transition states with **L2**.

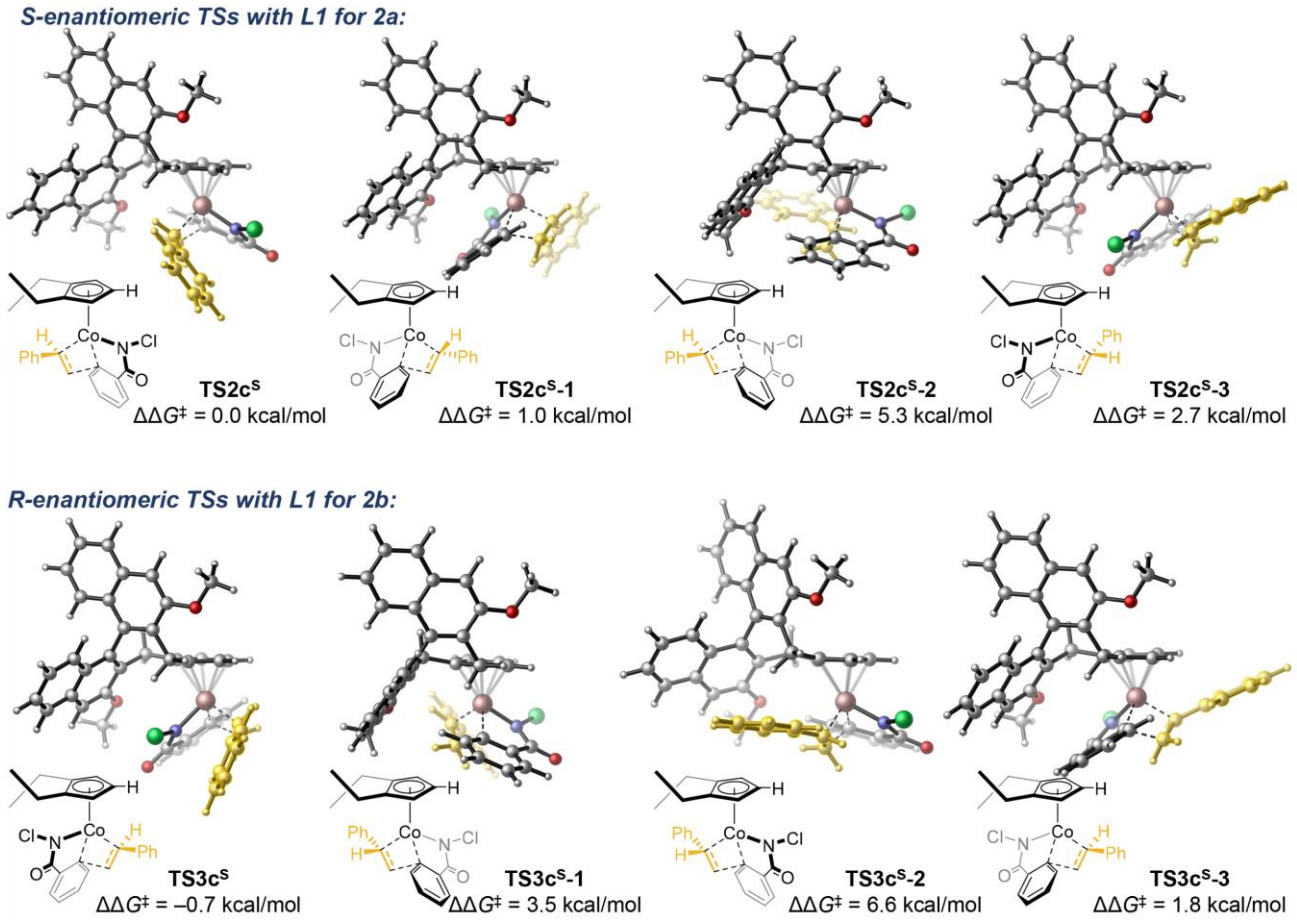

Fig. S6 Conformers of styrene insertion transition states with **L1**.

Non-Covalent Interactions in Styrene Insertion Transition States

Based on geometries of the most favorable transition states, the *S*-enantiomer (**2a**) is derived from the transition states of styrene insertion from the binaphthyl side. These structures are stabilized by the non-covalent interactions between styrene and the binaphthyl moieties, which are evidenced by the NCI plots shown in Fig. S7. For the transition states with **L1**, the greater dispersion interaction in **TS2c^{S}**, in which styrene inserts into the Co–C bond from the binaphthyl side, is mostly due to the non-covalent interactions between styrene and the binaphthyl moieties. The incoming styrene from the other side in **TS3c^{S}** results in relatively weaker non-covalent interactions with the Cp ring. In contrast, the addition of extra substituents on the Cp ring, such as **L2** with ^{i}Pr and **L3** with ^{t}Bu, can also introduce non-covalent interactions with styrene in **TS3b^{S}** and **TS3^{S}**. This can partially offset the non-covalent interactions between styrene and the binaphthyl groups in **TS2b^{S}** and **TS2^{S}**. Therefore, the EDA results shown in the main text indicate that the two transition states with **L1** showcase a larger difference in dispersion interactions than those with **L2** and **L3**. However, although having stronger dispersion interactions, **TS2c^{S}** is less favorable than **TS3c^{S}** which is stabilized by electronic effects.

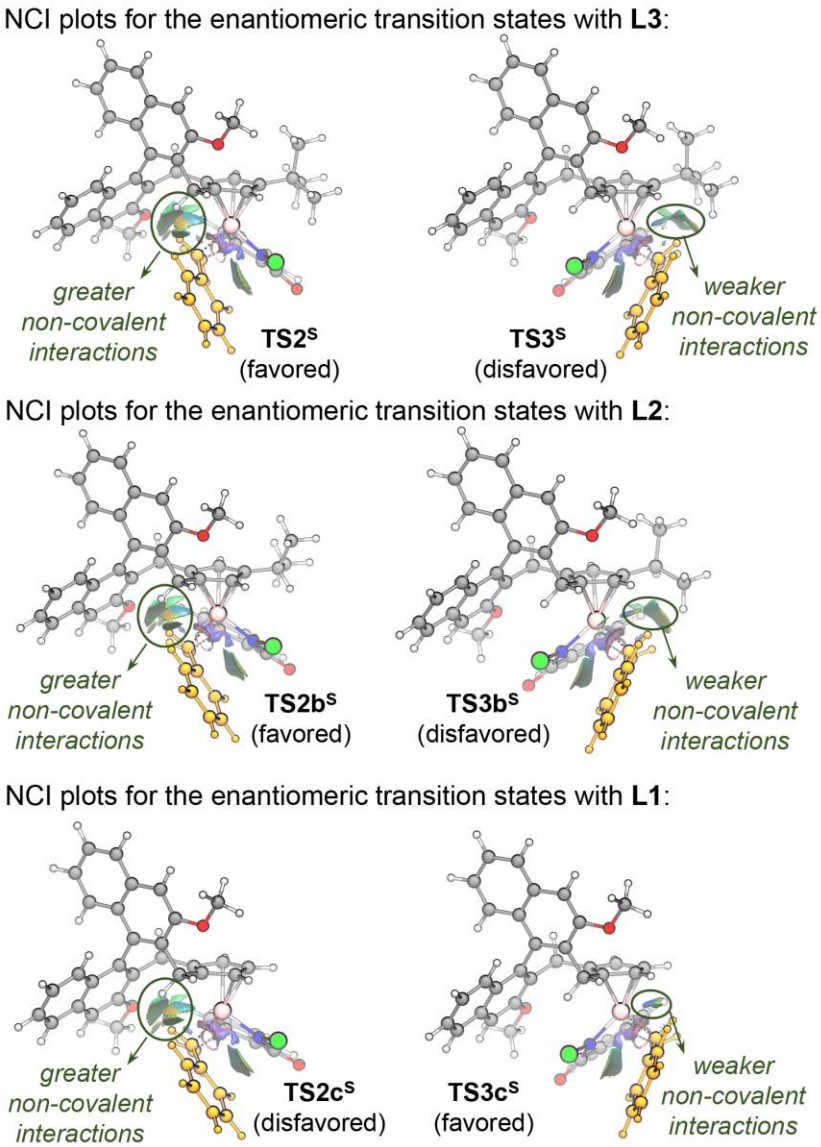

Fig. S7 NCI plots for the enantiomeric transition states with **L1** and **L2**.

Comparison of Different Spin States of Co Complexes Involved in Styrene Insertion

Except for the closed-shell singlet and triplet states of Co complexes reported in the manuscript, we further computed the open-shell singlet states of Co complexes involved in the enantioselectivity-determining styrene insertion step. Unfortunately, only the open-shell singlet states of the seven-membered aza-cobaltacycles (**int3^{OSS}** and **int4^{OSS}**) can be computationally located. These open-shell singlet complexes are extremely unstable, having higher or comparable energy compared with the closed-shell singlet transition states of styrene insertion (**int3^{OSS}** vs. **TS2^{S}**; **int4^{OSS}** vs. **TS3^{S}**). This indicates that the open-shell singlet styrene insertion transition states are much less favorable in kinetics.

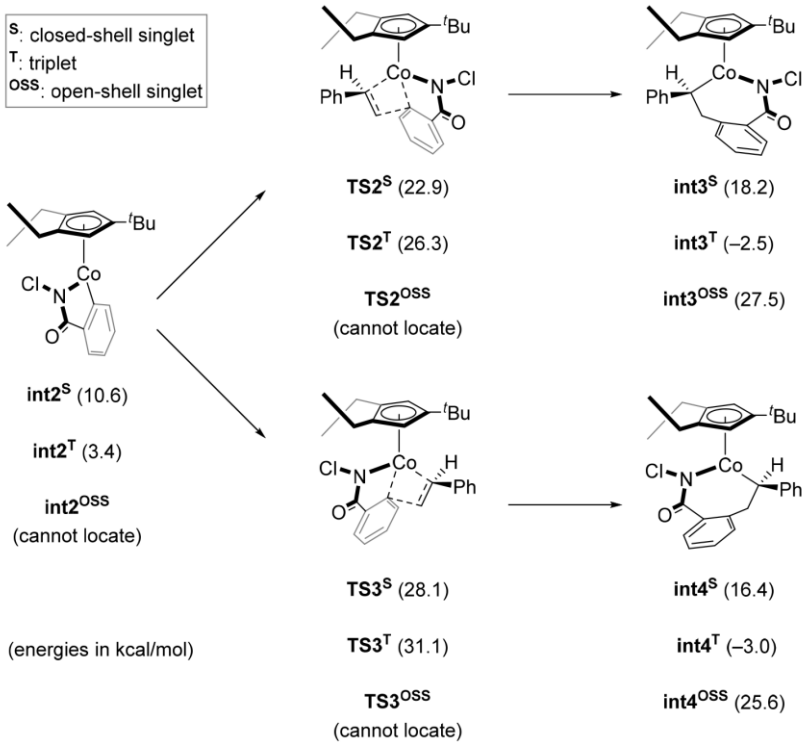

Fig. S8 Relative energies of Co complexes with different spin states.

Cartesian Coordinates (Å) and Energies of the Optimized Structures

int1[T]

B3LYP SCF energy: -2660.09940794 a.u.
B3LYP enthalpy: -2659.338511 a.u.
B3LYP free energy: -2659.469593 a.u.
M06 SCF energy in solution: -2660.03210255 a.u.
M06 enthalpy in solution: -2659.271206 a.u.
M06 free energy in solution: -2659.402288 a.u.
Three lowest frequencies (cm-1): 11.3792 20.9460 26.3502

Cartesian coordinates

ATOM	X	Y	Z
Co	1.681330	-0.539367	-0.250640
O	-1.454151	3.497934	1.691899
O	-0.981848	-2.700558	-2.330579
C	1.882792	1.673863	-1.123945
C	1.258147	1.690551	0.170356
H	1.660900	2.146458	1.063558
C	0.040911	0.996982	0.100362
C	-0.134077	0.543843	-1.300857
C	1.001914	0.931279	-2.004536
H	1.185893	0.732810	-3.051660
C	3.043521	2.533629	-1.580321
C	2.390788	3.812156	-2.186605
H	1.765504	3.571976	-3.053206
H	3.181057	4.497219	-2.515367
H	1.770675	4.333425	-1.448943
C	3.945487	2.956255	-0.405677
H	3.393674	3.541481	0.338715
H	4.759590	3.586787	-0.779820
H	4.392620	2.094344	0.095559
C	3.886725	1.848648	-2.676398
H	4.397196	0.954198	-2.312259
H	4.649119	2.550299	-3.033996
H	3.277014	1.562798	-3.540283
C	-0.980042	0.848296	1.197241
H	-0.591898	1.309344	2.107101
H	-1.145421	-0.211546	1.405835
C	-2.298324	1.490238	0.793688
C	-2.497876	2.882898	1.059926
C	-3.667183	3.512528	0.695331
H	-3.828069	4.564414	0.903531
C	-4.688217	2.794541	0.017796
C	-5.889798	3.432260	-0.391981
H	-6.023545	4.487227	-0.163932
C	-6.866166	2.735909	-1.069045
H	-7.779038	3.238475	-1.377294
C	-6.680966	1.366450	-1.370030
H	-7.450750	0.823619	-1.911379
C	-5.528341	0.718512	-0.981064
H	-5.391579	-0.331507	-1.215925

C	-4.504763	1.404510	-0.271699
C	-3.287502	0.764060	0.146612
C	-3.062730	-0.692334	-0.136002
C	-3.755523	-1.688761	0.635386
C	-4.669255	-1.362806	1.674720
H	-4.860142	-0.319202	1.900400
C	-5.311177	-2.347886	2.394290
H	-6.005824	-2.075837	3.184155
C	-5.067641	-3.711958	2.110626
H	-5.579338	-4.482665	2.680928
C	-4.179423	-4.062384	1.118492
H	-3.982559	-5.109512	0.900155
C	-3.497683	-3.070754	0.361403
C	-2.564625	-3.426094	-0.646949
H	-2.380011	-4.477996	-0.834249
C	-1.895812	-2.452123	-1.355626
C	-2.143552	-1.065274	-1.103775
C	-1.380932	-0.038298	-1.920970
H	-1.111359	-0.469184	-2.887613
H	-2.048783	0.810177	-2.124670
C	-1.586702	4.869646	2.030473
H	-1.716573	5.492904	1.136123
H	-0.658066	5.145526	2.533169
H	-2.432430	5.033856	2.710643
C	-0.470328	-4.021441	-2.454457
H	-1.244397	-4.720967	-2.796840
H	-0.050124	-4.358930	-1.501274
H	0.322084	-3.964446	-3.202006
N	3.523957	-1.201835	-0.573435
C	5.299346	-0.324184	0.858168
C	6.549017	0.316740	0.880215
H	7.115447	0.370634	-0.043325
C	7.046771	0.854393	2.064751
H	8.013900	1.350773	2.068404
C	6.307808	0.747575	3.246843
H	6.697515	1.162207	4.173301
C	5.073403	0.096063	3.233700
H	4.499602	-0.005183	4.151448
C	4.567881	-0.441308	2.047379
C	4.862231	-0.893943	-0.470721
O	5.692157	-1.073851	-1.361739
Cl	3.158523	-1.976560	-2.139212
O	1.526448	-1.172594	1.935236
C	0.900521	-2.152868	1.456676
O	0.648404	-2.182510	0.196040
H	3.613268	-0.951946	2.053263
C	0.444378	-3.309041	2.313939
H	-0.580908	-3.588544	2.055269
H	1.087222	-4.174572	2.114982
H	0.513941	-3.051215	3.372311

TS1^{T}

B3LYP SCF energy: -2660.05887191 a.u.
B3LYP enthalpy: -2659.303523 a.u.
B3LYP free energy: -2659.431057 a.u.
M06 SCF energy in solution: -2659.99403639 a.u.
M06 enthalpy in solution: -2659.238687 a.u.
M06 free energy in solution: -2659.366221 a.u.
Three lowest frequencies (cm-1): -1333.7391 17.6677 26.6691
Imaginary frequency: -1333.7391 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.910618	-0.015964	-0.386020
O	2.021282	3.580128	-1.668008
O	0.128228	-2.758977	1.907894
C	-1.958638	2.225764	0.513886
C	-1.156777	2.077008	-0.701266
H	-1.335541	2.592703	-1.636271
C	-0.033745	1.252997	-0.444867
C	-0.205743	0.723197	0.866993
C	-1.384261	1.367918	1.445972
H	-1.743921	1.172046	2.446798
C	-3.085452	3.224636	0.730350
C	-2.419851	4.608991	0.955418
H	-1.749769	4.590276	1.822469
H	-3.188033	5.371635	1.132125
H	-1.834137	4.916100	0.081258
C	-4.022278	3.322172	-0.491689
H	-3.476003	3.566506	-1.408754
H	-4.759335	4.116701	-0.325457
H	-4.562841	2.388737	-0.664939
C	-3.915724	2.862395	1.976748
H	-4.380343	1.875826	1.876719
H	-4.714821	3.599282	2.116506
H	-3.305152	2.865279	2.887179
C	1.121087	1.001737	-1.384462
H	0.953382	1.558252	-2.309142
H	1.174351	-0.058383	-1.640564
C	2.410408	1.456108	-0.724341
C	2.827330	2.818709	-0.868737
C	3.958170	3.285120	-0.236416
H	4.283103	4.313286	-0.350326
C	4.718820	2.426385	0.601536
C	5.872014	2.895659	1.285591
H	6.174373	3.931140	1.146492
C	6.593226	2.063816	2.113307
H	7.472132	2.438529	2.631123
C	6.188189	0.721337	2.294931
H	6.755865	0.070262	2.954001

C	5.076352	0.235411	1.640321
H	4.771270	-0.795449	1.785029
C	4.314484	1.064204	0.772576
C	3.145574	0.597365	0.076075
C	2.711548	-0.832059	0.213070
C	3.452125	-1.855151	-0.475656
C	4.561950	-1.568782	-1.317070
H	4.870170	-0.537681	-1.449818
C	5.242321	-2.576758	-1.966243
H	6.086172	-2.334572	-2.606279
C	4.846116	-3.924680	-1.805809
H	5.389844	-4.713342	-2.319007
C	3.769604	-4.235814	-1.005356
H	3.454728	-5.269538	-0.881791
C	3.044609	-3.217875	-0.328960
C	1.923566	-3.526812	0.484119
H	1.640114	-4.567090	0.593982
C	1.212144	-2.525769	1.108349
C	1.592207	-1.149939	0.968591
C	0.782001	-0.081128	1.688314
H	0.248118	-0.538449	2.524519
H	1.482401	0.644450	2.128158
C	2.378399	4.935576	-1.885763
H	2.386566	5.504048	-0.946555
H	1.615125	5.344102	-2.550505
H	3.362101	5.018719	-2.366040
C	-0.302204	-4.105048	2.082511
H	0.488126	-4.717354	2.534366
H	-0.622022	-4.541149	1.130201
H	-1.158063	-4.059201	2.757201
N	-3.512621	-0.004102	-1.434139
C	-4.488850	-0.909093	0.480551
C	-5.564479	-0.979008	1.368337
H	-6.558967	-0.733538	1.006951
C	-5.332484	-1.339737	2.695974
H	-6.161865	-1.388408	3.397132
C	-4.032544	-1.630142	3.129871
H	-3.857737	-1.904492	4.167680
C	-2.967250	-1.577954	2.230146
H	-1.965750	-1.832285	2.563926
C	-3.174486	-1.239643	0.876789
C	-4.721728	-0.403477	-0.915501
O	-5.821298	-0.324284	-1.447387
Cl	-3.546208	0.642037	-3.049241
H	-2.540657	-2.110728	0.052906
O	-0.858019	-1.440015	-1.453597
C	-1.248782	-2.641409	-1.460839
O	-2.126190	-3.097549	-0.652953
C	-0.646239	-3.592305	-2.469759
H	-0.831240	-3.205471	-3.477259
H	0.438056	-3.632681	-2.325340

