Supporting Information for:

Computational Study of the Double C-Cl Bond Activation of Dichloromethane and Phosphine Alkylation at $[CoCl(PR_3)_3]$.

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Functional Testing. Several functional were tested to check the dependency of results on the methodology employed (see Table S1). This focussed on the singlet/triplet energy gap of the reacting adduct ($^{3}\mathbf{1}\cdot\mathbf{CH_2Cl_2}$ and $^{1}\mathbf{1}\cdot\mathbf{CH_2Cl_2}$) and the transition states involved in the first C-Cl cleavage process ($^{3}\mathbf{TS(1\text{-}2^{+})}$,$^{1}\mathbf{TS(1\text{-}2^{+})}$ and $^{3}\mathbf{TS(1\text{-}3)}$). For B3P86 and OPBE both recomputation of the energy at the BP86 optimised geometry and full reoptimisation were assessed. Both approaches give similar results, although the latter allowed for the computation of free energies in solution for comparison with the original BP86 values (data in parenthesis in Table S1). For B3P86 and OPBE the location of a fully optimised minimum structure for $^{1}\mathbf{1}\cdot\mathbf{CH_2Cl_2}$ proved problematic and so no data are reported. Other functionals were tested via single point energy calculations at the BP86 geometry.

As expected, hybrid functionals tend to favour the higher spin state, whereas results with M06 and PBE are similar to those obtained with the pure functional BP86. Barriers are also higher with the hybrid functionals, although in all cases the order of the transition states is $^{3}\mathbf{TS(1\text{-}3)}$ < $^{3}\mathbf{TS(1\text{-}2^{+})}$ < $^{1}\mathbf{TS(1\text{-}2^{+})}$. This difference can be quite small in terms of the SCF (i.e. electronic) energy (e.g. BP86, PBE) but increases significantly upon inclusion of zero-point energy, entropy and solvation effects.

Species	BP86(opt)	B3P86//BP86	B3P86(opt)	B3LYP//BP86	OPBE//BP86	OPBE(opt)	PBE//BP86	M06//BP86
^{3}**1**·CH_2Cl_2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{1}**1**·CH_2Cl_2	16.3(19.6)	29.7	a	32.4	21.6	a	16.5	23.9
^{3}**TS(1-2^{+})**	23.8(29.7)	31.5	30.7(37.5)	32.1	38.1	38.2(42.6)	21.9	24.9
^{1}**TS(1-2^{+})**	24.5(35.2)	43.0	43.2(54.2)	46.3	42.7	42.9 (51.5)	22.1	31.1
^{3}**TS(1-3)**	14.9(19.1)	21.1	21.4(26.4)	22.6	29.5	30.1(33.3)	13.7	17.9

Table S1. Computed SCF energies and (in parenthesis) free energies in dichloromethane solution for key stationary points involved in the first C-Cl activation of CH_2Cl_2 at [$CoCl(PMe_3)_3$]. [a] optimisation of a true minimium not possible.

Computed Cartesian coordinates (Å) and energies (hartrees) for all species computed in dichloromethane solution with the BP86 functional

^{1}1

SCF (BP86) Energy =-540.047319289
Enthalpy 0K = -539.712134
Enthalpy 298K = -539.685654
Free Energy 298K = -539.767296