H -1.075640 -4.590898 -2.373198

TS1^{S}

B3LYP SCF energy: -2660.06813610 a.u.
B3LYP enthalpy: -2659.311062 a.u.
B3LYP free energy: -2659.434212 a.u.
M06 SCF energy in solution: -2659.99799002 a.u.
M06 enthalpy in solution: -2659.240916 a.u.
M06 free energy in solution: -2659.364066 a.u.
Three lowest frequencies (cm-1): -1009.0222 20.9478 28.1135
Imaginary frequency: -1009.0222 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.859361	0.071198	-0.263622
O	2.024191	3.608315	-1.577975
O	0.095500	-2.690552	1.991049
C	-2.045220	2.107962	0.500254
C	-1.187014	2.082486	-0.654846
H	-1.383366	2.567952	-1.601097
C	-0.049454	1.286604	-0.387013
C	-0.198776	0.737041	0.941722
C	-1.403473	1.284994	1.472143
H	-1.796274	1.057225	2.453351
C	-3.214119	3.057284	0.734625
C	-2.589376	4.429172	1.106487
H	-1.958584	4.351449	1.999808
H	-3.381827	5.158978	1.311834
H	-1.972546	4.819829	0.289127
C	-4.083597	3.238861	-0.525920
H	-3.491844	3.570134	-1.385918
H	-4.844668	4.004993	-0.336028
H	-4.592941	2.315119	-0.808676
C	-4.101080	2.589156	1.904129
H	-4.542233	1.607609	1.709930
H	-4.919009	3.303397	2.052222
H	-3.541144	2.536260	2.845173
C	1.100048	1.042270	-1.328924
H	0.933867	1.608886	-2.247346
H	1.129235	-0.017783	-1.593206
C	2.405947	1.464223	-0.678592
C	2.841003	2.821998	-0.815385
C	3.998054	3.259869	-0.210724
H	4.336375	4.284291	-0.318917
C	4.768445	2.375779	0.590774
C	5.948452	2.816165	1.247863
H	6.263937	3.848473	1.114787
C	6.678392	1.960773	2.043104
H	7.577752	2.313448	2.540865

C	6.255818	0.622726	2.217982
H	6.830500	-0.046679	2.852099
C	5.118040	0.164467	1.588740
H	4.799713	-0.862955	1.728625
C	4.346163	1.017958	0.754106
C	3.149649	0.579995	0.086379
C	2.688756	-0.840718	0.229305
C	3.382710	-1.882800	-0.478659
C	4.478892	-1.626782	-1.347083
H	4.813347	-0.604498	-1.485428
C	5.114058	-2.652847	-2.013533
H	5.948907	-2.434197	-2.673521
C	4.682595	-3.988928	-1.844912
H	5.190253	-4.792092	-2.372329
C	3.617548	-4.270419	-1.018418
H	3.276079	-5.294879	-0.888889
C	2.939378	-3.233850	-0.321925
C	1.830207	-3.513212	0.518732
H	1.516961	-4.544762	0.630209
C	1.165836	-2.493660	1.164850
C	1.584901	-1.130665	1.017416
C	0.823416	-0.038407	1.750018
H	0.320273	-0.471554	2.617673
H	1.549620	0.687732	2.139193
C	2.395127	4.962044	-1.784702
H	2.440019	5.514273	-0.836961
H	1.618222	5.392326	-2.419084
H	3.364993	5.038468	-2.293297
C	-0.379755	-4.021302	2.169299
H	0.398128	-4.664201	2.600052
H	-0.736620	-4.438234	1.221810
H	-1.216859	-3.947714	2.864968
N	-3.344592	0.013860	-1.478968
C	-4.463198	-0.853801	0.350490
C	-5.602165	-0.992477	1.142647
H	-6.575452	-0.809033	0.696967
C	-5.460188	-1.347095	2.485784
H	-6.341695	-1.452122	3.113482
C	-4.187933	-1.566092	3.031017
H	-4.088500	-1.840666	4.078413
C	-3.054721	-1.447066	2.226573
H	-2.071068	-1.658084	2.636602
C	-3.170199	-1.106188	0.861771
C	-4.580167	-0.391922	-1.076932
O	-5.634037	-0.383028	-1.707472
Cl	-3.197346	0.527125	-3.133779
H	-2.501857	-1.952992	0.132762
O	-0.918460	-1.208988	-1.384223
C	-1.218249	-2.443177	-1.400348
O	-2.036756	-2.976311	-0.593921
C	-0.561015	-3.300057	-2.458214

H	0.520704	-3.141670	-2.447846
H	-0.790999	-4.354379	-2.297492
H	-0.937532	-2.990507	-3.439251

int2[T]

B3LYP SCF energy: -2430.99601585 a.u.
B3LYP enthalpy: -2430.303494 a.u.
B3LYP free energy: -2430.419572 a.u.
M06 SCF energy in solution: -2430.96979383 a.u.
M06 enthalpy in solution: -2430.277272 a.u.
M06 free energy in solution: -2430.393350 a.u.
Three lowest frequencies (cm-1): 19.0254 23.0933 26.6650

Cartesian coordinates

ATOM	X	Y	Z
Co	2.142404	0.374561	0.150876
O	-2.390182	3.360863	1.580807
O	0.755209	-2.291224	-1.943669
C	1.988405	2.525712	-0.395243
C	1.140667	2.332363	0.720330
H	1.255424	2.789282	1.695217
C	0.092340	1.407726	0.389123
C	0.287248	0.997346	-0.955154
C	1.491036	1.633946	-1.416994
H	1.884832	1.540181	-2.420227
C	3.137884	3.520850	-0.496230
C	2.524807	4.939116	-0.613237
H	1.882223	5.020062	-1.497611
H	3.318915	5.690872	-0.699492
H	1.919454	5.183190	0.266722
C	4.029280	3.456916	0.763080
H	3.459837	3.665062	1.675469
H	4.830525	4.202323	0.695609
H	4.488981	2.468357	0.870643
C	4.007281	3.252112	-1.739013
H	4.455500	2.253827	-1.705506
H	4.820400	3.985187	-1.789828
H	3.427966	3.341256	-2.665724
C	-1.031721	0.994134	1.313368
H	-0.970202	1.589515	2.226343
H	-0.913980	-0.053464	1.605836
C	-2.390587	1.189597	0.662073
C	-3.062073	2.444486	0.821076
C	-4.290531	2.669726	0.240599
H	-4.807854	3.614281	0.367210
C	-4.903584	1.667311	-0.557192
C	-6.158464	1.888805	-1.185336
H	-6.656507	2.843549	-1.032026
C	-6.735170	0.921111	-1.977816

H	-7.695116	1.106593	-2.452381
C	-6.076647	-0.313812	-2.180689
H	-6.531447	-1.071081	-2.813278
C	-4.860251	-0.559944	-1.580445
H	-4.358888	-1.508459	-1.740335
C	-4.243126	0.412038	-0.746886
C	-2.975294	0.193342	-0.105010
C	-2.250156	-1.107819	-0.276909
C	-2.707920	-2.284061	0.411933
C	-3.848071	-2.285510	1.261280
H	-4.402101	-1.363731	1.401807
C	-4.254768	-3.434624	1.904783
H	-5.129181	-3.413180	2.549354
C	-3.537081	-4.641048	1.733603
H	-3.864753	-5.542607	2.244290
C	-2.419926	-4.670477	0.929212
H	-1.855906	-5.591661	0.802886
C	-1.972325	-3.501774	0.256635
C	-0.803790	-3.518332	-0.549358
H	-0.255992	-4.449032	-0.644226
C	-0.371903	-2.370480	-1.176283
C	-1.104632	-1.145450	-1.057359
C	-0.594507	0.088668	-1.783678
H	-0.038511	-0.220448	-2.671994
H	-1.454770	0.673946	-2.132904
C	-3.001091	4.620093	1.810435
H	-3.163889	5.164217	0.870855
H	-2.306341	5.180762	2.438406
H	-3.959655	4.511126	2.334461
C	1.568284	-3.450247	-2.069975
H	1.026090	-4.261878	-2.572560
H	1.920350	-3.796043	-1.090738
H	2.425286	-3.147931	-2.672379
N	2.602219	-0.538985	1.695302
C	4.178268	-1.494324	0.261405
C	5.213853	-2.361238	-0.091769
H	5.624026	-3.026227	0.663263
C	5.694175	-2.345814	-1.402104
H	6.503313	-3.010514	-1.693267
C	5.134517	-1.472839	-2.341406
H	5.510807	-1.462952	-3.361903
C	4.093245	-0.607600	-1.978899
H	3.673333	0.054432	-2.730298
C	3.609559	-0.610701	-0.666274
C	3.628691	-1.476971	1.655833
O	4.027944	-2.164535	2.579503
Cl	1.845770	-0.326699	3.250315

int2^{S}

B3LYP SCF energy: -2430.98793037 a.u.
B3LYP enthalpy: -2430.294961 a.u.
B3LYP free energy: -2430.409287 a.u.
M06 SCF energy in solution: -2430.96055933 a.u.
M06 enthalpy in solution: -2430.267590 a.u.
M06 free energy in solution: -2430.381916 a.u.
Three lowest frequencies (cm-1): 18.5366 23.0033 28.3620

Cartesian coordinates

ATOM	X	Y	Z
Co	-2.081518	-0.447237	0.185271
O	2.288477	-3.428083	1.519346
O	-0.688940	2.470530	-1.881697
C	-2.077116	-2.423229	-0.441069
C	-1.173971	-2.331589	0.688712
H	-1.319866	-2.807204	1.649855
C	-0.144117	-1.429269	0.396509
C	-0.380665	-0.919135	-0.948167
C	-1.521643	-1.593826	-1.461741
H	-1.942953	-1.429458	-2.442260
C	-3.270895	-3.359451	-0.541199
C	-2.721017	-4.804101	-0.651478
H	-2.082087	-4.918618	-1.534721
H	-3.550675	-5.515997	-0.736905
H	-2.131362	-5.076490	0.231039
C	-4.158536	-3.247579	0.717757
H	-3.602913	-3.482119	1.632299
H	-4.994342	-3.953459	0.647649
H	-4.568810	-2.237932	0.821685
C	-4.121976	-3.048722	-1.786504
H	-4.506534	-2.024145	-1.761191
H	-4.977554	-3.732019	-1.831465
H	-3.548424	-3.180987	-2.711659
C	0.980196	-1.027277	1.319093
H	0.914316	-1.622547	2.231717
H	0.869803	0.022118	1.607191
C	2.327993	-1.236950	0.651081
C	2.969598	-2.511568	0.768046
C	4.179885	-2.753479	0.156878
H	4.675057	-3.713731	0.249486
C	4.801486	-1.747421	-0.629657
C	6.036667	-1.985565	-1.289989
H	6.512126	-2.956593	-1.171427
C	6.622189	-1.013302	-2.070179
H	7.566549	-1.211681	-2.570061
C	5.993265	0.243591	-2.227349
H	6.455271	1.004675	-2.849999
C	4.796779	0.506340	-1.595198
H	4.318220	1.471736	-1.719791
C	4.170665	-0.470834	-0.774326
C	2.921846	-0.236162	-0.101623

C	2.234326	1.091268	-0.221884
C	2.745269	2.225033	0.499868
C	3.888159	2.151479	1.342596
H	4.404139	1.203584	1.450362
C	4.343986	3.260650	2.022060
H	5.218914	3.181760	2.661418
C	3.675840	4.500642	1.894393
H	4.041976	5.370279	2.433522
C	2.558991	4.603132	1.095854
H	2.033917	5.550736	1.001505
C	2.061503	3.476924	0.386403
C	0.900278	3.570759	-0.423222
H	0.400193	4.529585	-0.498194
C	0.417625	2.463996	-1.087427
C	1.083433	1.198457	-0.988608
C	0.510171	0.009509	-1.743436
H	-0.052870	0.369398	-2.607397
H	1.341082	-0.595196	-2.130719
C	2.870861	-4.708056	1.706800
H	3.000530	-5.233178	0.751419
H	2.174519	-5.265637	2.335682
H	3.842157	-4.635894	2.213239
C	-1.464746	3.659472	-1.953038
H	-0.895251	4.478298	-2.412220
H	-1.810972	3.964527	-0.958482
H	-2.327677	3.413140	-2.571516
N	-2.597422	0.437725	1.676633
C	-4.048065	1.532842	0.207940
C	-5.041902	2.435217	-0.168894
H	-5.502176	3.064214	0.588498
C	-5.420745	2.502259	-1.511939
H	-6.197679	3.192764	-1.829292
C	-4.792643	1.671478	-2.442141
H	-5.082666	1.717764	-3.489973
C	-3.789700	0.772232	-2.043581
H	-3.323664	0.156914	-2.808076
C	-3.401484	0.682035	-0.702563
C	-3.602763	1.420336	1.627858
O	-4.025685	2.060643	2.571597
Cl	-1.959549	0.135717	3.273897

TS2^{S}

B3LYP SCF energy: -2740.60780699 a.u.
B3LYP enthalpy: -2739.771545 a.u.
B3LYP free energy: -2739.900307 a.u.
M06 SCF energy in solution: -2740.44270078 a.u.
M06 enthalpy in solution: -2739.606439 a.u.
M06 free energy in solution: -2739.735201 a.u.
Three lowest frequencies (cm-1): -293.2935 13.8277 18.5270

Imaginary frequency: -293.2935 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	1.826281	-0.201819	0.130244
O	-0.566071	2.034549	3.006308
O	-2.023184	-2.979286	-2.454626
C	1.697031	-2.397761	0.352369
C	1.024504	-1.802243	1.442875
H	1.301798	-1.903097	2.483574
C	-0.054249	-0.982960	0.977064
C	-0.087710	-1.109768	-0.455307
C	1.017513	-1.916379	-0.828790
H	1.284568	-2.151503	-1.849840
C	2.736590	-3.510540	0.427019
C	1.945435	-4.845247	0.467545
H	1.279240	-4.886862	1.337179
H	2.638572	-5.693428	0.527245
H	1.333795	-4.970719	-0.433542
C	3.668099	-3.531844	-0.800012
H	4.341356	-4.394714	-0.731689
H	4.275736	-2.627223	-0.865041
H	3.107066	-3.627128	-1.735828
C	3.588879	-3.402835	1.707221
H	4.147563	-2.463104	1.741119
H	4.309945	-4.227865	1.739846
H	2.975821	-3.470942	2.613453
C	-1.129992	-0.437709	1.900118
H	-0.687103	-0.259721	2.882637
H	-1.865855	-1.242979	2.034382
C	-1.878145	0.808628	1.457736
C	-1.554185	2.071883	2.053578
C	-2.213501	3.224343	1.689397
H	-1.968923	4.178699	2.141695
C	-3.228707	3.190018	0.698659
C	-3.897027	4.373956	0.286618
H	-3.617339	5.317957	0.748450
C	-4.873841	4.333245	-0.682813
H	-5.374430	5.247133	-0.991027
C	-5.223218	3.101759	-1.284324
H	-5.989100	3.075642	-2.054437
C	-4.596240	1.935862	-0.900659
H	-4.868421	0.996484	-1.369081
C	-3.587890	1.940380	0.102291
C	-2.906324	0.746692	0.525758
C	-3.316144	-0.576576	-0.055277
C	-4.547460	-1.189472	0.367966
C	-5.393643	-0.618101	1.357033
H	-5.107013	0.321990	1.815843
C	-6.563844	-1.239003	1.738858
H	-7.195010	-0.784224	2.497358

C	-6.946528	-2.465692	1.149032
H	-7.871780	-2.947331	1.453755
C	-6.144676	-3.050845	0.194308
H	-6.428936	-3.997903	-0.258610
C	-4.930112	-2.439091	-0.216185
C	-4.089606	-3.049702	-1.184908
H	-4.400662	-3.995335	-1.614748
C	-2.902629	-2.455393	-1.550802
C	-2.504230	-1.199989	-0.989143
C	-1.165393	-0.603526	-1.384809
H	-0.911889	-0.882038	-2.409540
H	-1.243752	0.485015	-1.349572
C	-0.300771	3.218822	3.747530
H	0.462727	2.948682	4.478917
H	-1.201184	3.569864	4.266611
H	0.082723	4.020174	3.103280
C	-2.349720	-4.213414	-3.073900
H	-3.281378	-4.137921	-3.649732
H	-2.446439	-5.018941	-2.334435
H	-1.522544	-4.437739	-3.749467
N	3.446138	-0.112999	-0.910714
C	4.378157	0.313924	1.160859
C	5.430728	0.206651	2.072505
H	6.433917	0.072945	1.677910
C	5.175086	0.249294	3.442999
H	5.991783	0.163153	4.154647
C	3.859213	0.396440	3.896955
H	3.651259	0.418872	4.964176
C	2.809278	0.531967	2.987556
H	1.798261	0.692556	3.353678
C	3.053978	0.497572	1.604200
C	4.640264	0.130299	-0.305605
O	5.762741	0.169991	-0.807076
Cl	3.519713	-0.394754	-2.628773
C	1.981687	1.892213	0.779786
H	2.851555	2.540286	0.737915
H	1.353230	2.066181	1.645030
C	1.271290	1.698602	-0.456194
H	0.193594	1.624196	-0.346558
C	1.679814	2.307779	-1.737368
C	2.970138	2.815383	-1.983774
C	0.709455	2.476078	-2.743802
C	3.272222	3.454835	-3.182501
H	3.755969	2.689520	-1.246928
C	1.011994	3.110964	-3.946643
H	-0.301555	2.115619	-2.572957
C	2.297678	3.604994	-4.172663
H	4.279112	3.828522	-3.347664
H	0.240260	3.225945	-4.703510
H	2.538391	4.103216	-5.107942

TS2[T]

B3LYP SCF energy: -2740.59742901 a.u.
B3LYP enthalpy: -2739.762781 a.u.
B3LYP free energy: -2739.894730 a.u.
M06 SCF energy in solution: -2740.43257909 a.u.
M06 enthalpy in solution: -2739.597931 a.u.
M06 free energy in solution: -2739.729880 a.u.
Three lowest frequencies (cm-1): -376.6812 15.8899 17.2171
Imaginary frequency: -376.6812 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	1.913104	0.173806	-0.085766
O	-2.037241	3.029649	2.413543
O	-0.549590	-1.880590	-3.115491
C	1.690832	2.472465	-0.382280
C	0.990472	2.056780	0.773118
H	1.232524	2.311615	1.795652
C	-0.072618	1.174583	0.393720
C	-0.076652	1.093363	-1.048842
C	1.030467	1.839817	-1.499445
H	1.312359	1.955994	-2.538656
C	2.764288	3.549603	-0.476282
C	2.051961	4.866425	-0.883290
H	1.559755	4.769204	-1.857992
H	2.778291	5.686142	-0.950310
H	1.289804	5.145186	-0.146636
C	3.466307	3.762370	0.877886
H	2.760530	4.084862	1.651989
H	4.228766	4.544541	0.782776
H	3.953084	2.846075	1.222706
C	3.824456	3.212403	-1.544748
H	4.385060	2.311918	-1.280382
H	4.535814	4.042161	-1.635289
H	3.376374	3.054504	-2.532159
C	-1.152349	0.672604	1.326510
H	-0.898240	0.960048	2.348769
H	-1.218558	-0.417311	1.305500
C	-2.502937	1.250169	0.942409
C	-2.916819	2.495693	1.516445
C	-4.118494	3.071613	1.169568
H	-4.439628	4.009352	1.609204
C	-4.962545	2.451638	0.210172
C	-6.193666	3.043884	-0.178874
H	-6.487473	3.983560	0.283311
C	-6.999688	2.449596	-1.124463
H	-7.937805	2.916354	-1.412653
C	-6.604059	1.233119	-1.726528
H	-7.238224	0.770932	-2.478069

C	-5.417081	0.631513	-1.365814
H	-5.120838	-0.300373	-1.835079
C	-4.566360	1.212089	-0.386015
C	-3.318003	0.619061	0.016172
C	-2.890728	-0.687609	-0.589233
C	-3.540890	-1.903161	-0.178416
C	-4.531991	-1.938156	0.841055
H	-4.813533	-1.013052	1.331912
C	-5.130814	-3.123294	1.210844
H	-5.884345	-3.127273	1.993501
C	-4.768763	-4.335387	0.578107
H	-5.247394	-5.264644	0.875132
C	-3.807674	-4.337988	-0.407944
H	-3.518819	-5.267097	-0.893794
C	-3.168278	-3.133531	-0.806868
C	-2.166806	-3.128558	-1.812698
H	-1.908423	-4.069454	-2.285363
C	-1.533682	-1.956151	-2.161438
C	-1.878445	-0.710773	-1.539982
C	-1.162145	0.559349	-1.965417
H	-0.734852	0.413375	-2.960319
H	-1.918129	1.350792	-2.065064
C	-2.369977	4.262412	3.031179
H	-2.486134	5.063080	2.289184
H	-1.536335	4.499746	3.694247
H	-3.292891	4.179378	3.620163
C	-0.290113	-3.035195	-3.903236
H	-1.198710	-3.378738	-4.413227
H	0.116603	-3.855087	-3.297219
H	0.452447	-2.731936	-4.643413
N	3.518935	0.091986	1.117983
C	4.599475	-0.440701	-0.865696
C	5.757379	-0.377422	-1.647671
H	6.714070	-0.344650	-1.134118
C	5.663929	-0.335603	-3.038152
H	6.564376	-0.283328	-3.644210
C	4.405726	-0.354719	-3.650058
H	4.324962	-0.309598	-4.733588
C	3.247775	-0.452356	-2.875264
H	2.277441	-0.512201	-3.362701
C	3.336527	-0.495283	-1.477773
C	4.723489	-0.330130	0.632207
O	5.773696	-0.540527	1.234186
Cl	3.498593	0.412919	2.838891
C	2.071414	-2.016857	-0.873693
H	2.947703	-2.639409	-0.730737
H	1.618926	-2.074928	-1.855713
C	1.160245	-1.898391	0.205935
H	0.124870	-1.715114	-0.062172
C	1.354772	-2.448615	1.550231
C	0.211523	-2.704857	2.337325

C	2.611794	-2.827140	2.066458
C	0.317777	-3.306979	3.588280
H	-0.771266	-2.458716	1.944963
C	2.714557	-3.430245	3.314979
H	3.515889	-2.624297	1.504146
C	1.571335	-3.671004	4.083965
H	-0.578904	-3.498223	4.171486
H	3.694984	-3.701605	3.695622
H	1.658985	-4.139009	5.060672

TS3^{S}

B3LYP SCF energy: -2740.60021556 a.u.
B3LYP enthalpy: -2739.763857 a.u.
B3LYP free energy: -2739.891362 a.u.
M06 SCF energy in solution: -2740.43576327 a.u.
M06 enthalpy in solution: -2739.599405 a.u.
M06 free energy in solution: -2739.726910 a.u.
Three lowest frequencies (cm-1): -302.3052 15.3793 17.5486
Imaginary frequency: -302.3052 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	1.981223	0.473403	-0.234569
O	-2.003540	3.359182	1.842396
O	-0.317432	-2.715121	-2.313506
C	1.540431	2.524577	-0.900127
C	0.914474	2.273051	0.362638
H	1.104538	2.797054	1.289237
C	-0.021157	1.220849	0.235198
C	-0.027369	0.806359	-1.154237
C	0.926153	1.607823	-1.821373
H	1.171385	1.512091	-2.871441
C	2.284049	3.814993	-1.259331
C	3.212237	3.670408	-2.479164
H	4.092263	3.063474	-2.244264
H	3.573000	4.657990	-2.789717
H	2.702374	3.221542	-3.337967
C	1.185328	4.855538	-1.608467
H	0.590064	4.528069	-2.468018
H	1.640370	5.822423	-1.856887
H	0.502906	5.005217	-0.764703
C	3.113820	4.365331	-0.081872
H	2.503182	4.533254	0.811733
H	3.555970	5.329256	-0.359452
H	3.935538	3.692508	0.185705
C	-1.027725	0.839479	1.291930
H	-0.770556	1.337165	2.229419
H	-1.018080	-0.234174	1.472950
C	-2.401761	1.273822	0.813239

C	-2.859283	2.601986	1.088160
C	-4.074712	3.045071	0.616444
H	-4.431559	4.046747	0.829689
C	-4.886739	2.196705	-0.183255
C	-6.129954	2.643505	-0.705389
H	-6.460411	3.653265	-0.472068
C	-6.903181	1.822117	-1.495887
H	-7.851223	2.179407	-1.889338
C	-6.463025	0.513343	-1.800792
H	-7.073382	-0.129057	-2.429596
C	-5.263842	0.049179	-1.303586
H	-4.931284	-0.955998	-1.539509
C	-4.444876	0.868058	-0.479402
C	-3.185573	0.421740	0.052363
C	-2.713240	-0.979232	-0.202049
C	-3.323093	-2.059365	0.524902
C	-4.340556	-1.859100	1.498166
H	-4.681725	-0.850646	1.705220
C	-4.892065	-2.921484	2.181466
H	-5.667227	-2.744566	2.922202
C	-4.450301	-4.240890	1.926837
H	-4.889024	-5.073055	2.471225
C	-3.461482	-4.468571	0.996547
H	-3.109122	-5.478743	0.801579
C	-2.872100	-3.393862	0.277097
C	-1.852827	-3.620568	-0.680443
H	-1.527493	-4.639203	-0.854088
C	-1.273678	-2.566978	-1.353588
C	-1.681430	-1.216345	-1.099349
C	-1.018239	-0.088750	-1.874360
H	-0.528630	-0.504505	-2.757764
H	-1.812262	0.577296	-2.242429
C	-2.414129	4.665545	2.209726
H	-2.559609	5.305096	1.328944
H	-1.608818	5.073038	2.824038
H	-3.342797	4.644361	2.794863
C	0.084395	-4.037634	-2.655825
H	0.788311	-3.923963	-3.481314
H	-0.774220	-4.635764	-2.988342
H	0.585794	-4.518751	-1.809810
N	1.776758	-1.364479	0.374633
C	2.991539	-1.816647	-1.542481
C	3.334991	-2.650193	-2.608825
H	3.147527	-3.713603	-2.498749
C	3.889934	-2.115479	-3.769295
H	4.157111	-2.763331	-4.599900
C	4.102528	-0.735705	-3.854026
H	4.528168	-0.302026	-4.755655
C	3.802738	0.090166	-2.770871
H	4.040400	1.144851	-2.841070
C	3.250010	-0.433220	-1.588389

C	2.287379	-2.390370	-0.354852
O	2.206955	-3.602440	-0.138744
Cl	0.927961	-1.871610	1.808170
C	4.181513	0.366242	-0.088400
H	4.791339	-0.524750	0.022797
H	4.677536	1.139305	-0.666944
C	3.500885	0.827812	1.095025
H	3.437888	1.906922	1.185987
C	3.568935	0.165004	2.412080
C	3.190542	0.907291	3.547087
C	4.060968	-1.137256	2.614251
C	3.293609	0.375252	4.829943
H	2.813088	1.919456	3.414388
C	4.170561	-1.668504	3.896694
H	4.340949	-1.753035	1.765890
C	3.787215	-0.918464	5.011189
H	2.992866	0.971277	5.687789
H	4.548347	-2.679259	4.024394
H	3.871591	-1.338524	6.009775

TS3^{T}

B3LYP SCF energy: -2740.59096699 a.u.
B3LYP enthalpy: -2739.756416 a.u.
B3LYP free energy: -2739.887445 a.u.
M06 SCF energy in solution: -2740.42562635 a.u.
M06 enthalpy in solution: -2739.591075 a.u.
M06 free energy in solution: -2739.722104 a.u.
Three lowest frequencies (cm-1): -403.1563 16.1077 17.5762
Imaginary frequency: -403.1563 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	2.078212	0.285866	-0.229076
O	-2.000188	3.584947	1.417715
O	-0.354516	-2.917818	-2.011793
C	1.579024	2.376940	-1.204272
C	0.996335	2.229656	0.096512
H	1.189239	2.856956	0.956994
C	-0.035038	1.232789	0.060645
C	-0.037924	0.677928	-1.240593
C	0.990728	1.354585	-1.993454
H	1.211342	1.146939	-3.034044
C	2.396974	3.567601	-1.710339
C	1.468162	4.395454	-2.637393
H	1.150702	3.807858	-3.505357
H	1.987615	5.290546	-3.002745
H	0.567446	4.716680	-2.102748
C	2.846812	4.485863	-0.556133
H	1.991440	4.861457	0.015616

H	3.382641	5.353215	-0.958684
H	3.524695	3.979975	0.140627
C	3.635623	3.143697	-2.522751
H	4.353475	2.595322	-1.902396
H	4.148617	4.026389	-2.923579
H	3.359965	2.508770	-3.371270
C	-1.052651	1.008074	1.155675
H	-0.787471	1.618871	2.021715
H	-1.062348	-0.033372	1.478052
C	-2.423465	1.400175	0.633155
C	-2.865698	2.756387	0.754757
C	-4.075961	3.158582	0.235769
H	-4.420109	4.182113	0.335069
C	-4.899398	2.235923	-0.463897
C	-6.136745	2.636631	-1.034834
H	-6.454239	3.670388	-0.916701
C	-6.920058	1.741698	-1.729986
H	-7.863337	2.064421	-2.162883
C	-6.495747	0.401848	-1.885201
H	-7.113362	-0.299641	-2.439443
C	-5.302473	-0.018147	-1.336778
H	-4.981874	-1.047173	-1.458811
C	-4.473641	0.877271	-0.607812
C	-3.218875	0.478730	-0.028282
C	-2.761315	-0.946425	-0.129465
C	-3.385350	-1.937909	0.704347
C	-4.402715	-1.624694	1.647299
H	-4.729709	-0.595509	1.747695
C	-4.971219	-2.603413	2.434055
H	-5.746189	-2.340575	3.149110
C	-4.547413	-3.947931	2.318654
H	-5.000003	-4.713660	2.943370
C	-3.557974	-4.283380	1.422089
H	-3.218611	-5.312865	1.334264
C	-2.950829	-3.296346	0.599367
C	-1.926489	-3.633024	-0.319895
H	-1.611269	-4.667643	-0.382413
C	-1.328381	-2.660945	-1.091541
C	-1.728582	-1.287820	-0.991202
C	-1.047721	-0.256049	-1.877690
H	-0.565763	-0.771028	-2.711907
H	-1.828342	0.383388	-2.316757
C	-2.384913	4.934556	1.612524
H	-2.527308	5.455104	0.656005
H	-1.567340	5.404864	2.162609
H	-3.308800	5.008716	2.201423
C	0.026745	-4.273883	-2.217348
H	-0.837008	-4.884965	-2.511098
H	0.497715	-4.686118	-1.318519
H	0.752173	-4.253204	-3.031796
N	1.799592	-1.535047	0.611312

C	3.050648	-2.235981	-1.223650
C	3.392801	-3.215628	-2.162010
H	3.190334	-4.250629	-1.903639
C	3.961394	-2.857116	-3.381937
H	4.227771	-3.620939	-4.107619
C	4.189926	-1.506803	-3.665622
H	4.625224	-1.212642	-4.617579
C	3.892754	-0.529348	-2.714225
H	4.135674	0.505478	-2.928590
C	3.324494	-0.884853	-1.483531
C	2.316892	-2.649048	0.021551
O	2.202095	-3.828613	0.359148
Cl	0.832772	-1.879995	2.027491
C	4.409355	0.092395	-0.008722
H	4.787860	-0.859127	0.346809
H	5.019301	0.560135	-0.771823
C	3.816088	0.970345	0.933767
H	3.821392	2.021766	0.666400
C	3.623069	0.717677	2.365891
C	3.331222	1.816995	3.201010
C	3.798579	-0.544106	2.967936
C	3.225488	1.665949	4.579821
H	3.200594	2.800951	2.756316
C	3.696871	-0.692131	4.347484
H	3.994831	-1.415810	2.354065
C	3.409859	0.408063	5.160290
H	3.003611	2.528440	5.202441
H	3.830989	-1.675397	4.788938
H	3.327725	0.285320	6.236638

int3^{S}

B3LYP SCF energy: -2740.62778076 a.u.
B3LYP enthalpy: -2739.789697 a.u.
B3LYP free energy: -2739.918268 a.u.
M06 SCF energy in solution: -2740.45230490 a.u.
M06 enthalpy in solution: -2739.614221 a.u.
M06 free energy in solution: -2739.742792 a.u.
Three lowest frequencies (cm-1): 18.9607 21.4631 28.1227

Cartesian coordinates

ATOM	X	Y	Z
Co	1.997549	-0.046705	-0.009777
O	-1.468224	3.163908	2.299968
O	-0.658087	-2.340169	-2.854882
C	2.025821	2.207998	-0.433806
C	1.329973	1.790419	0.754694
H	1.579494	2.073879	1.768783
C	0.194851	0.991363	0.407375
C	0.249680	0.785767	-1.009228

C	1.373271	1.544683	-1.492164
H	1.683451	1.559011	-2.530369
C	3.085151	3.301368	-0.529135
C	2.358162	4.646340	-0.262344
H	1.548624	4.809393	-0.983406
H	3.064207	5.481862	-0.345478
H	1.924244	4.669547	0.743816
C	4.206632	3.137610	0.516566
H	3.808118	3.069050	1.533255
H	4.872702	4.008443	0.478684
H	4.812226	2.244899	0.341683
C	3.705142	3.356184	-1.938246
H	4.191692	2.411565	-2.200496
H	4.460810	4.148958	-1.980459
H	2.952537	3.578701	-2.704318
C	-0.938685	0.646416	1.338785
H	-0.666443	0.926379	2.358123
H	-1.148672	-0.422977	1.341550
C	-2.165509	1.415762	0.882046
C	-2.382992	2.742110	1.377228
C	-3.444856	3.498586	0.934454
H	-3.619646	4.499397	1.313591
C	-4.330053	2.986702	-0.051422
C	-5.413810	3.763211	-0.541646
H	-5.562814	4.761918	-0.137493
C	-6.258122	3.270444	-1.511860
H	-7.081696	3.877775	-1.877787
C	-6.050871	1.974478	-2.037679
H	-6.714220	1.591806	-2.808468
C	-5.011136	1.194654	-1.577445
H	-4.859207	0.201882	-1.987276
C	-4.126433	1.668562	-0.570696
C	-3.027016	0.888800	-0.066363
C	-2.822721	-0.513749	-0.562274
C	-3.718419	-1.543905	-0.106582
C	-4.744201	-1.305150	0.849492
H	-4.861209	-0.307846	1.258344
C	-5.580543	-2.318912	1.264736
H	-6.355350	-2.113898	1.998228
C	-5.434141	-3.625846	0.744106
H	-6.099366	-4.418379	1.076172
C	-4.446190	-3.893407	-0.176660
H	-4.321006	-4.897265	-0.575837
C	-3.565461	-2.870117	-0.619353
C	-2.535290	-3.138892	-1.556816
H	-2.444760	-4.147308	-1.943856
C	-1.668265	-2.143171	-1.949331
C	-1.786360	-0.806971	-1.439917
C	-0.831752	0.266460	-1.942220
H	-0.357074	-0.085384	-2.861089
H	-1.437866	1.140351	-2.223048

C	-1.627247	4.456510	2.862366
H	-1.567685	5.238202	2.093823
H	-0.805071	4.578966	3.569576
H	-2.582913	4.546397	3.395130
C	-0.593231	-3.593847	-3.518629
H	-1.532030	-3.816340	-4.041551
H	-0.366657	-4.409687	-2.820161
H	0.215103	-3.507943	-4.247371
N	3.567909	-0.251667	1.114336
C	4.319018	-0.784181	-1.011597
C	5.063407	-0.200886	-2.051923
H	5.926641	0.399245	-1.782411
C	4.706617	-0.401232	-3.378503
H	5.290937	0.053677	-4.173935
C	3.587356	-1.188258	-3.689071
H	3.298460	-1.340765	-4.725591
C	2.874896	-1.806290	-2.670882
H	2.042218	-2.460302	-2.911217
C	3.233139	-1.647471	-1.312420
C	4.712730	-0.421533	0.408672
O	5.882837	-0.263583	0.747071
Cl	3.774436	0.306304	2.755988
C	2.577261	-2.552027	-0.258013
H	3.317938	-2.793921	0.505773
H	2.293043	-3.494139	-0.749016
C	1.347797	-1.896370	0.375055
H	0.501064	-1.970309	-0.309257
C	0.947997	-2.380497	1.722864
C	-0.391342	-2.757825	1.952031
C	1.857966	-2.546542	2.785368
C	-0.810496	-3.252022	3.187381
H	-1.107846	-2.689075	1.137828
C	1.441185	-3.041470	4.019318
H	2.896067	-2.269852	2.648736
C	0.104635	-3.391870	4.231519
H	-1.850874	-3.535146	3.326403
H	2.166296	-3.151311	4.821829
H	-0.215546	-3.777089	5.196137

int3^{T}

B3LYP SCF energy: -2740.65581712 a.u.
B3LYP enthalpy: -2739.818208 a.u.
B3LYP free energy: -2739.948973 a.u.
M06 SCF energy in solution: -2740.48252976 a.u.
M06 enthalpy in solution: -2739.644921 a.u.
M06 free energy in solution: -2739.775686 a.u.
Three lowest frequencies (cm-1): 18.8080 22.9397 27.9116