Co	-0.00200	-0.26734	-0.21764
Cl	-0.00113	-2.25862	-1.36492
P	0.00344	1.87810	-0.22994
P	-2.12595	-0.54040	0.32605
P	2.12186	-0.54568	0.32761
C	-1.42352	2.65648	-1.17203
H	-1.27159	3.74547	-1.26790
H	-1.46795	2.20500	-2.17639
H	-2.38030	2.47295	-0.66023
C	1.40818	2.62864	-1.22652
H	1.27473	3.72040	-1.31788
H	2.38025	2.42510	-0.75246
H	1.40465	2.17550	-2.23112
C	0.03918	2.96216	1.30310
H	0.94563	2.74017	1.88687
H	0.03279	4.03118	1.02792
H	-0.84051	2.73928	1.92646
C	-2.97551	0.58575	1.56391
H	-3.97519	0.19194	1.81634
H	-2.36312	0.63245	2.47917
H	-3.08808	1.60554	1.16361
C	-2.35100	-2.17849	1.20786
H	-1.74205	-2.18504	2.12604
H	-3.41259	-2.33162	1.46888
H	-2.00158	-2.98252	0.54321
C	-3.44918	-0.68420	-0.99801
H	-3.11388	-1.43040	-1.73582
H	-4.41607	-0.99580	-0.56635
H	-3.57104	0.28564	-1.50618
C	3.42958	-0.74200	-1.00510
H	4.39688	-1.05577	-0.57604
H	3.07578	-1.50056	-1.72117
H	3.55839	0.21395	-1.53760
C	2.32706	-2.16209	1.25335
H	3.38811	-2.32700	1.50925
H	1.72651	-2.13091	2.17653
H	1.95742	-2.97861	0.61532
C	3.00387	0.59858	1.52570
H	2.40227	0.68345	2.44540
H	3.99786	0.19167	1.77968
H	3.13377	1.60389	1.09503

^{3}1

SCF (BP86) Energy = -540.072528124
Enthalpy 0K = -539.738988
Enthalpy 298K = -539.711405
Free Energy 298K = -539.798428

Co	-0.00150	-0.00468	0.60553
Cl	0.00093	-0.03423	2.92112
P	0.22857	2.07268	-0.31634
P	1.68176	-1.22822	-0.33502
P	-1.91135	-0.83319	-0.33339
C	1.91074	2.88182	-0.11959
H	1.91000	3.91899	-0.49737
H	2.18129	2.88099	0.94900
H	2.66584	2.29660	-0.66997
C	-0.86398	3.39095	0.45110
H	-0.66332	4.38516	0.01596
H	-1.92210	3.12963	0.28960
H	-0.67512	3.41951	1.53653
C	-0.08856	2.38558	-2.13716
H	-1.13122	2.11747	-2.37302
H	0.08316	3.44359	-2.40047
H	0.57872	1.74734	-2.73792
C	2.11861	-1.08754	-2.15273
H	2.95268	-1.75960	-2.41902
H	1.23638	-1.34307	-2.76100
H	2.40602	-0.04718	-2.37606
C	1.54740	-3.09226	-0.15934
H	0.66673	-3.45114	-0.71722
H	2.44949	-3.60269	-0.53903
H	1.40821	-3.33844	0.90611
C	3.36513	-0.94532	0.44263
H	3.29043	-1.13615	1.52552
H	4.13003	-1.60876	0.00350
H	3.66559	0.10448	0.29528
C	-3.45134	0.22113	-0.13348
H	-4.35004	-0.29540	-0.51298
H	-3.58567	0.45249	0.93586
H	-3.32092	1.16935	-0.68078
C	-2.51208	-2.43777	0.42899
H	-3.47154	-2.76009	-0.01098
H	-1.75658	-3.22417	0.27154
H	-2.63664	-2.28842	1.51383
C	-2.02196	-1.25789	-2.15619
H	-1.27248	-2.03052	-2.39278
H	-3.02561	-1.63226	-2.42223
H	-1.79713	-0.36063	-2.75440

^{1}1.CH_2Cl_2

SCF (BP86) Energy =-609.410370247
Enthalpy 0K = -609.047092
Enthalpy 298K = -609.014400
Free Energy 298K =-609.118717

Co	1.57012	-0.00795	0.45313
Cl	1.34146	0.04215	2.73922
P	2.82293	-0.07342	-1.28724
P	0.91210	-2.11534	0.39416
P	1.02906	2.13038	0.31966
C	4.00642	-1.53175	-1.33620
H	4.72902	-1.41252	-2.16182
H	4.55014	-1.57443	-0.37860
H	3.46001	-2.47695	-1.47391
C	4.10194	1.30063	-1.35491
H	4.81142	1.12716	-2.18234
H	3.61940	2.27947	-1.49638
H	4.65112	1.31331	-0.39952