Cartesian coordinates

ATOM	X	Y	Z
Co	1.954953	0.114876	0.274997
O	-1.957018	3.410777	2.000194
O	-0.435485	-2.535348	-2.496973
C	1.813803	2.385855	-0.468399
C	1.029879	2.171326	0.717915
H	1.172447	2.664279	1.670845
C	0.022919	1.213594	0.455625
C	0.191270	0.781883	-0.920453
C	1.297056	1.512957	-1.454780
H	1.659134	1.412390	-2.469752
C	2.844257	3.487718	-0.685042
C	2.053537	4.820505	-0.773466
H	1.316984	4.792223	-1.584745
H	2.740619	5.654215	-0.963921
H	1.519644	5.027219	0.160799
C	3.856235	3.591332	0.473862
H	3.358111	3.692671	1.443330
H	4.488707	4.475946	0.330309
H	4.507197	2.715160	0.523834
C	3.613195	3.284824	-2.004851
H	4.142001	2.326077	-2.018984
H	4.355800	4.081496	-2.128000
H	2.946269	3.320296	-2.874141
C	-1.140671	0.875593	1.357907
H	-0.961398	1.300528	2.347738
H	-1.245880	-0.204632	1.480388
C	-2.408235	1.458485	0.757746
C	-2.771323	2.805834	1.085400
C	-3.865975	3.407163	0.506474
H	-4.148415	4.423406	0.757989
C	-4.643096	2.710633	-0.456607
C	-5.753501	3.328493	-1.091450
H	-6.008081	4.349471	-0.816125
C	-6.490992	2.657868	-2.041820
H	-7.335804	3.145405	-2.521018
C	-6.145098	1.334777	-2.399769
H	-6.723219	0.811036	-3.156130
C	-5.077340	0.706096	-1.794888
H	-4.819574	-0.308333	-2.078943
C	-4.299563	1.365793	-0.804363
C	-3.170018	0.749261	-0.156711
C	-2.831418	-0.676730	-0.483972
C	-3.680647	-1.723809	0.020323
C	-4.762640	-1.474850	0.909192
H	-4.958447	-0.456860	1.227114
C	-5.553703	-2.503321	1.374333
H	-6.372529	-2.289876	2.055758
C	-5.304175	-3.835923	0.971358
H	-5.934508	-4.640221	1.341113
C	-4.260550	-4.113047	0.116880

H	-4.057058	-5.135792	-0.191960
C	-3.423873	-3.074706	-0.373630
C	-2.335950	-3.352524	-1.241704
H	-2.167082	-4.380267	-1.542619
C	-1.508570	-2.337883	-1.669854
C	-1.732669	-0.975664	-1.278845
C	-0.819465	0.106431	-1.830893
H	-0.287266	-0.288243	-2.698816
H	-1.461366	0.917857	-2.205039
C	-2.261187	4.737954	2.397596
H	-2.221325	5.431043	1.547144
H	-1.497999	5.014742	3.127091
H	-3.252391	4.798830	2.865854
C	-0.225488	-3.834606	-3.028379
H	-1.101506	-4.180951	-3.591474
H	0.005785	-4.560849	-2.238295
H	0.628669	-3.746397	-3.701620
N	3.714501	0.076174	1.060759
C	4.573427	-0.809519	-0.982655
C	5.304750	-0.333476	-2.081684
H	6.027362	0.458234	-1.910425
C	5.125768	-0.875261	-3.351116
H	5.694002	-0.489989	-4.193320
C	4.226073	-1.929427	-3.527988
H	4.087187	-2.372048	-4.511042
C	3.527652	-2.434063	-2.432601
H	2.866116	-3.287242	-2.563707
C	3.679767	-1.891882	-1.147400
C	4.863217	-0.146728	0.350544
O	6.004622	0.163188	0.674358
Cl	3.963909	0.790297	2.644521
C	2.949740	-2.531010	0.023516
H	3.608005	-2.542399	0.894294
H	2.749523	-3.583605	-0.230363
C	1.605219	-1.888525	0.401671
H	0.859132	-2.070361	-0.371378
C	1.083974	-2.197576	1.758033
C	-0.260967	-2.592317	1.922424
C	1.893566	-2.139186	2.912461
C	-0.773319	-2.917228	3.177035
H	-0.900765	-2.667615	1.049225
C	1.378794	-2.460530	4.166550
H	2.925948	-1.819725	2.829635
C	0.044141	-2.850437	4.307839
H	-1.811373	-3.226591	3.266834
H	2.024602	-2.402536	5.038807
H	-0.352743	-3.101731	5.287795

int4^{S}

B3LYP SCF energy: -2740.63134554 a.u.
B3LYP enthalpy: -2739.793178 a.u.
B3LYP free energy: -2739.921221 a.u.
M06 SCF energy in solution: -2740.45570744 a.u.
M06 enthalpy in solution: -2739.617540 a.u.
M06 free energy in solution: -2739.745583 a.u.
Three lowest frequencies (cm-1): 15.5910 19.5459 25.8796

Cartesian coordinates

ATOM	X	Y	Z
Co	2.017530	0.061571	-0.072858
O	-1.574516	3.686562	0.953042
O	-0.537019	-3.123516	-2.063849
C	2.013479	1.824109	-1.364789
C	1.275523	2.013813	-0.168222
H	1.504731	2.701195	0.633511
C	0.188289	1.079625	-0.130619
C	0.151037	0.412153	-1.426137
C	1.280291	0.829824	-2.127794
H	1.572911	0.450187	-3.098917
C	3.078040	2.759400	-1.938391
C	2.344571	4.049324	-2.390976
H	1.552476	3.819799	-3.112712
H	3.049511	4.741268	-2.868562
H	1.885567	4.564343	-1.539566
C	4.149902	3.143389	-0.900198
H	3.707096	3.565388	0.009005
H	4.821603	3.901533	-1.320481
H	4.756498	2.278341	-0.615394
C	3.770661	2.137785	-3.167108
H	4.245259	1.182492	-2.924507
H	4.546147	2.817432	-3.539685
H	3.063540	1.971246	-3.987464
C	-0.898340	1.029183	0.915801
H	-0.613106	1.660867	1.759363
H	-1.013916	0.009863	1.288474
C	-2.207990	1.507015	0.310759
C	-2.509866	2.907187	0.328558
C	-3.662089	3.393951	-0.246177
H	-3.898807	4.451934	-0.225767
C	-4.563550	2.513788	-0.901726
C	-5.741153	3.000224	-1.529764
H	-5.951109	4.066669	-1.487349
C	-6.599411	2.145911	-2.185875
H	-7.495468	2.533592	-2.663378
C	-6.312732	0.762597	-2.243839
H	-6.987967	0.092442	-2.768776
C	-5.180879	0.260091	-1.637884
H	-4.968016	-0.802105	-1.687031
C	-4.278152	1.112017	-0.944456
C	-3.082674	0.625370	-0.306528

C	-2.778758	-0.845102	-0.328413
C	-3.536971	-1.735683	0.507283
C	-4.530654	-1.281683	1.417552
H	-4.729573	-0.217989	1.492626
C	-5.235101	-2.167727	2.204032
H	-5.988001	-1.798011	2.894855
C	-4.979545	-3.556373	2.119049
H	-5.539243	-4.248682	2.742579
C	-4.018183	-4.028427	1.253911
H	-3.808945	-5.093762	1.190176
C	-3.271288	-3.140156	0.433264
C	-2.268729	-3.619824	-0.446811
H	-2.077470	-4.686035	-0.477946
C	-1.525511	-2.742742	-1.205277
C	-1.771880	-1.332417	-1.148589
C	-0.957596	-0.415487	-2.041739
H	-0.533133	-0.999962	-2.860819
H	-1.648162	0.308067	-2.498936
C	-1.823124	5.078394	1.056177
H	-1.891582	5.549673	0.066695
H	-0.972908	5.496280	1.598572
H	-2.746181	5.280651	1.615146
C	-0.200045	-4.506641	-2.128760
H	-1.064642	-5.108835	-2.437667
H	0.196181	-4.852539	-1.169846
H	0.580854	-4.583874	-2.887489
N	1.593496	-1.698855	0.615556
C	3.434975	-1.966750	-0.763397
C	3.682714	-2.366082	-2.092882
H	3.009394	-3.089339	-2.541905
C	4.782014	-1.886699	-2.787275
H	4.967104	-2.208706	-3.808428
C	5.672562	-1.005404	-2.153468
H	6.551640	-0.646370	-2.682149
C	5.442977	-0.608337	-0.843006
H	6.157305	0.042266	-0.343801
C	4.327397	-1.073888	-0.113750
C	2.302221	-2.653103	-0.016866
O	2.159337	-3.875317	-0.045262
Cl	0.318934	-2.265251	1.658544
C	4.172913	-0.682314	1.353940
H	3.829941	-1.546816	1.925169
H	5.158908	-0.400507	1.751795
C	3.193304	0.488913	1.484694
H	3.683259	1.398303	1.131911
C	2.579758	0.750378	2.815594
C	2.411867	2.082731	3.247553
C	2.178488	-0.268238	3.699763
C	1.852691	2.386631	4.487105
H	2.748193	2.893178	2.603331
C	1.622363	0.032575	4.942832

H	2.287204	-1.306846	3.411017
C	1.450007	1.359012	5.343330
H	1.742074	3.425234	4.789316
H	1.319704	-0.777840	5.601013
H	1.016115	1.589106	6.312718

int4^{T}

B3LYP SCF energy: -2740.65716618 a.u.
B3LYP enthalpy: -2739.819686 a.u.
B3LYP free energy: -2739.950571 a.u.
M06 SCF energy in solution: -2740.48312151 a.u.
M06 enthalpy in solution: -2739.645641 a.u.
M06 free energy in solution: -2739.776526 a.u.
Three lowest frequencies (cm-1): 15.7717 17.6991 24.2100

Cartesian coordinates

ATOM	X	Y	Z
Co	1.970952	0.195601	0.009127
O	-2.124215	3.768570	0.794669
O	-0.541890	-3.179906	-1.672944
C	1.718702	1.901741	-1.357139
C	0.956882	2.126512	-0.142847
H	1.160642	2.880430	0.605986
C	-0.137646	1.227743	-0.100703
C	-0.082081	0.427660	-1.291725
C	1.063168	0.826239	-2.027657
H	1.357630	0.401010	-2.979451
C	2.703839	2.858001	-2.029278
C	1.895663	3.660058	-3.084611
H	1.470413	2.997439	-3.845519
H	2.544752	4.387094	-3.588486
H	1.070307	4.207762	-2.615562
C	3.318096	3.870611	-1.044116
H	2.546579	4.442914	-0.516878
H	3.942311	4.585921	-1.591976
H	3.955574	3.388430	-0.297609
C	3.832484	2.092642	-2.747205
H	4.436466	1.513500	-2.042466
H	4.493312	2.794702	-3.270239
H	3.437067	1.393836	-3.492114
C	-1.219712	1.184397	0.954224
H	-0.988714	1.914605	1.733155
H	-1.256177	0.198424	1.424816
C	-2.566398	1.499077	0.327417
C	-2.987242	2.865406	0.236584
C	-4.177424	3.204086	-0.366477
H	-4.504826	4.236048	-0.428214
C	-5.000864	2.200156	-0.942248
C	-6.218112	2.531766	-1.595153

H	-6.518921	3.576340	-1.636159
C	-7.002390	1.557051	-2.171241
H	-7.930196	1.827109	-2.668727
C	-6.597914	0.203293	-2.121150
H	-7.214686	-0.562444	-2.583587
C	-5.424511	-0.149765	-1.489027
H	-5.120625	-1.190175	-1.455291
C	-4.596483	0.829070	-0.875109
C	-3.362398	0.499966	-0.209781
C	-2.936605	-0.936088	-0.107321
C	-3.624525	-1.808985	0.805683
C	-4.651338	-1.357085	1.679561
H	-4.933774	-0.309913	1.663422
C	-5.284023	-2.223775	2.544826
H	-6.064216	-1.855462	3.205474
C	-4.919770	-3.590035	2.579247
H	-5.423738	-4.267410	3.263747
C	-3.923968	-4.058597	1.751880
H	-3.632151	-5.105964	1.778535
C	-3.249462	-3.189085	0.852330
C	-2.215133	-3.663227	0.006485
H	-1.946244	-4.711690	0.058882
C	-1.544136	-2.799724	-0.831072
C	-1.890529	-1.409449	-0.886131
C	-1.134664	-0.509767	-1.848279
H	-0.668673	-1.127302	-2.618554
H	-1.866874	0.131549	-2.360793
C	-2.488137	5.138331	0.782496
H	-2.591662	5.518705	-0.242430
H	-1.677720	5.669328	1.285596
H	-3.427385	5.309188	1.324984
C	-0.151700	-4.549903	-1.679289
H	-1.000609	-5.199167	-1.931126
H	0.284864	-4.835597	-0.717964
H	0.610392	-4.634781	-2.455848
N	1.899663	-1.626694	0.607873
C	3.719236	-2.153595	-0.847401
C	3.860094	-2.768242	-2.100180
H	3.144593	-3.534531	-2.381269
C	4.905004	-2.423977	-2.952993
H	4.996510	-2.903503	-3.923769
C	5.847032	-1.478039	-2.540919
H	6.679302	-1.215269	-3.188538
C	5.730479	-0.886128	-1.284121
H	6.485972	-0.177182	-0.951879
C	4.669306	-1.199123	-0.421401
C	2.596239	-2.654325	0.039555
O	2.390909	-3.857484	0.177448
Cl	0.659510	-2.123587	1.740228
C	4.597247	-0.547942	0.948804
H	4.287735	-1.288855	1.688765

H	5.609895	-0.224585	1.235492
C	3.680960	0.681556	1.025819
H	4.092856	1.502806	0.438971
C	3.275349	1.136461	2.381515
C	3.307307	2.509808	2.705185
C	2.859269	0.238794	3.386283
C	2.947696	2.965181	3.970816
H	3.633128	3.224187	1.953750
C	2.495855	0.695796	4.651973
H	2.798812	-0.821708	3.169740
C	2.537387	2.058884	4.952878
H	2.993289	4.028123	4.194024
H	2.175395	-0.018864	5.405286
H	2.255155	2.411527	5.941107

TS4^{S}

B3LYP SCF energy: -2430.94400297 a.u.
B3LYP enthalpy: -2430.253010 a.u.
B3LYP free energy: -2430.366328 a.u.
M06 SCF energy in solution: -2430.91027689 a.u.
M06 enthalpy in solution: -2430.219284 a.u.
M06 free energy in solution: -2430.332602 a.u.
Three lowest frequencies (cm-1): -209.3573 15.4689 18.1534
Imaginary frequency: -209.3573 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	2.278550	-0.044701	-0.232137
O	-1.151596	3.300384	2.052312
O	-0.149135	-2.230226	-2.928085
C	2.455226	2.145662	-0.796743
C	1.783299	1.961461	0.426083
H	2.093222	2.334892	1.391067
C	0.629185	1.130725	0.209171
C	0.515705	0.921575	-1.233375
C	1.661903	1.475350	-1.813033
H	1.920487	1.404544	-2.860943
C	3.674722	3.023638	-1.034673
C	3.166946	4.489927	-1.078012
H	2.426174	4.632132	-1.873221
H	4.006861	5.167734	-1.271929
H	2.705711	4.781109	-0.127690
C	4.697402	2.877715	0.110887
H	4.261997	3.141039	1.081643
H	5.544699	3.551481	-0.061382
H	5.075105	1.852654	0.169508
C	4.358208	2.695946	-2.376856
H	5.238647	3.335498	-2.506006
H	3.691381	2.883729	-3.226455

C	-0.408917	0.780275	1.250445
H	-0.086334	1.172706	2.216729
H	-0.490345	-0.304681	1.349011
C	-1.762410	1.352638	0.874044
C	-2.107757	2.674417	1.300481
C	-3.319329	3.233057	0.960145
H	-3.591446	4.230391	1.286992
C	-4.239777	2.512721	0.152420
C	-5.484949	3.079961	-0.229418
H	-5.730995	4.079795	0.120927
C	-6.364257	2.385292	-1.030163
H	-7.312419	2.833591	-1.314853
C	-6.033264	1.088870	-1.487981
H	-6.727418	0.547501	-2.124728
C	-4.834329	0.509860	-1.131092
H	-4.585766	-0.484383	-1.485991
C	-3.907687	1.195241	-0.298968
C	-2.645605	0.627200	0.090764
C	-2.263711	-0.748025	-0.373588
C	-2.856476	-1.901298	0.246310
C	-3.786171	-1.807588	1.317945
H	-4.074711	-0.826741	1.680816
C	-4.317557	-2.938436	1.899937
H	-5.025780	-2.844479	2.718614
C	-3.941444	-4.221770	1.438883
H	-4.364470	-5.108477	1.903587
C	-3.037604	-4.347489	0.407835
H	-2.739434	-5.331109	0.052766
C	-2.470704	-3.201386	-0.212881
C	-1.544027	-3.324186	-1.279854
H	-1.280773	-4.317333	-1.625258
C	-0.992478	-2.203530	-1.863915
C	-1.319298	-0.893233	-1.379170
C	-0.628016	0.303634	-2.007365
H	-0.257154	0.027108	-2.995804
H	-1.368737	1.102060	-2.153759
C	-1.430682	4.602229	2.542390
H	-1.590771	5.314165	1.722178
H	-0.551965	4.902255	3.116262
H	-2.311448	4.603500	3.197678
C	0.415766	-3.478184	-3.319258
H	-0.358347	-4.168360	-3.680345
H	0.973301	-3.924903	-2.489923
H	1.100270	-3.245761	-4.136630
N	2.060630	-1.624816	-0.861863
C	2.616058	-2.219219	1.424657
C	2.872445	-3.036662	2.530518
H	2.873338	-4.116613	2.409688
C	3.113680	-2.437214	3.763494
H	3.316970	-3.045183	4.640517
C	3.092152	-1.040858	3.867745

H	3.289242	-0.573299	4.830041
C	2.827037	-0.228867	2.755196
H	2.830332	0.849270	2.883810
C	2.590580	-0.816923	1.512682
C	2.339338	-2.706165	0.069385
O	2.211119	-3.860434	-0.306218
H	4.682095	1.652220	-2.412866
Cl	4.382994	-0.723728	-0.935166

TS4^{T}

B3LYP SCF energy: -2430.92744076 a.u.
B3LYP enthalpy: -2430.237367 a.u.
B3LYP free energy: -2430.353742 a.u.
M06 SCF energy in solution: -2430.89935335 a.u.
M06 enthalpy in solution: -2430.209280 a.u.
M06 free energy in solution: -2430.325655 a.u.
Three lowest frequencies (cm-1): -143.2381 15.2305 21.4676
Imaginary frequency: -143.2381 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	2.212254	0.211405	-0.138855
O	-1.627834	3.372469	1.933514
O	0.267328	-2.150784	-2.684695
C	2.325628	2.344258	-0.682896
C	1.603344	2.147115	0.525560
H	1.864550	2.545041	1.495721
C	0.456569	1.324345	0.264733
C	0.448050	1.042746	-1.154938
C	1.611585	1.634626	-1.706781
H	1.921637	1.536510	-2.737990
C	3.592250	3.169719	-0.852163
C	3.192804	4.661073	-0.714968
H	2.451034	4.944916	-1.470383
H	4.075522	5.297059	-0.850850
H	2.769640	4.873723	0.273319
C	4.625475	2.813239	0.239922
H	4.225880	2.970831	1.248048
H	5.511697	3.449294	0.131381
H	4.943929	1.769309	0.153117
C	4.227413	2.940672	-2.237225
H	5.136811	3.545118	-2.327832
H	3.551604	3.241927	-3.046369
C	-0.598825	0.919712	1.268328
H	-0.367196	1.384076	2.228878
H	-0.574612	-0.163184	1.415928
C	-1.986355	1.331734	0.809791
C	-2.482539	2.624580	1.171504
C	-3.729878	3.042335	0.764767

H	-4.116089	4.016896	1.042328
C	-4.537403	2.204344	-0.049727
C	-5.815734	2.627927	-0.501973
H	-6.177088	3.608153	-0.199433
C	-6.583797	1.821516	-1.312232
H	-7.558852	2.160881	-1.651473
C	-6.102992	0.552386	-1.709704
H	-6.709255	-0.076969	-2.355225
C	-4.868711	0.111228	-1.283092
H	-4.505047	-0.862788	-1.591979
C	-4.054602	0.913915	-0.438011
C	-2.759722	0.491574	0.023428
C	-2.217366	-0.849928	-0.375023
C	-2.727630	-2.044967	0.239460
C	-3.730040	-2.025300	1.247531
H	-4.137004	-1.071843	1.567195
C	-4.186041	-3.193083	1.820427
H	-4.952577	-3.155602	2.589584
C	-3.657808	-4.440669	1.413989
H	-4.022649	-5.356794	1.870800
C	-2.679204	-4.494071	0.446807
H	-2.262620	-5.449209	0.136054
C	-2.185805	-3.308237	-0.161662
C	-1.170927	-3.357579	-1.152457
H	-0.775683	-4.324431	-1.441851
C	-0.688421	-2.197219	-1.718610
C	-1.201513	-0.919794	-1.316056
C	-0.616114	0.327240	-1.953726
H	-0.197292	0.071027	-2.928826
H	-1.423467	1.051042	-2.128862
C	-2.058813	4.655109	2.360784
H	-2.251435	5.318427	1.507562
H	-1.242076	5.062651	2.959298
H	-2.964626	4.588248	2.977234
C	0.858649	-3.372562	-3.126055
H	0.100627	-4.041982	-3.553182
H	1.390399	-3.866028	-2.306753
H	1.572145	-3.086871	-3.900128
N	2.578889	-1.392242	-0.698119
C	2.723087	-2.021561	1.525394
C	2.962275	-2.827157	2.639675
H	3.088180	-3.898744	2.511725
C	3.034174	-2.222007	3.893935
H	3.216740	-2.821190	4.781650
C	2.873381	-0.836889	4.003528
H	2.936715	-0.366030	4.982044
C	2.630816	-0.041113	2.873935
H	2.514855	1.029983	3.009999
C	2.550424	-0.627550	1.608003
C	2.653918	-2.539777	0.134868
O	2.637053	-3.692516	-0.249288

H	4.501740	1.890388	-2.380806
Cl	4.711224	-0.958883	-1.549686

TS5^{T}

B3LYP SCF energy: -2740.61750116 a.u.
B3LYP enthalpy: -2739.782914 a.u.
B3LYP free energy: -2739.915003 a.u.
M06 SCF energy in solution: -2740.44550900 a.u.
M06 enthalpy in solution: -2739.610922 a.u.
M06 free energy in solution: -2739.743011 a.u.
Three lowest frequencies (cm-1): -403.4282 14.2361 22.7096
Imaginary frequency: -403.4282 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	2.086835	-0.115334	-0.393211
O	-1.200939	3.376688	2.187429
O	-0.976336	-1.982895	-3.034512
C	2.091977	2.130275	-1.026591
C	1.513328	1.845758	0.268354
H	1.870791	2.227879	1.215779
C	0.232382	1.198298	0.085104
C	0.062728	1.010383	-1.301430
C	1.220451	1.545452	-1.961343
H	1.375040	1.505988	-3.032589
C	3.292107	3.014602	-1.366304
C	2.825776	4.088943	-2.380056
H	2.486183	3.638003	-3.318315
H	3.654335	4.767914	-2.616467
H	2.000689	4.685774	-1.974212
C	3.816925	3.740325	-0.113562
H	3.035077	4.356493	0.346969
H	4.646492	4.402823	-0.387467
H	4.191324	3.037422	0.635573
C	4.432631	2.192843	-2.006977
H	4.840109	1.459735	-1.304929
H	5.250450	2.855463	-2.317827
H	4.081663	1.647935	-2.889838
C	-0.779102	0.874477	1.162931
H	-0.379882	1.171390	2.135543
H	-0.971869	-0.201150	1.201526
C	-2.082107	1.609787	0.895349
C	-2.247639	2.929846	1.427358
C	-3.386583	3.660890	1.177671
H	-3.518973	4.655924	1.587738
C	-4.412847	3.130695	0.351513
C	-5.579943	3.883845	0.054399
H	-5.682798	4.876445	0.487254
C	-6.559878	3.377754	-0.770482

H	-7.445773	3.967467	-0.990871
C	-6.409820	2.091935	-1.338420
H	-7.179134	1.699183	-1.997572
C	-5.291240	1.334607	-1.062079
H	-5.184523	0.350518	-1.504826
C	-4.266118	1.820807	-0.205277
C	-3.080440	1.062261	0.102967
C	-2.924573	-0.320669	-0.461845
C	-3.733704	-1.394838	0.053463
C	-4.625316	-1.229924	1.147842
H	-4.700744	-0.257022	1.621387
C	-5.386033	-2.281510	1.614968
H	-6.060692	-2.131391	2.453448
C	-5.292923	-3.554196	1.005392
H	-5.899593	-4.377260	1.373924
C	-4.431299	-3.750643	-0.051912
H	-4.348092	-4.729091	-0.519704
C	-3.627579	-2.688999	-0.549364
C	-2.703358	-2.896670	-1.608221
H	-2.635645	-3.883966	-2.052081
C	-1.897744	-1.865873	-2.044846
C	-2.010300	-0.551871	-1.477615
C	-1.163642	0.562523	-2.064755
H	-0.850789	0.273544	-3.069895
H	-1.804578	1.449389	-2.177265
C	-1.294330	4.670569	2.759286
H	-1.385140	5.445523	1.986872
H	-0.367505	4.821157	3.316172
H	-2.147998	4.745906	3.445838
C	-0.668013	-3.276029	-3.541349
H	-1.535012	-3.724315	-4.044670
H	-0.314862	-3.939064	-2.743181
H	0.136999	-3.124333	-4.260811
N	1.310007	-1.969264	-0.534597
C	0.676507	-2.848937	1.131425
C	-0.666357	-3.175037	1.355050
H	-1.295114	-3.472174	0.524740
C	-1.168527	-3.128945	2.652775
H	-2.206567	-3.388439	2.837774
C	-0.334189	-2.734055	3.704722
H	-0.724662	-2.691878	4.717976
C	0.996965	-2.384324	3.463548
H	1.634217	-2.076982	4.289529
C	1.524563	-2.419884	2.168897
C	1.357374	-3.226377	-0.262160
O	1.656936	-4.334793	-0.651201
C	2.942841	-2.004777	1.871463
H	3.391116	-2.685045	1.140953
H	3.536964	-2.113408	2.791970
C	3.109345	-0.545843	1.414949
H	2.635689	0.129267	2.129985

C	4.522796	-0.162750	1.159476
C	5.101911	0.915260	1.860469
C	5.346794	-0.899587	0.282546
C	6.447957	1.238937	1.702514
H	4.489299	1.484741	2.555971
C	6.690709	-0.568752	0.119447
H	4.921598	-1.715585	-0.293202
C	7.248560	0.498646	0.828380
H	6.873400	2.066156	2.264610
H	7.303823	-1.146739	-0.566610
H	8.297772	0.751036	0.701851
Cl	2.826406	-1.500219	-2.277760

int5^{T}

B3LYP SCF energy: -2740.64069193 a.u.
B3LYP enthalpy: -2739.805562 a.u.
B3LYP free energy: -2739.941924 a.u.
M06 SCF energy in solution: -2740.47536125 a.u.
M06 enthalpy in solution: -2739.640231 a.u.
M06 free energy in solution: -2739.776593 a.u.
Three lowest frequencies (cm-1): 9.6062 14.9182 24.4065

Cartesian coordinates

ATOM	X	Y	Z
Co	2.228906	-0.231347	-0.708133
O	-0.938762	3.152111	2.309342
O	-1.398329	-1.151873	-3.612043
C	1.729702	2.425267	-1.658997
C	1.456210	1.888725	-0.338565
H	2.004561	2.149653	0.557327
C	0.142685	1.377908	-0.346368
C	-0.378425	1.503792	-1.721623
C	0.601598	2.102342	-2.484836
H	0.518215	2.321898	-3.541704
C	2.862668	3.344515	-2.058627
C	2.264902	4.779764	-2.131200
H	1.462782	4.844737	-2.873847
H	3.052871	5.487263	-2.416168
H	1.859720	5.092738	-1.162179
C	4.010598	3.336929	-1.031844
H	3.673485	3.667657	-0.042715
H	4.797525	4.026692	-1.358104
H	4.449977	2.340329	-0.937144
C	3.413561	2.962097	-3.452521
H	3.833326	1.952546	-3.440688
H	4.204214	3.666283	-3.737608
H	2.636277	3.008646	-4.223161
C	-0.628729	0.859118	0.838037
H	-0.042439	1.027442	1.744462

H	-0.762322	-0.222644	0.722491
C	-1.994622	1.511750	0.983497
C	-2.110325	2.709601	1.758031
C	-3.327143	3.335076	1.916626
H	-3.422943	4.238432	2.508844
C	-4.489648	2.813527	1.289194
C	-5.749601	3.456943	1.419187
H	-5.814847	4.357823	2.025138
C	-6.867792	2.958300	0.788550
H	-7.824262	3.462886	0.896418
C	-6.773416	1.792077	-0.006162
H	-7.657003	1.407705	-0.508044
C	-5.565881	1.142941	-0.147975
H	-5.497830	0.249797	-0.759581
C	-4.394489	1.624232	0.498212
C	-3.118098	0.976666	0.370330
C	-2.966950	-0.261211	-0.461833
C	-3.442955	-1.526746	0.022724
C	-4.095418	-1.679390	1.277004
H	-4.250241	-0.805037	1.900454
C	-4.530361	-2.914197	1.707963
H	-5.027927	-3.008043	2.669418
C	-4.329060	-4.061424	0.904866
H	-4.676619	-5.031296	1.251132
C	-3.689160	-3.950370	-0.309193
H	-3.524067	-4.829021	-0.928482
C	-3.224601	-2.692020	-0.781471
C	-2.540674	-2.579438	-2.018412
H	-2.354202	-3.479663	-2.591239
C	-2.075223	-1.356309	-2.451575
C	-2.297170	-0.176749	-1.672527
C	-1.763204	1.144752	-2.194533
H	-1.759933	1.131776	-3.286921
H	-2.446345	1.947287	-1.885469
C	-0.974504	4.328825	3.100546
H	-1.314418	5.194362	2.517124
H	0.050930	4.498010	3.434441
H	-1.627305	4.205006	3.974500
C	-0.989824	-2.294223	-4.366484
H	-1.860452	-2.842341	-4.751402
H	-0.362259	-2.946356	-3.752375
H	-0.415778	-1.898257	-5.206295
N	1.198498	-1.695634	-0.781808
C	1.337361	-3.790313	0.472763
C	0.485385	-4.869277	0.748825
H	-0.307869	-5.086205	0.041223
C	0.653351	-5.640878	1.895042
H	-0.021129	-6.467945	2.099218
C	1.697588	-5.346373	2.772909
H	1.847040	-5.942576	3.669301
C	2.558863	-4.285508	2.493857

H	3.382386	-4.072820	3.171932
C	2.398708	-3.489062	1.351342
C	1.051305	-3.034091	-0.800347
O	0.618753	-3.630428	-1.798669
C	3.389682	-2.366332	1.106256
H	3.812421	-2.426523	0.096159
H	4.237500	-2.504855	1.790905
C	2.799610	-0.982205	1.362516
H	1.801757	-0.993954	1.799041
C	3.646634	0.098184	1.857645
C	3.102498	1.073255	2.728096
C	5.023062	0.184845	1.541871
C	3.896830	2.081517	3.263800
H	2.050762	1.013676	2.997680
C	5.812572	1.195864	2.078731
H	5.455907	-0.529338	0.850346
C	5.256490	2.148361	2.940197
H	3.461218	2.810133	3.942267
H	6.866841	1.246425	1.821439
H	5.878316	2.935360	3.357822
Cl	4.185964	-0.306277	-1.844346

TS6^{T}

B3LYP SCF energy: -2740.63293613 a.u.
B3LYP enthalpy: -2739.798750 a.u.
B3LYP free energy: -2739.932183 a.u.
M06 SCF energy in solution: -2740.46626138 a.u.
M06 enthalpy in solution: -2739.632075 a.u.
M06 free energy in solution: -2739.765508 a.u.
Three lowest frequencies (cm-1): -54.1611 5.3581 17.6044
Imaginary frequency: -54.1611 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	1.525108	-0.110739	-0.191165
N	2.687167	-0.751320	-1.418270
C	5.043145	-1.217989	-1.815688
C	5.979088	-2.185438	-2.208977
H	5.603961	-3.173791	-2.453368
C	7.334807	-1.884307	-2.287223
H	8.046934	-2.644246	-2.597291
C	7.767901	-0.596735	-1.965960
H	8.823058	-0.341747	-2.021883
C	6.842171	0.369201	-1.572186
H	7.189017	1.370263	-1.326347
C	5.470310	0.089984	-1.490346
C	3.608577	-1.673386	-1.758406
O	3.282109	-2.835714	-2.055148
C	4.537659	1.212364	-1.060663

H	3.747826	1.376299	-1.804521
H	5.126265	2.139639	-1.035918
C	3.924561	1.006820	0.313773
H	4.169668	0.075525	0.818439
C	3.605638	2.118220	1.172851
C	3.528074	1.933370	2.577238
C	3.429154	3.433858	0.673887
C	3.299510	3.000183	3.435758
H	3.676424	0.937394	2.984199
C	3.204357	4.499037	1.537837
H	3.450176	3.604519	-0.395939
C	3.137787	4.292612	2.920883
H	3.259224	2.832213	4.508744
H	3.079742	5.499793	1.132652
H	2.968470	5.130392	3.591901
Cl	0.922753	1.901242	-1.054727
O	-2.358075	-3.875837	-0.859687
O	-1.144647	3.313036	1.172678
C	1.301006	-1.754444	1.353269
C	0.584803	-2.102294	0.109112
H	0.873698	-2.891817	-0.573140
C	-0.502738	-1.241246	-0.061849
C	-0.479180	-0.302288	1.039240
C	0.642037	-0.628611	1.876590
H	0.884189	-0.108672	2.793295
C	2.263287	-2.679343	2.087712
C	1.437544	-3.940408	2.465372
H	0.570396	-3.678837	3.082317
H	2.065664	-4.635751	3.034656
H	1.077953	-4.464009	1.573510
C	3.459374	-3.118548	1.222132
H	3.151727	-3.550096	0.266599
H	4.045482	-3.869892	1.764681
H	4.122132	-2.275286	1.002742
C	2.786943	-2.037113	3.384789
H	3.366226	-1.131398	3.178682
H	3.448087	-2.739787	3.903702
H	1.974470	-1.776510	4.072220
C	-1.528745	-1.285503	-1.166252
H	-1.242087	-2.053847	-1.886945
H	-1.556365	-0.326786	-1.691230
C	-2.889325	-1.598250	-0.569821
C	-3.268152	-2.968741	-0.394038
C	-4.464382	-3.303325	0.199481
H	-4.760570	-4.338837	0.325637
C	-5.334514	-2.288799	0.680542
C	-6.558960	-2.613568	1.323465
H	-6.828304	-3.661913	1.430966
C	-7.389548	-1.627031	1.807071
H	-8.322304	-1.891915	2.297957
C	-7.027374	-0.267261	1.669696

H	-7.681769	0.508113	2.058441
C	-5.848082	0.079283	1.045093
H	-5.577211	1.124424	0.943054
C	-4.971769	-0.912796	0.526926
C	-3.729713	-0.590651	-0.126294
C	-3.348853	0.847018	-0.326744
C	-4.030861	1.615856	-1.333994
C	-5.007815	1.054483	-2.200858
H	-5.257214	0.003550	-2.103152
C	-5.632272	1.820000	-3.162204
H	-6.373274	1.368644	-3.816271
C	-5.309222	3.189396	-3.304120
H	-5.805719	3.786533	-4.064496
C	-4.362085	3.762427	-2.485417
H	-4.102274	4.812898	-2.594300
C	-3.697199	2.998552	-1.488525
C	-2.720664	3.581827	-0.642069
H	-2.496959	4.635788	-0.761338
C	-2.064030	2.820257	0.298518
C	-2.350017	1.423222	0.442774
C	-1.569975	0.641426	1.486191
H	-1.141952	1.338285	2.208509
H	-2.275482	0.004091	2.042827
C	-2.678524	-5.254933	-0.774284
H	-2.801200	-5.575299	0.268833
H	-1.836370	-5.786603	-1.220777
H	-3.594719	-5.488124	-1.332290
C	-0.659849	4.630772	0.970494
H	-1.453314	5.376697	1.115778
H	-0.227780	4.735868	-0.031003
H	0.120800	4.777474	1.718156

int6^{T}

B3LYP SCF energy: -2740.75971426 a.u.
B3LYP enthalpy: -2739.921428 a.u.
B3LYP free energy: -2740.055460 a.u.
M06 SCF energy in solution: -2740.57927678 a.u.
M06 enthalpy in solution: -2739.740991 a.u.
M06 free energy in solution: -2739.875023 a.u.
Three lowest frequencies (cm-1): 12.9349 14.7114 20.5395