C	2.20113	-0.06811	-3.05978
H	1.61057	0.84425	-3.23646
H	3.04434	-0.10336	-3.77130
H	1.55015	-0.94169	-3.21948
C	0.53202	-2.97686	-1.22941
H	0.07512	-3.96367	-1.04060
H	-0.17371	-2.35516	-1.80402
H	1.44496	-3.11955	-1.82850
C	-0.76272	-2.28598	1.21796
H	-1.49035	-1.64856	0.69050
H	-1.10213	-3.33597	1.18757
H	-0.67712	-1.94194	2.25943
C	1.87455	-3.45503	1.29165
H	2.04572	-3.11957	2.32696
H	1.32157	-4.41017	1.29649
H	2.85061	-3.59978	0.80154
C	2.03399	3.43620	1.22020
H	1.53074	4.41805	1.19279
H	2.16014	3.11146	2.26523
H	3.02875	3.52162	0.75407
C	-0.65762	2.40035	1.09043
H	-0.94288	3.46519	1.03150
H	-1.40143	1.78980	0.55380
H	-0.61848	2.07317	2.14019
C	0.74047	2.98191	-1.32837
H	0.01648	2.39024	-1.91198
H	0.33351	3.99514	-1.16731
H	1.67532	3.06456	-1.90466
C	-6.41421	0.04635	0.35463
H	-7.42577	0.15569	0.77510
H	-5.62733	-0.07154	1.11559
Cl	-6.40499	-1.43806	-0.68639
Cl	-6.04472	1.54473	-0.59661

^{3}1.CH_2Cl_2

SCF (BP86) Energy =-609.436266941
Enthalpy 0K = -609.074669
Enthalpy 298K = -609.040915
Free Energy 298K =-609.149899

Co	0.94559	-0.19102	-0.19342
Cl	-0.96646	-1.05318	-1.17725
P	0.72770	1.95356	0.57038
P	1.71325	-1.35857	1.61411
P	2.73681	-0.10783	-1.61217
C	-0.29670	2.19717	2.12324
H	-0.43320	3.26808	2.35312
H	-1.28237	1.72549	1.97786
H	0.20364	1.70528	2.97348
C	-0.18084	3.10278	-0.60182
H	-0.31196	4.10739	-0.16400
H	0.38522	3.18558	-1.54366
H	-1.16814	2.66798	-0.82786
C	2.22572	3.00340	0.98353
H	2.85714	3.10128	0.08529
H	1.92994	4.00879	1.33002
H	2.81421	2.50451	1.77031
C	3.02456	-0.64924	2.75113
H	3.28086	-1.35414	3.56093
H	3.92891	-0.42150	2.16438
H	2.65078	0.28907	3.19286
C	2.44333	-3.05024	1.26057
H	3.35501	-2.93528	0.65167
H	2.69459	-3.58574	2.19245
H	1.71134	-3.64041	0.68515
C	0.39181	-1.82525	2.86156
H	-0.39970	-2.39061	2.34292
H	0.80554	-2.43869	3.68047
H	-0.05423	-0.90901	3.28106
C	2.65557	1.17267	-2.98112
H	3.49989	1.06712	-3.68420
H	1.70647	1.04912	-3.52810
H	2.67616	2.18288	-2.54027
C	2.97914	-1.66330	-2.63238
H	3.81079	-1.55224	-3.34940
H	3.18711	-2.51161	-1.96035
H	2.04649	-1.87523	-3.18025
C	4.48519	0.16724	-0.99156
H	4.75103	-0.63966	-0.28915
H	5.21022	0.17571	-1.82382
H	4.53558	1.12792	-0.45415
C	-5.24069	-0.11735	-0.66010
H	-4.28906	-0.60432	-0.39445
H	-5.20234	0.44253	-1.60722
Cl	-6.49956	-1.41046	-0.83183
Cl	-5.65280	1.05615	0.65991

^{1}TS(1-2^{+})

SCF (BP86) Energy =-609.397244346
Enthalpy 0K = -609.033162
Enthalpy 298K = -609.002091
Free Energy 298K = -609.093760

Co	-0.06976	-0.47177	-0.38903
Cl	0.13464	-0.18755	-2.67235
P	-0.23634	-1.38314	1.59200
P	-2.28521	-0.11596	-0.80956
P	2.20124	-0.79068	-0.51866
C	-1.87148	-1.73236	2.43429
H	-1.67400	-2.30245	3.35807
H	-2.37844	-0.79189	2.69429
H	-2.51846	-2.33376	1.77720
C	0.63792	-0.60859	3.05959
H	0.56196	-1.27459	3.93596
H	1.69634	-0.41535	2.84160
H	0.14185	0.34871	3.28895
C	0.41423	-3.14375	1.58776
H	1.45890	-3.19075	1.24972
H	0.34127	-3.57757	2.59956
H	-0.20379	-3.73554	0.89268
C	-3.66779	0.09003	0.44422
H	-4.56224	0.45433	-0.08889
H	-3.91094	-0.86763	0.92362
H	-3.38253	0.82437	1.21244
C	-3.00979	-1.48738	-1.85415
H	-2.99575	-2.42703	-1.27764
H	-4.04929	-1.24585	-2.13384
H	-2.39407	-1.60956	-2.75750
C	-2.64014	1.40581	-1.84034
H	-1.97936	1.41745	-2.71738

H	-3.69705	1.39346	-2.15631
H	-2.45771	2.30398	-1.22845
C	3.11762	0.56925	-1.41664
H	4.18247	0.29652	-1.50989
H	2.67040	0.71028	-2.40995
H	3.02844	1.50689	-0.84415
C	2.63711	-2.30319	-1.52751
H	3.72796	-2.35159	-1.68480
H	2.30421	-3.21242	-1.00162
H	2.11792	-2.23660	-2.49469
C	3.38729	-0.99048	0.92440
H	3.09931	-1.81436	1.59387
H	4.39414	-1.19594	0.52329
H	3.42505	-0.05266	1.50249
C	0.33326	2.10080	0.47018
H	1.03407	1.42775	0.96540
H	0.10710	2.04072	-0.59897
Cl	-1.04638	2.54456	1.48702
Cl	1.65122	3.85444	0.38543

^{3}TS(1-2^{+})

SCF (BP86) Energy =-609.398323056
Enthalpy 0K = -609.036653
Enthalpy 298K = -609.004205
Free Energy 298K =-609.102633

Co	-0.20526	0.01747	-0.21229
Cl	0.08836	-0.06982	-2.51480
P	0.18587	0.10728	2.01515
P	-1.37329	2.05978	-0.41108
P	-1.67700	-1.82550	-0.27281
C	1.09447	1.59584	2.70295
H	1.16601	1.51897	3.80103
H	2.11035	1.66726	2.28119
H	0.54562	2.51437	2.44069
C	1.12395	-1.30169	2.81645
H	1.15738	-1.16166	3.91015
H	0.61772	-2.25280	2.58513
H	2.15126	-1.35198	2.42358
C	-1.33107	0.14166	3.10934
H	-1.91235	-0.78042	2.97204
H	-1.01957	0.21840	4.16494
H	-1.96690	1.00241	2.85692
C	-2.31353	2.96193	0.93619
H	-2.70289	3.91811	0.54654
H	-3.16037	2.34275	1.27468
H	-1.65749	3.17153	1.79599
C	-2.64183	2.11605	-1.78127
H	-3.52273	1.52164	-1.49116
H	-2.95210	3.15812	-1.96969
H	-2.19775	1.68168	-2.68904
C	-0.17703	3.38348	-0.96707
H	0.34230	3.02666	-1.87043
H	-0.71121	4.32256	-1.19095
H	0.56947	3.56716	-0.17749
C	-0.81204	-3.32629	-0.97264
H	-1.53614	-4.13705	-1.16207
H	-0.31268	-3.03942	-1.91060
H	-0.04992	-3.67325	-0.25672
C	-3.08430	-1.61006	-1.48192
H	-3.60423	-2.57064	-1.63897
H	-3.79866	-0.87187	-1.08336
H	-2.67892	-1.24110	-2.43601
C	-2.59390	-2.60171	1.16463
H	-3.30621	-1.87668	1.59021
H	-3.15113	-3.48863	0.81707
H	-1.88328	-2.91226	1.94793
C	2.48957	-0.09706	-0.26187
H	2.12712	0.46770	-1.12230
H	2.65115	0.27474	0.74663
Cl	2.67096	-1.81415	-0.47342
Cl	4.69179	0.81430	-0.71659