Cartesian coordinates

ATOM	X	Y	Z
Co	1.511173	-0.281126	1.055989
O	-1.602077	-2.760118	-2.807522
O	-0.975775	1.033179	3.423917
C	1.599398	-2.642493	0.690200
C	1.101435	-2.074241	-0.483906
H	1.561693	-2.105126	-1.461105

C	-0.111482	-1.361401	-0.186723
C	-0.413887	-1.552816	1.225661
C	0.651893	-2.272181	1.763500
H	0.754472	-2.556392	2.802763
C	2.751751	-3.617980	0.836238
C	2.121075	-5.028430	0.999953
H	1.495466	-5.088111	1.897690
H	2.915613	-5.778360	1.092710
H	1.501957	-5.290196	0.134400
C	3.645401	-3.609777	-0.418175
H	3.089634	-3.914325	-1.312898
H	4.470729	-4.318355	-0.287532
H	4.077313	-2.620338	-0.596443
C	3.612445	-3.309939	2.079834
H	5.077572	-0.158572	-3.286361
H	4.389244	-4.077190	2.181875
H	3.019755	-3.309086	3.000342
C	-0.985724	-0.648893	-1.180989
H	-0.538213	-0.726478	-2.174225
H	-1.030673	0.410494	-0.909148
C	-2.390358	-1.235066	-1.192549
C	-2.664189	-2.346983	-2.051881
C	-3.914257	-2.923587	-2.087620
H	-4.130159	-3.758553	-2.744869
C	-4.950134	-2.444465	-1.242130
C	-6.237555	-3.045131	-1.239739
H	-6.425690	-3.877032	-1.914659
C	-7.228690	-2.592636	-0.397194
H	-8.207698	-3.064382	-0.405366
C	-6.973318	-1.517536	0.485567
H	-7.755897	-1.170413	1.154474
C	-5.736017	-0.910356	0.502081
H	-5.543725	-0.087308	1.181875
C	-4.694126	-1.345221	-0.361945
C	-3.390320	-0.740334	-0.367311
C	-3.079868	0.415525	0.536082
C	-3.588869	1.725757	0.232638
C	-4.425519	1.990790	-0.885743
H	-4.698572	1.173975	-1.545273
C	-4.893437	3.262088	-1.141662
H	-5.533237	3.440394	-2.001611
C	-4.542762	4.335829	-0.290573
H	-4.918203	5.334745	-0.496827
C	-3.722800	4.116439	0.793935
H	-3.442495	4.938897	1.448115
C	-3.219372	2.818282	1.082430
C	-2.345840	2.593806	2.177599
H	-2.059261	3.437748	2.795122
C	-1.848034	1.333832	2.426885
C	-2.233162	0.220521	1.615136
C	-1.674901	-1.150271	1.956641

H	-1.475835	-1.201681	3.029462
H	-2.440317	-1.905092	1.735246
C	-1.798506	-3.837735	-3.709064
H	-2.085363	-4.756133	-3.180415
H	-0.839581	-3.990848	-4.207461
H	-2.564746	-3.598602	-4.457943
C	-0.306681	2.102042	4.086099
H	-1.002476	2.680128	4.708871
H	0.181702	2.756792	3.356867
H	0.451578	1.632330	4.712476
N	2.524671	0.922691	-0.415740
C	1.554264	3.118707	-0.939989
C	0.407025	3.919171	-0.946560
H	-0.469232	3.592053	-0.396134
C	0.405212	5.117343	-1.659535
H	-0.485410	5.739478	-1.672374
C	1.549605	5.512211	-2.358040
H	1.549661	6.444144	-2.917689
C	2.697142	4.714570	-2.343028
H	3.586208	5.030632	-2.884015
C	2.712262	3.510976	-1.635648
C	1.595268	1.826827	-0.219507
O	0.677692	1.511806	0.640671
Cl	2.773317	0.128559	2.901533
C	3.932671	2.625217	-1.531944
H	4.498049	2.887106	-0.625277
H	4.606977	2.782167	-2.381401
C	3.547574	1.128959	-1.440093
H	3.127867	0.834520	-2.417419
C	4.783147	0.278969	-1.195879
C	5.468624	-0.286814	-2.278452
C	5.294383	0.100412	0.097428
C	6.644824	-1.013377	-2.080120
H	4.093372	-2.332328	1.999876
C	6.469240	-0.628008	0.296367
H	4.755837	0.510627	0.946656
C	7.149504	-1.184794	-0.789708
H	7.162381	-1.447603	-2.931898
H	6.850901	-0.761693	1.305386
H	8.063312	-1.751762	-0.631352

TS7[T]

B3LYP SCF energy: -2969.84340272 a.u.
B3LYP enthalpy: -2968.940755 a.u.
B3LYP free energy: -2969.090177 a.u.
M06 SCF energy in solution: -2969.55040696 a.u.
M06 enthalpy in solution: -2968.647759 a.u.
M06 free energy in solution: -2968.797181 a.u.
Three lowest frequencies (cm-1): -927.1365 8.4599 12.0845

Imaginary frequency: -927.1365 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-1.917829	1.171401	-0.229310
O	4.690203	3.088436	-1.301850
O	-0.118489	-2.308855	1.050921
C	0.169770	3.251526	0.255628
C	1.149531	3.052229	-0.784354
H	1.420197	3.781639	-1.537737
C	1.673602	1.788311	-0.688070
C	1.040103	1.133881	0.463640
C	0.037407	2.008456	0.958725
H	-0.443505	1.890580	1.922097
C	-0.410608	4.598900	0.636178
C	-1.007229	5.302400	-0.606243
H	-0.256817	5.441741	-1.392046
H	-1.379403	6.295176	-0.323610
H	-1.835531	4.720291	-1.017410
C	-1.487625	4.480420	1.730640
H	-2.319787	3.850464	1.407499
H	-1.881589	5.475174	1.970776
H	-1.077192	4.056767	2.654117
C	0.760090	5.462070	1.183901
H	1.215713	4.998079	2.066098
H	0.384326	6.451015	1.474376
H	1.543673	5.602271	0.431690
C	2.731605	1.186884	-1.571182
H	2.955125	1.882785	-2.382332
H	2.353904	0.263101	-2.020248
C	3.985881	0.903364	-0.764172
C	4.965874	1.938867	-0.617282
C	6.089026	1.748475	0.156021
H	6.837413	2.525858	0.261985
C	6.283040	0.526039	0.852791
C	7.419919	0.321982	1.679594
H	8.153283	1.121094	1.761904
C	7.592965	-0.857501	2.369654
H	8.467265	-0.997542	2.999887
C	6.629181	-1.886380	2.263150
H	6.764525	-2.812660	2.814891
C	5.518373	-1.719814	1.463501
H	4.783584	-2.513882	1.388475
C	5.313249	-0.519431	0.730231
C	4.164807	-0.303870	-0.111055
C	3.151012	-1.397828	-0.270497
C	3.483305	-2.542811	-1.074730
C	4.696184	-2.640964	-1.810381
H	5.404915	-1.821030	-1.769570
C	4.975901	-3.751279	-2.577660
H	5.906697	-3.802466	-3.135886

C	4.055225	-4.822717	-2.646487
H	4.283778	-5.694465	-3.253942
C	2.869420	-4.757415	-1.949872
H	2.152986	-5.574047	-2.002759
C	2.550772	-3.623554	-1.155352
C	1.333700	-3.546579	-0.432292
H	0.652431	-4.388399	-0.481791
C	1.022696	-2.423767	0.301808
C	1.920249	-1.308285	0.364906
C	1.525752	-0.094109	1.194300
H	0.766746	-0.386108	1.923100
H	2.409024	0.223163	1.770691
C	5.619196	4.156318	-1.223186
H	5.737168	4.511129	-0.190795
H	5.206526	4.958856	-1.837342
H	6.601627	3.864523	-1.617510
C	-0.847371	-3.498050	1.319392
H	-0.191299	-4.276421	1.730230
H	-1.339537	-3.885085	0.417590
H	-1.606282	-3.228713	2.054546
N	-3.537172	-0.236030	0.337425
C	-3.560676	-1.070912	2.673525
C	-3.087246	-0.931298	3.985032
H	-2.496056	-0.055863	4.233110
C	-3.379247	-1.903881	4.936691
H	-3.013603	-1.799880	5.954190
C	-4.144282	-3.017844	4.574101
H	-4.371452	-3.782954	5.311893
C	-4.616790	-3.157064	3.267462
H	-5.211109	-4.025965	2.994782
C	-4.332562	-2.187322	2.301187
C	-3.251004	-0.036739	1.660727
O	-2.699906	1.049409	1.962584
C	-4.846393	-2.277151	0.883386
H	-5.829044	-1.788477	0.825631
H	-5.003919	-3.322468	0.593831
C	-3.885174	-1.606011	-0.118819
H	-2.950795	-2.179850	-0.133759
C	-4.441007	-1.612448	-1.535121
C	-3.679387	-2.161772	-2.573239
C	-5.715479	-1.107794	-1.832497
C	-4.177085	-2.215813	-3.876020
H	-2.677422	-2.525242	-2.364335
C	-6.214204	-1.157316	-3.134562
H	-6.321724	-0.655770	-1.053027
C	-5.448044	-1.715684	-4.160151
H	-3.565509	-2.639087	-4.668110
H	-7.202925	-0.758698	-3.346885
H	-5.837683	-1.754504	-5.174078
Cl	-0.992533	0.295409	-2.117061
C	-4.409931	2.657518	-0.692032

O	-5.077367	1.626721	-0.331217
H	-4.348497	0.711731	-0.039645
O	-3.149591	2.725311	-0.696107
C	-5.196115	3.857878	-1.165018
H	-5.087676	3.941355	-2.252526
H	-6.253634	3.755138	-0.916761
H	-4.785292	4.769187	-0.721890

int7^{T}

B3LYP SCF energy: -2260.44189152 a.u.
B3LYP enthalpy: -2259.794887 a.u.
B3LYP free energy: -2259.908494 a.u.
M06 SCF energy in solution: -2260.52503804 a.u.
M06 enthalpy in solution: -2259.878034 a.u.
M06 free energy in solution: -2259.991641 a.u.
Three lowest frequencies (cm-1): 18.1952 23.5620 31.6868

Cartesian coordinates

ATOM	X	Y	Z
Co	2.553835	-0.577403	0.089039
O	-0.911538	3.415165	1.828635
O	0.577370	-2.478828	-2.137669
C	2.980403	1.629660	-0.390989
C	2.136633	1.641879	0.741362
H	2.402403	1.980844	1.733150
C	0.904856	1.016618	0.409169
C	0.943759	0.664146	-1.016701
C	2.206779	1.013456	-1.481867
H	2.574138	0.854011	-2.486248
C	4.350157	2.275640	-0.501637
C	4.135467	3.812114	-0.444808
H	3.491074	4.155840	-1.262306
H	5.101763	4.321716	-0.537591
H	3.677720	4.118230	0.502105
C	5.248026	1.841438	0.679109
H	4.801744	2.097037	1.646440
H	6.215498	2.352680	0.612141
H	5.422028	0.761537	0.657878
C	5.043099	1.914290	-1.829735
H	5.171917	0.832281	-1.927576
H	6.032939	2.382880	-1.864325
H	4.476937	2.281945	-2.694068
C	-0.267899	0.807706	1.328649
H	-0.041192	1.254274	2.299149
H	-0.407746	-0.268502	1.476759
C	-1.545349	1.411869	0.761757
C	-1.838735	2.783636	1.047939
C	-2.979019	3.380762	0.557896
H	-3.211201	4.416443	0.779691

C	-3.872502	2.651014	-0.270249
C	-5.040234	3.255855	-0.807933
H	-5.250952	4.293605	-0.559823
C	-5.888465	2.549743	-1.631625
H	-6.776916	3.027172	-2.036236
C	-5.602575	1.203582	-1.958364
H	-6.270546	0.653760	-2.615485
C	-4.479940	0.587684	-1.448549
H	-4.263982	-0.444330	-1.703214
C	-3.589709	1.283564	-0.585556
C	-2.408206	0.675495	-0.038365
C	-2.061955	-0.749578	-0.350642
C	-2.784145	-1.828558	0.266066
C	-3.878377	-1.620472	1.149697
H	-4.187609	-0.605585	1.375835
C	-4.548603	-2.683287	1.716515
H	-5.383990	-2.501056	2.387000
C	-4.152368	-4.010660	1.430631
H	-4.687527	-4.843304	1.879493
C	-3.085537	-4.246679	0.592718
H	-2.767935	-5.264613	0.378880
C	-2.369759	-3.173173	-0.003575
C	-1.242623	-3.411048	-0.831962
H	-0.923816	-4.434701	-0.993545
C	-0.547829	-2.356942	-1.381650
C	-0.977241	-1.009357	-1.172552
C	-0.191956	0.106007	-1.838998
H	0.217329	-0.253338	-2.786215
H	-0.876430	0.930442	-2.074129
C	-1.139966	4.771124	2.179361
H	-1.180247	5.413769	1.290253
H	-0.293926	5.066381	2.802434
H	-2.070897	4.885671	2.749671
C	1.233612	-3.742822	-2.177872
H	0.630432	-4.485409	-2.716576
H	1.448639	-4.094253	-1.163268
H	2.171727	-3.571796	-2.706146
O	1.521570	-2.030894	0.959793
C	2.197820	-1.960987	2.056515
O	3.062099	-1.057368	2.179407
Cl	4.300770	-1.631995	-0.881634
C	1.947525	-2.985406	3.134615
H	0.882266	-3.222715	3.198622
H	2.482229	-3.906473	2.874018
H	2.320626	-2.625140	4.095424

TS8^{T}

B3LYP SCF energy: -2740.61460397 a.u.

B3LYP enthalpy: -2739.780448 a.u.

B3LYP free energy: -2739.914206 a.u.
M06 SCF energy in solution: -2740.44025321 a.u.
M06 enthalpy in solution: -2739.606097 a.u.
M06 free energy in solution: -2739.739855 a.u.
Three lowest frequencies (cm-1): -417.6075 7.2643 18.1391
Imaginary frequency: -417.6075 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	1.734947	0.055653	0.168996
N	2.516496	-1.665668	-0.505700
C	4.421650	-1.671340	-1.065267
C	4.829935	-1.886550	-2.386677
H	4.260119	-2.553308	-3.026598
C	5.991208	-1.268530	-2.843194
H	6.336255	-1.440550	-3.858620
C	6.713835	-0.431112	-1.985539
H	7.622138	0.049094	-2.339067
C	6.273134	-0.196497	-0.679838
H	6.840554	0.464474	-0.028874
C	5.103936	-0.794459	-0.198672
C	3.353560	-2.634764	-0.380904
O	3.539038	-3.767713	0.005496
C	4.572171	-0.521050	1.190801
H	4.225565	-1.453696	1.645294
H	5.406550	-0.168621	1.816640
C	3.475442	0.552735	1.264306
H	3.793605	1.461572	0.755704
C	2.934691	0.845893	2.612959
C	2.743018	2.185637	3.019732
C	2.619836	-0.172021	3.538505
C	2.267202	2.494657	4.289825
H	2.990257	2.988795	2.330067
C	2.141078	0.139724	4.809217
H	2.722573	-1.212076	3.249968
C	1.961176	1.470898	5.192361
H	2.139764	3.534313	4.580182
H	1.900800	-0.663113	5.500744
H	1.586702	1.709591	6.183994
Cl	0.847920	-2.015107	1.123410
O	-2.275538	3.614581	0.982363
O	-0.575409	-3.099710	-1.875958
C	1.584812	1.914993	-1.264686
C	0.849171	2.013405	-0.012018
H	1.029033	2.732334	0.775708
C	-0.271476	1.135942	-0.059292
C	-0.212956	0.443803	-1.307423
C	0.929973	0.916479	-2.015846
H	1.226852	0.562184	-2.995809
C	2.603614	2.902023	-1.829497
C	1.849529	3.779807	-2.864907

H	1.452014	3.170897	-3.683276
H	2.525998	4.530338	-3.293362
H	1.008730	4.305442	-2.398064
C	3.181833	3.843365	-0.755076
H	2.391316	4.394868	-0.233502
H	3.841388	4.581007	-1.226930
H	3.775310	3.308459	-0.007093
C	3.758043	2.174310	-2.547024
H	4.343363	1.568648	-1.849283
H	4.432136	2.901684	-3.016242
H	3.387527	1.510485	-3.335312
C	-1.367384	1.022453	0.977068
H	-1.145046	1.697603	1.806759
H	-1.408167	0.005977	1.378132
C	-2.709351	1.379649	0.361723
C	-3.133732	2.747806	0.361120
C	-4.321901	3.124793	-0.223313
H	-4.651357	4.157913	-0.215639
C	-5.140266	2.161245	-0.870983
C	-6.354565	2.533323	-1.507271
H	-6.658510	3.577463	-1.478867
C	-7.131981	1.598104	-2.154081
H	-8.057489	1.899111	-2.638008
C	-6.723720	0.245051	-2.194170
H	-7.335360	-0.488880	-2.711800
C	-5.553218	-0.147142	-1.579996
H	-5.245358	-1.186490	-1.614584
C	-4.732163	0.789940	-0.895635
C	-3.501330	0.418799	-0.247948
C	-3.065788	-1.017627	-0.241931
C	-3.738928	-1.956612	0.614925
C	-4.789211	-1.581341	1.496798
H	-5.102421	-0.543410	1.531616
C	-5.407742	-2.510492	2.305946
H	-6.207459	-2.200259	2.973167
C	-5.003524	-3.865323	2.274489
H	-5.496257	-4.592265	2.915023
C	-3.982117	-4.260007	1.439613
H	-3.658328	-5.298103	1.417306
C	-3.321639	-3.325304	0.597273
C	-2.257798	-3.722958	-0.251735
H	-1.953800	-4.763468	-0.244622
C	-1.608220	-2.798656	-1.038710
C	-2.004709	-1.422136	-1.037334
C	-1.259710	-0.451495	-1.937100
H	-0.787797	-1.010019	-2.747984
H	-1.997674	0.216862	-2.404705
C	-2.642029	4.981241	1.054640
H	-2.744397	5.424480	0.055070
H	-1.833835	5.481881	1.591531
H	-3.582836	5.116934	1.604561

C	0.022088	-4.384309	-1.773268
H	-0.682352	-5.179334	-2.052815
H	0.402707	-4.558539	-0.760824
H	0.855940	-4.381802	-2.477556

int8^{T}

B3LYP SCF energy: -2740.64242717 a.u.
B3LYP enthalpy: -2739.807202 a.u.
B3LYP free energy: -2739.943373 a.u.
M06 SCF energy in solution: -2740.47279954 a.u.
M06 enthalpy in solution: -2739.637574 a.u.
M06 free energy in solution: -2739.773745 a.u.
Three lowest frequencies (cm-1): 11.2514 13.6625 23.4467

Cartesian coordinates

ATOM	X	Y	Z
Co	2.418580	0.347370	-0.476359
O	-1.785963	3.072811	1.866068
O	-1.009014	-1.850831	-3.501147
C	1.083277	2.581193	-1.990377
C	0.944821	2.135732	-0.619010
H	1.356183	2.659556	0.237298
C	-0.220405	1.333539	-0.557177
C	-0.731184	1.165480	-1.923941
C	0.082131	1.897273	-2.760592
H	-0.036027	1.972076	-3.834724
C	1.943564	3.705085	-2.527621
C	0.984925	4.844982	-2.973861
H	0.299250	4.514949	-3.761043
H	1.573875	5.683209	-3.365209
H	0.385421	5.212638	-2.133184
C	2.908968	4.264731	-1.466772
H	2.365910	4.667151	-0.603347
H	3.494606	5.083740	-1.900072
H	3.605625	3.497415	-1.119870
C	2.748833	3.220674	-3.759168
H	3.447119	2.426934	-3.480623
H	3.322278	4.059198	-4.172586
H	2.090688	2.844618	-4.550224
C	-0.857877	0.783116	0.687830
H	-0.352671	1.208401	1.557083
H	-0.697060	-0.301624	0.703911
C	-2.350392	1.063274	0.770575
C	-2.790987	2.273198	1.395737
C	-4.131990	2.569225	1.500542
H	-4.471562	3.480271	1.980846
C	-5.105753	1.686159	0.962754
C	-6.493034	1.982756	1.039065
H	-6.803493	2.899757	1.534841

C	-7.429982	1.133625	0.493248
H	-8.487531	1.375439	0.558490
C	-7.018402	-0.051757	-0.159452
H	-7.761208	-0.713596	-0.596036
C	-5.679899	-0.369167	-0.245768
H	-5.368184	-1.278003	-0.749003
C	-4.687425	0.478546	0.317663
C	-3.283183	0.181377	0.245240
C	-2.794992	-1.058480	-0.442293
C	-2.925148	-2.341765	0.189522
C	-3.540153	-2.520127	1.459154
H	-3.940526	-1.654420	1.976262
C	-3.634424	-3.768500	2.035793
H	-4.110742	-3.882687	3.005846
C	-3.110224	-4.902241	1.371170
H	-3.187192	-5.883193	1.832804
C	-2.497761	-4.762220	0.146141
H	-2.083456	-5.627968	-0.364976
C	-2.383421	-3.488919	-0.476159
C	-1.735233	-3.338545	-1.728262
H	-1.306436	-4.215526	-2.197916
C	-1.612649	-2.093882	-2.307997
C	-2.150655	-0.934751	-1.663417
C	-1.973127	0.415283	-2.334280
H	-1.952851	0.284081	-3.418738
H	-2.845168	1.040911	-2.103178
C	-2.137399	4.294891	2.493040
H	-2.680385	4.957078	1.806057
H	-1.195019	4.764656	2.780796
H	-2.750479	4.126326	3.388409
C	-0.356333	-2.933851	-4.162182
H	-1.075863	-3.716586	-4.438259
H	0.435520	-3.341208	-3.528610
H	0.072812	-2.505015	-5.069869
N	1.688603	-1.304090	-0.453134
C	2.945998	-3.239632	0.410200
C	3.560265	-4.439151	0.022782
H	3.353892	-4.809436	-0.975617
C	4.399544	-5.131131	0.890228
H	4.872059	-6.055849	0.570428
C	4.624792	-4.628476	2.172503
H	5.274832	-5.157131	2.864748
C	4.008040	-3.442401	2.568545
H	4.178906	-3.061135	3.572888
C	3.166616	-2.726164	1.705783
C	2.067045	-2.591082	-0.630895
O	1.695084	-3.231495	-1.625130
C	2.534763	-1.446468	2.219812
H	1.449435	-1.461075	2.067433
H	2.691036	-1.408800	3.308672
C	3.142509	-0.186270	1.626112

H	4.131846	-0.318355	1.189065
C	2.918807	1.108523	2.250776
C	3.793139	2.189634	1.969248
C	1.862067	1.330798	3.168035
C	3.613330	3.428372	2.574401
H	4.601390	2.037733	1.260123
C	1.687528	2.573696	3.767219
H	1.185372	0.519419	3.416141
C	2.558946	3.629049	3.473091
H	4.298530	4.240556	2.348295
H	0.873271	2.720076	4.471470
H	2.422168	4.597445	3.946489
Cl	4.430226	0.887786	-1.357760

TS9^{T}

B3LYP SCF energy: -2740.64149100 a.u.
B3LYP enthalpy: -2739.806842 a.u.
B3LYP free energy: -2739.939141 a.u.
M06 SCF energy in solution: -2740.47335076 a.u.
M06 enthalpy in solution: -2739.638702 a.u.
M06 free energy in solution: -2739.771001 a.u.
Three lowest frequencies (cm-1): -41.4014 12.3763 13.8762
Imaginary frequency: -41.4014 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	1.631606	-0.082660	-0.542511
O	-2.111795	3.264200	1.498672
O	-0.920229	-2.797896	-2.653430
C	1.368723	1.994478	-1.378353
C	0.751087	1.923764	-0.088773
H	1.055801	2.458767	0.798543
C	-0.325452	1.019464	-0.144783
C	-0.453656	0.561720	-1.545920
C	0.587099	1.136119	-2.259955
H	0.802590	0.963608	-3.305541
C	2.374865	3.039283	-1.833037
C	1.596587	4.384318	-1.883813
H	0.737208	4.319438	-2.560568
H	2.258952	5.176692	-2.252052
H	1.229817	4.675830	-0.893443
C	3.545761	3.183648	-0.840279
H	3.196886	3.380304	0.180273
H	4.180276	4.025921	-1.138823
H	4.167446	2.284573	-0.832137
C	2.928560	2.731209	-3.237911
H	3.435787	1.762148	-3.269887
H	3.653968	3.503550	-3.519012
H	2.132696	2.745424	-3.991864

C	-1.295294	0.704284	0.961421
H	-0.966728	1.198838	1.877802
H	-1.295724	-0.374381	1.141718
C	-2.690047	1.171652	0.575975
C	-3.068702	2.523401	0.860942
C	-4.310282	3.002405	0.507884
H	-4.605017	4.021789	0.730803
C	-5.231923	2.168920	-0.179678
C	-6.506203	2.652625	-0.579856
H	-6.774458	3.677996	-0.335482
C	-7.385473	1.846993	-1.268840
H	-8.356001	2.232374	-1.569980
C	-7.024897	0.518124	-1.591311
H	-7.718443	-0.111231	-2.142069
C	-5.797752	0.018504	-1.211127
H	-5.526488	-1.001127	-1.461785
C	-4.870221	0.819266	-0.490021
C	-3.578888	0.334097	-0.081829
C	-3.178185	-1.078750	-0.388224
C	-3.751176	-2.162640	0.363002
C	-4.680167	-1.963039	1.420417
H	-4.975000	-0.951633	1.679028
C	-5.205208	-3.029235	2.118958
H	-5.913292	-2.853073	2.924193
C	-4.823507	-4.351757	1.794309
H	-5.242374	-5.187428	2.348875
C	-3.916967	-4.578931	0.783107
H	-3.610528	-5.592621	0.535370
C	-3.353597	-3.501161	0.047813
C	-2.403784	-3.728640	-0.980526
H	-2.109683	-4.749740	-1.195360
C	-1.845436	-2.670975	-1.662914
C	-2.231563	-1.324715	-1.369598
C	-1.597813	-0.202705	-2.171194
H	-1.255598	-0.593788	-3.131548
H	-2.374971	0.542732	-2.392299
C	-2.422260	4.604367	1.842678
H	-2.635650	5.209242	0.951528
H	-1.536746	4.998720	2.344678
H	-3.280758	4.654782	2.525165
C	-0.311084	-4.066626	-2.847001
H	-1.037095	-4.810152	-3.202767
H	0.157767	-4.416212	-1.920397
H	0.454451	-3.916037	-3.609959
N	3.224602	-0.560974	-1.225189
C	5.600055	-0.817401	-0.636309
C	6.906888	-0.738233	-1.141713
H	7.027950	-0.395611	-2.163808
C	8.004661	-1.089402	-0.363356
H	9.008469	-1.025610	-0.774520
C	7.801838	-1.523239	0.947511

H	8.646679	-1.800683	1.572656
C	6.507063	-1.598273	1.459067
H	6.356740	-1.933266	2.482704
C	5.385337	-1.257197	0.689656
C	4.510916	-0.395296	-1.592478
O	4.797076	0.049491	-2.717926
C	4.015833	-1.379680	1.334791
H	3.391153	-2.104791	0.799840
H	4.152563	-1.793448	2.342822
C	3.291685	-0.050510	1.461819
H	3.801030	0.807125	1.030738
C	2.449970	0.253821	2.597288
C	2.323858	1.597026	3.035239
C	1.785203	-0.748810	3.345387
C	1.572434	1.922111	4.158053
H	2.851498	2.378581	2.493161
C	1.028673	-0.416682	4.463630
H	1.841020	-1.779653	3.016577
C	0.915727	0.915796	4.876887
H	1.503784	2.957151	4.482402
H	0.519211	-1.200698	5.017083
H	0.325503	1.167814	5.753591
Cl	0.801155	-2.037701	0.328067

int9^{T}

B3LYP SCF energy: -2740.75672502 a.u.
B3LYP enthalpy: -2739.917882 a.u.
B3LYP free energy: -2740.049731 a.u.
M06 SCF energy in solution: -2740.58205673 a.u.
M06 enthalpy in solution: -2739.743214 a.u.
M06 free energy in solution: -2739.875063 a.u.
Three lowest frequencies (cm-1): 13.6879 19.0561 24.6736

Cartesian coordinates

ATOM	X	Y	Z
Co	1.780038	1.639265	-0.083996
O	-3.403538	2.655889	1.628896
O	0.979719	-1.754231	-2.642776
C	0.603272	3.493591	-0.719921
C	-0.061650	2.979090	0.464102
H	-0.116176	3.481125	1.419819
C	-0.565826	1.710127	0.195374
C	-0.238400	1.395242	-1.210505
C	0.446475	2.505377	-1.739683
H	0.838455	2.565528	-2.746056
C	1.141804	4.898847	-0.927162
C	0.074130	5.670688	-1.749735
H	-0.088031	5.210173	-2.730388
H	0.408430	6.702933	-1.908585

H	-0.887486	5.702424	-1.224409
C	1.360669	5.627677	0.412677
H	0.420636	5.747675	0.964840
H	1.758508	6.631210	0.223221
H	2.072686	5.087789	1.042972
C	2.466659	4.869943	-1.720344
H	3.241421	4.338129	-1.160879
H	2.808499	5.895399	-1.903529
H	2.347312	4.381555	-2.693958
C	-1.398482	0.857245	1.114319
H	-1.462312	1.340000	2.091135
H	-0.925483	-0.115447	1.261357
C	-2.782640	0.672375	0.518196
C	-3.792569	1.651670	0.788362
C	-5.045972	1.549976	0.227648
H	-5.816772	2.283588	0.436096
C	-5.352326	0.482574	-0.657868
C	-6.629959	0.378039	-1.270016
H	-7.381451	1.129109	-1.037297
C	-6.915411	-0.646474	-2.145115
H	-7.896977	-0.711280	-2.607026
C	-5.929090	-1.612951	-2.448653
H	-6.155307	-2.415162	-3.145625
C	-4.681790	-1.541491	-1.865708
H	-3.930837	-2.286339	-2.105584
C	-4.356297	-0.502680	-0.951162
C	-3.064299	-0.388248	-0.327459
C	-2.010742	-1.418839	-0.609261
C	-2.132042	-2.726922	-0.022407
C	-3.171009	-3.068944	0.885855
H	-3.907221	-2.317757	1.150292
C	-3.250995	-4.331280	1.435511
H	-4.053260	-4.570366	2.128161
C	-2.293862	-5.317193	1.100396
H	-2.365273	-6.310690	1.535047
C	-1.271479	-5.016924	0.227719
H	-0.529413	-5.768826	-0.031207
C	-1.158473	-3.722882	-0.349348
C	-0.103338	-3.402392	-1.242965
H	0.607425	-4.178683	-1.503350
C	0.011429	-2.131328	-1.764109
C	-0.936597	-1.107448	-1.429622
C	-0.775863	0.266232	-2.059761
H	-0.141930	0.181447	-2.944249
H	-1.764830	0.598360	-2.409256
C	-4.351990	3.655214	1.966234
H	-4.690484	4.203430	1.077311
H	-3.837611	4.341246	2.641550
H	-5.223048	3.224975	2.477626
C	1.881056	-2.738560	-3.129105
H	1.343700	-3.544083	-3.647021

H	2.488212	-3.162558	-2.321057
H	2.535573	-2.219017	-3.829759
N	2.323093	-0.230138	0.374317
C	4.224894	-1.304153	-0.754062
C	5.182515	-1.250287	-1.773600
H	5.126106	-0.443290	-2.497015
C	6.185288	-2.215264	-1.835872
H	6.933115	-2.175216	-2.623125
C	6.231879	-3.229494	-0.873938
H	7.017825	-3.979414	-0.913171
C	5.279862	-3.278685	0.146940
H	5.327637	-4.064873	0.897078
C	4.266945	-2.318149	0.219708
C	3.157014	-0.280948	-0.665899
O	3.015897	0.625771	-1.548560
C	3.192396	-2.339113	1.283142
H	2.342336	-2.930652	0.916119
H	3.555418	-2.829519	2.193704
C	2.709452	-0.913240	1.619305
H	3.562317	-0.366038	2.049769
C	1.599447	-0.882605	2.660744
C	1.612320	0.128031	3.632758
C	0.566586	-1.830012	2.697747
C	0.623170	0.190514	4.616489
H	2.402368	0.874188	3.608525
C	-0.421000	-1.774591	3.684200
H	0.519667	-2.619196	1.953967
C	-0.395833	-0.763885	4.647471
H	0.654831	0.980766	5.362391
H	-1.211956	-2.519859	3.690682
H	-1.162444	-0.722436	5.417085
Cl	3.400032	2.642130	1.163605

TS10^{T}

B3LYP SCF energy: -2969.84542908 a.u.
B3LYP enthalpy: -2968.941504 a.u.
B3LYP free energy: -2969.087658 a.u.
M06 SCF energy in solution: -2969.62566128 a.u.
M06 enthalpy in solution: -2968.721736 a.u.
M06 free energy in solution: -2968.867890 a.u.
Three lowest frequencies (cm-1): -270.5951 9.6999 14.5372
Imaginary frequency: -270.5951 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	1.600776	0.286926	0.222387
O	-2.130581	-3.138568	-2.189026
O	-1.988831	1.349794	3.564855
C	0.775409	-2.343568	1.707542

C	0.528647	-1.789609	0.369782
H	1.051880	-2.104080	-0.529469
C	-0.785442	-1.295646	0.366135
C	-1.311403	-1.393622	1.732504
C	-0.354022	-2.026539	2.506757
H	-0.453749	-2.232064	3.564316
C	1.957818	-3.195725	2.121493
C	1.683936	-3.900031	3.466091
H	1.555555	-3.179433	4.281207
H	2.531259	-4.544740	3.725369
H	0.786228	-4.526793	3.416616
C	2.220819	-4.268217	1.034277
H	1.341210	-4.905859	0.887026
H	3.054792	-4.909058	1.345227
H	2.483423	-3.813915	0.074387
C	3.226021	-2.318814	2.277612
H	3.502481	-1.845628	1.331398
H	4.067791	-2.948627	2.591286
H	3.075153	-1.528816	3.018037
C	-1.543443	-0.818338	-0.846382
H	-0.988515	-1.117911	-1.739178
H	-1.566255	0.276261	-0.834173
C	-2.970844	-1.332757	-0.932525
C	-3.234388	-2.541992	-1.651953
C	-4.518314	-3.027943	-1.772654
H	-4.724163	-3.939464	-2.322606
C	-5.605297	-2.347398	-1.162787
C	-6.933866	-2.841946	-1.257948
H	-7.110753	-3.753727	-1.823978
C	-7.979365	-2.188181	-0.644385
H	-8.989700	-2.580351	-0.725597
C	-7.740451	-1.008074	0.097927
H	-8.567684	-0.500517	0.586427
C	-6.463058	-0.501404	0.205839
H	-6.283913	0.402605	0.778306
C	-5.363320	-1.144922	-0.424324
C	-4.018401	-0.649348	-0.333705
C	-3.703367	0.584385	0.458894
C	-3.996216	1.888316	-0.068346
C	-4.632058	2.086402	-1.324530
H	-4.921920	1.219441	-1.908883
C	-4.886205	3.354925	-1.802092
H	-5.377028	3.484021	-2.762950
C	-4.512157	4.489636	-1.044603
H	-4.718918	5.486280	-1.425798
C	-3.881995	4.332013	0.169877
H	-3.583408	5.200901	0.751924
C	-3.600051	3.038718	0.687424
C	-2.923799	2.870475	1.923984
H	-2.620715	3.755384	2.472284
C	-2.642259	1.608076	2.400774

C	-3.041151	0.444424	1.667876
C	-2.660632	-0.922647	2.209418
H	-2.654445	-0.900165	3.301709
H	-3.423898	-1.650257	1.905424
C	-2.302489	-4.336281	-2.929108
H	-2.732164	-5.132872	-2.307618
H	-1.304205	-4.629986	-3.257700
H	-2.944487	-4.177392	-3.805630
C	-1.357797	2.429631	4.240634
H	-2.094462	3.156527	4.608483
H	-0.631756	2.925355	3.586977
H	-0.833447	1.983599	5.086758
N	3.293096	0.240499	-1.035696
C	5.113678	-1.450884	-1.069743
C	5.571958	-2.694990	-1.523967
H	4.888662	-3.320795	-2.088708
C	6.870982	-3.107511	-1.243757
H	7.227468	-4.069685	-1.600992
C	7.714132	-2.279036	-0.495254
H	8.729661	-2.596220	-0.272395
C	7.260723	-1.040864	-0.038931
H	7.922835	-0.397463	0.535842
C	5.961104	-0.610700	-0.323441
C	3.688111	-1.064397	-1.317479
O	2.870274	-1.899439	-1.720943
C	5.431111	0.731577	0.122481
H	4.942225	0.644812	1.102990
H	6.249135	1.453187	0.230139
C	4.418249	1.225786	-0.916773
H	4.938175	1.218138	-1.886901
C	3.935752	2.654703	-0.713502
C	3.771531	3.480145	-1.837422
C	3.686030	3.198037	0.553659
C	3.354585	4.804662	-1.703835
H	3.972746	3.077952	-2.827311
C	3.268752	4.524326	0.690348
H	3.794814	2.587751	1.442468
C	3.100659	5.331463	-0.434875
H	3.241202	5.427221	-2.587859
H	3.074993	4.922079	1.682736
H	2.780626	6.364442	-0.325431
Cl	1.710274	1.005180	2.379201
H	2.418989	0.701820	-2.086682
O	0.489152	1.496560	-0.972086
C	0.730275	1.708666	-2.187663
O	1.739828	1.206513	-2.817030
C	-0.169421	2.620094	-2.978904
H	0.216749	3.642038	-2.880431
H	-0.157434	2.349367	-4.036849
H	-1.185463	2.598755	-2.579994

TS2b[S]

B3LYP SCF energy: -2701.30005524 a.u.
B3LYP enthalpy: -2700.492991 a.u.
B3LYP free energy: -2700.619098 a.u.
M06 SCF energy in solution: -2701.14968457 a.u.
M06 enthalpy in solution: -2700.342620 a.u.
M06 free energy in solution: -2700.468727 a.u.
Three lowest frequencies (cm-1): -291.3428 14.2866 22.8786
Imaginary frequency: -291.3428 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	1.878432	-0.258815	0.158420
O	-2.012555	-3.113058	-2.241287
O	-0.481510	2.335641	2.727046
C	1.664995	-2.390294	0.509347
C	1.003806	-1.972788	-0.707934
H	1.272162	-2.289176	-1.706828
C	-0.083056	-1.122910	-0.390294
C	-0.044536	-0.892002	1.027703
C	1.005204	-1.718730	1.558953
H	1.284180	-1.755161	2.603439
C	2.781636	-3.404937	0.592098
C	2.252381	-4.799186	0.192469
H	1.808992	-4.789866	-0.809280
H	1.487079	-5.145574	0.898280
H	3.069715	-5.529679	0.192698
C	3.447868	-3.454254	1.974136
H	4.272743	-4.175031	1.966795
H	2.737719	-3.773944	2.747835
H	3.855512	-2.480488	2.261933
C	-1.149757	-0.663704	-1.355218
H	-0.898378	-1.014112	-2.358232
H	-1.216319	0.426181	-1.391766
C	-2.491057	-1.225251	-0.917043
C	-2.889191	-2.521145	-1.377916
C	-4.073308	-3.086619	-0.960411
H	-4.383974	-4.063871	-1.312422
C	-4.910182	-2.403920	-0.037720
C	-6.121401	-2.983455	0.426028
H	-6.406639	-3.963326	0.050050
C	-6.918671	-2.326737	1.337085
H	-7.841266	-2.784640	1.683601
C	-6.535014	-1.057350	1.827867
H	-7.162817	-0.546129	2.552416
C	-5.368199	-0.466424	1.392105
H	-5.080163	0.507039	1.774292
C	-4.526904	-1.112175	0.445695
C	-3.299102	-0.533011	-0.029863

C	-2.884510	0.832749	0.434926
C	-3.567147	1.985366	-0.088080
C	-4.595040	1.893620	-1.067123
H	-4.882034	0.916765	-1.440169
C	-5.222988	3.022615	-1.547094
H	-6.004376	2.929354	-2.296155
C	-4.854611	4.302977	-1.072093
H	-5.356480	5.187196	-1.455571
C	-3.857776	4.427892	-0.130774
H	-3.563239	5.409165	0.233933
C	-3.188242	3.283023	0.378432
C	-2.150138	3.402505	1.337635
H	-1.888347	4.393735	1.689644
C	-1.491165	2.284634	1.798551
C	-1.839175	0.971635	1.339697
C	-1.104874	-0.238288	1.897370
H	-0.652917	0.027858	2.855479
H	-1.853559	-1.013062	2.114787
C	-2.335878	-4.395750	-2.755336
H	-2.426529	-5.137763	-1.951503
H	-1.509844	-4.671658	-3.412946
H	-3.269688	-4.372104	-3.332141
C	-0.188182	3.587589	3.334699
H	-1.070212	3.995529	3.843570
H	0.176439	4.316035	2.599518
H	0.598416	3.388536	4.064300
N	3.600350	-0.418173	-0.706970
C	4.354578	0.257805	1.371860
C	5.302603	0.222112	2.397026
H	6.325085	-0.033417	2.134117
C	4.920325	0.483246	3.712547
H	5.655535	0.453337	4.512210
C	3.581767	0.775872	3.997318
H	3.272930	0.967526	5.022404
C	2.637967	0.840057	2.970762
H	1.611835	1.111302	3.200513
C	3.011964	0.587798	1.640072
C	4.744952	-0.172583	-0.012251
O	5.910824	-0.296023	-0.382434
Cl	3.836008	-1.046323	-2.318030
C	2.130513	1.895259	0.504213
H	3.053831	2.459622	0.418046
H	1.469556	2.263660	1.279905
C	1.478346	1.542183	-0.730734
H	0.392928	1.553095	-0.679261
C	1.992438	1.892311	-2.070058
C	1.087415	1.920024	-3.148573
C	3.322452	2.278243	-2.322974
C	1.489553	2.307495	-4.424989
H	0.050082	1.643384	-2.977435
C	3.724181	2.670820	-3.596733

H	4.059049	2.249428	-1.527402
C	2.812981	2.686592	-4.655998
H	0.766871	2.319794	-5.236962
H	4.759051	2.956838	-3.764140
H	3.131636	2.992249	-5.648933
H	3.542170	-3.115849	-0.143575

TS3b[S]

B3LYP SCF energy: -2701.29455449 a.u.
B3LYP enthalpy: -2700.487664 a.u.
B3LYP free energy: -2700.612278 a.u.
M06 SCF energy in solution: -2701.14720510 a.u.
M06 enthalpy in solution: -2700.340315 a.u.
M06 free energy in solution: -2700.464929 a.u.
Three lowest frequencies (cm-1): -291.9832 18.3842 22.4822
Imaginary frequency: -291.9832 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	2.044296	0.606504	-0.227477
O	-2.055544	3.469625	1.636278
O	-0.158676	-2.637714	-2.376059
C	1.627155	2.574246	-1.027988
C	0.948415	2.424748	0.219874
H	1.122432	3.000315	1.118950
C	0.027256	1.351046	0.132927
C	0.048388	0.870494	-1.237952
C	1.029781	1.615699	-1.918499
H	1.316349	1.463552	-2.951946
C	2.510183	3.723766	-1.471562
C	3.372696	4.332954	-0.355640
H	2.753742	4.721739	0.462150
H	3.957071	5.172622	-0.748072
H	4.076651	3.609563	0.068027
C	1.632170	4.817980	-2.119652
H	1.037310	4.414814	-2.945913
H	2.255426	5.630594	-2.511845
H	0.939527	5.245111	-1.384447
C	-0.980725	0.978380	1.191819
H	-0.752734	1.522612	2.111013
H	-0.922382	-0.087114	1.414670
C	-2.372581	1.328842	0.697123
C	-2.884749	2.646826	0.921806
C	-4.120473	3.019885	0.443309
H	-4.517494	4.013482	0.619457
C	-4.900860	2.106963	-0.315479
C	-6.164730	2.481495	-0.844726
H	-6.535662	3.484633	-0.646305
C	-6.907060	1.599872	-1.598939

H	-7.871420	1.902096	-1.998787
C	-6.413022	0.300685	-1.858253
H	-6.998396	-0.389900	-2.459117
C	-5.192655	-0.093888	-1.352508
H	-4.819856	-1.092001	-1.554752
C	-4.404307	0.787811	-0.563835
C	-3.122989	0.414726	-0.025088
C	-2.593756	-0.971587	-0.252568
C	-3.160847	-2.067435	0.485095
C	-4.169073	-1.893834	1.472786
H	-4.533677	-0.894318	1.684052
C	-4.681182	-2.969879	2.165408
H	-5.449239	-2.813249	2.918028
C	-4.208088	-4.277091	1.904367
H	-4.616056	-5.120369	2.455557
C	-3.227749	-4.479012	0.959119
H	-2.851775	-5.479687	0.759263
C	-2.677273	-3.389791	0.230624
C	-1.665051	-3.591223	-0.740580
H	-1.314234	-4.600860	-0.918153
C	-1.117549	-2.521834	-1.414628
C	-1.563620	-1.184018	-1.157477
C	-0.935762	-0.043976	-1.939254
H	-0.453063	-0.446820	-2.832050
H	-1.746034	0.611468	-2.290750
C	-2.509602	4.778538	1.936548
H	-2.688627	5.361859	1.023546
H	-1.712699	5.248524	2.516247
H	-3.429953	4.756986	2.534820
C	0.304371	-3.943306	-2.708746
H	-0.522945	-4.576677	-3.055469
H	0.814524	-4.399559	-1.855241
H	1.016844	-3.800353	-3.523023
N	1.881765	-1.267400	0.273324
C	3.262652	-1.533455	-1.566066
C	3.720231	-2.262727	-2.665818
H	3.551299	-3.335363	-2.669621
C	4.364867	-1.614326	-3.717631
H	4.720741	-2.179842	-4.574620
C	4.555994	-0.229218	-3.660624
H	5.057413	0.286932	-4.475709
C	4.128842	0.494412	-2.546972
H	4.340762	1.559339	-2.499388
C	3.474552	-0.145219	-1.480836
C	2.487076	-2.218999	-0.483974
O	2.441760	-3.445774	-0.360769
Cl	0.916346	-1.898108	1.577746
C	4.203010	0.571405	0.194824
H	4.781651	-0.335186	0.338209
H	4.769344	1.359638	-0.291120
C	3.374246	0.988680	1.292769

H	3.271582	2.064334	1.395576
C	3.283145	0.296756	2.593462
C	2.698862	0.987688	3.672043
C	3.818228	-0.979469	2.845047
C	2.642716	0.429976	4.946839
H	2.287810	1.981176	3.503017
C	3.769011	-1.535931	4.120507
H	4.261501	-1.554686	2.038881
C	3.180305	-0.838027	5.177741
H	2.183935	0.986325	5.760150
H	4.185696	-2.525603	4.286725
H	3.141722	-1.277899	6.170574
H	3.183672	3.348948	-2.253723

TS2c^{S}

B3LYP SCF energy: -2583.35517964 a.u.
B3LYP enthalpy: -2582.637436 a.u.
B3LYP free energy: -2582.753712 a.u.
M06 SCF energy in solution: -2583.26444442 a.u.
M06 enthalpy in solution: -2582.546701 a.u.
M06 free energy in solution: -2582.662977 a.u.
Three lowest frequencies (cm-1): -293.6255 15.1027 23.6506
Imaginary frequency: -293.6255 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-2.010400	-0.526369	-0.516661
O	2.101251	-3.813563	0.721111
O	0.164808	3.038350	-1.713106
C	-1.605367	-2.270426	-1.674021
C	-0.996070	-2.376250	-0.375067
H	-1.257868	-3.092085	0.391061
C	0.025618	-1.400129	-0.270625
C	0.000778	-0.614811	-1.476362
C	-0.978546	-1.204398	-2.344989
H	-1.244976	-0.826103	-3.323034
C	1.026215	-1.294613	0.855279
H	0.788610	-2.042932	1.614050
H	0.983833	-0.313287	1.334096
C	2.425733	-1.517920	0.310678
C	2.937461	-2.852648	0.230476
C	4.182628	-3.100552	-0.302816
H	4.579786	-4.107968	-0.358709
C	4.972314	-2.034768	-0.811106
C	6.247972	-2.274049	-1.388588
H	6.619272	-3.295622	-1.425345
C	7.001178	-1.239726	-1.898296
H	7.974554	-1.439721	-2.338154
C	6.506755	0.084303	-1.855563

H	7.100765	0.896222	-2.265918
C	5.274606	0.349031	-1.296616
H	4.901461	1.367231	-1.268915
C	4.475998	-0.693417	-0.752547
C	3.184082	-0.460592	-0.164578
C	2.644948	0.936359	-0.063893
C	3.189997	1.827803	0.924059
C	4.194741	1.430496	1.849296
H	4.573382	0.415054	1.812753
C	4.686085	2.312313	2.787582
H	5.451610	1.986961	3.486483
C	4.197215	3.638185	2.848683
H	4.591351	4.326227	3.591682
C	3.219503	4.053018	1.972681
H	2.832765	5.068400	2.018255
C	2.689596	3.165422	0.998161
C	1.671889	3.579245	0.100771
H	1.317928	4.601916	0.163033
C	1.146399	2.696667	-0.816445
C	1.615279	1.344472	-0.902719
C	1.020573	0.409035	-1.944370
H	0.573332	1.002049	-2.744993
H	1.846083	-0.154309	-2.401402
C	2.535432	-5.164448	0.690364
H	2.716770	-5.503336	-0.337803
H	1.724527	-5.749396	1.127501
H	3.448386	-5.304662	1.283676
C	-0.227921	4.403120	-1.792589
H	0.629201	5.047406	-2.023741
H	-0.696465	4.742543	-0.860191
H	-0.958015	4.457596	-2.601730
N	-3.717606	-1.160607	0.121472
C	-4.490948	0.192960	-1.587778
C	-5.398938	0.467431	-2.613055
H	-6.386488	0.019843	-2.548581
C	-5.019617	1.269792	-3.687981
H	-5.724302	1.482603	-4.487378
C	-3.722216	1.792019	-3.735965
H	-3.413945	2.407786	-4.577792
C	-2.820165	1.540336	-2.701026
H	-1.828570	1.982616	-2.732827
C	-3.194473	0.741622	-1.606997
C	-4.861522	-0.792774	-0.519061
O	-6.010213	-1.182843	-0.322362
Cl	-3.909499	-2.415590	1.315981
C	-2.476011	1.553699	0.005380
H	-3.454463	1.948006	0.262035
H	-1.847605	2.261351	-0.522459
C	-1.802139	0.794764	1.029143
H	-0.722258	0.920381	1.039219
C	-2.363067	0.527715	2.368102

C	-1.476820	0.205474	3.413849
C	-3.729755	0.649812	2.683174
C	-1.931537	0.003720	4.715222
H	-0.413591	0.124137	3.201832
C	-4.184533	0.453724	3.984059
H	-4.449730	0.874043	1.903737
C	-3.290858	0.127702	5.007699
H	-1.222738	-0.243425	5.501451
H	-5.246105	0.546313	4.196832
H	-3.651024	-0.026545	6.021288
H	-2.431672	-2.865923	-2.036914

TS3c^{S}

B3LYP SCF energy: -2583.35450371 a.u.
B3LYP enthalpy: -2582.637090 a.u.
B3LYP free energy: -2582.752836 a.u.
M06 SCF energy in solution: -2583.26666713 a.u.
M06 enthalpy in solution: -2582.549253 a.u.
M06 free energy in solution: -2582.664999 a.u.
Three lowest frequencies (cm-1): -294.9174 15.1532 20.0145
Imaginary frequency: -294.9174 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Co	-2.086633	-0.775879	-0.853955
O	2.295460	-3.828561	-0.305927
O	-0.217463	3.224499	-1.025098
C	-1.463877	-2.033264	-2.425528
C	-0.817599	-2.479966	-1.234566
H	-0.966903	-3.426212	-0.732956
C	0.015686	-1.441066	-0.755796
C	-0.019682	-0.363568	-1.731807
C	-0.917167	-0.749272	-2.746383
H	-1.196090	-0.136614	-3.593562
C	0.952154	-1.544412	0.422759
H	0.765342	-2.485651	0.944483
H	0.766128	-0.732916	1.127449
C	2.388869	-1.484425	-0.063923
C	3.044554	-2.693612	-0.460596
C	4.330377	-2.674877	-0.952154
H	4.835160	-3.588572	-1.245837
C	5.022129	-1.443411	-1.104339
C	6.337370	-1.398675	-1.639067
H	6.817125	-2.333408	-1.920676
C	6.994348	-0.199676	-1.806290
H	7.999690	-0.182035	-2.218837
C	6.359882	1.011515	-1.445967
H	6.879065	1.955716	-1.585649
C	5.086196	0.999732	-0.918460

H	4.604840	1.931940	-0.643543
C	4.382540	-0.220292	-0.725387
C	3.049530	-0.272494	-0.186288
C	2.360834	0.992927	0.234769
C	2.759804	1.639722	1.454867
C	3.754527	1.107925	2.320791
H	4.240385	0.175191	2.055274
C	4.102040	1.753619	3.487917
H	4.863103	1.327666	4.136156
C	3.468954	2.966025	3.848659
H	3.747822	3.468225	4.771344
C	2.496497	3.503906	3.036061
H	1.997853	4.430297	3.311248
C	2.113616	2.860545	1.828017
C	1.107865	3.405804	0.991379
H	0.630431	4.330277	1.293831
C	0.724866	2.753627	-0.160044
C	1.338021	1.516190	-0.542980
C	0.887812	0.845726	-1.829393
H	0.400645	1.587490	-2.465689
H	1.783733	0.507197	-2.369362
C	2.886603	-5.071432	-0.646887
H	3.158163	-5.109589	-1.710109
H	2.131136	-5.831490	-0.438581
H	3.780025	-5.270516	-0.040605
C	-0.826618	4.479301	-0.734332
H	-0.071874	5.273139	-0.658051
H	-1.419253	4.415897	0.183355
H	-1.485768	4.685637	-1.579262
N	-2.183059	0.594162	0.517832
C	-3.495969	1.632352	-1.082315
C	-3.991429	2.768693	-1.725475
H	-3.970777	3.709789	-1.184158
C	-4.482534	2.677406	-3.026970
H	-4.868211	3.560421	-3.529375
C	-4.477200	1.441626	-3.685193
H	-4.851906	1.363744	-4.702789
C	-4.015112	0.299758	-3.031179
H	-4.062190	-0.661149	-3.539555
C	-3.524139	0.378067	-1.716936
C	-2.862807	1.745357	0.271730
O	-2.968614	2.746551	0.984330
Cl	-1.344289	0.558828	2.042187
C	-4.253014	-1.129494	-0.696496
H	-4.911719	-0.465203	-0.146871
H	-4.728506	-1.577243	-1.563008
C	-3.431165	-2.017450	0.079772
H	-3.234223	-2.972329	-0.400909
C	-3.455566	-2.129723	1.551404
C	-2.881526	-3.273686	2.138424
C	-4.090963	-1.205223	2.399823

C	-2.934189	-3.487647	3.513482
H	-2.394123	-4.008402	1.500361
C	-4.151727	-1.421945	3.773981
H	-4.526373	-0.299922	1.990317
C	-3.573256	-2.560670	4.339712
H	-2.481937	-4.379735	3.938990
H	-4.646107	-0.690537	4.407397
H	-3.620368	-2.723583	5.412967
H	-2.163169	-2.599163	-3.028225