MECP between **^{3}2^{+}.Cl^{-} and ^{1}2^{+}.Cl^{-}**
SCF (BP86) Energy =-609.420320547
Enthalpy 0K = -609.056894
Enthalpy 298K = -609.026947
Free Energy 298K =-609.116282

Co	-0.34443	0.28936	-0.24777
Cl	-1.45688	1.21786	-1.99057
P	0.75335	-0.62303	1.48901
P	0.75054	2.45674	0.03698
P	-2.52258	-0.71379	0.35964
C	2.57648	-0.32846	1.63598
H	2.91355	-0.68259	2.62458
H	3.09337	-0.91554	0.84618
H	2.83615	0.73291	1.53053
C	0.69571	-2.47737	1.59438
H	1.21416	-2.80289	2.51136
H	-0.33704	-2.84583	1.61176
H	1.22262	-2.88893	0.71925
C	0.08602	-0.02561	3.12437
H	-0.99678	-0.19971	3.18821
H	0.59247	-0.54722	3.95392
H	0.27537	1.05475	3.21280
C	1.41993	3.17757	1.63083
H	1.97899	4.09915	1.39880
H	0.58204	3.43509	2.29671
H	2.09443	2.48863	2.15629
C	-0.15222	3.95634	-0.60096
H	-1.04704	4.14294	0.01268
H	0.52182	4.82802	-0.54605
H	-0.46296	3.77670	-1.63801
C	2.25768	2.41443	-1.05686
H	1.92959	2.21940	-2.08845
H	2.77665	3.38715	-1.01130
H	2.94054	1.61121	-0.73933
C	-3.36108	-1.51701	-1.09647
H	-4.41076	-1.73335	-0.83419
H	-3.30497	-0.84196	-1.96094
H	-2.83478	-2.45287	-1.33519
C	-3.73892	0.61309	0.84775
H	-4.74770	0.17780	0.95220
H	-3.44302	1.06915	1.80546
H	-3.74723	1.38582	0.06589
C	-2.86086	-2.02110	1.65898
H	-2.45440	-1.75128	2.64431
H	-3.95156	-2.15793	1.75333
H	-2.42386	-2.97878	1.33867

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C    0.94985 -0.74845 -1.36349
H    1.10789 -0.07868 -2.22497
H    1.89993 -1.15988 -0.96954
Cl -0.02338 -2.15633 -1.95632
Cl   4.04067 -2.19350 -0.82467
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$^{1}2^{+}.Cl^{-}$

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SCF (BP86) Energy = -609.446615739
Enthalpy 0K = -609.080641
Enthalpy 298K = -609.049441
Free Energy 298K = -609.141175

Co   0.37208   0.48026   0.04882
Cl   0.91419   2.45173 -0.98687
P   -0.04741 -0.99112   1.67292
P    2.64173   0.00935 -0.34044
P   -1.71070   1.52323   0.26022
C    1.25961 -2.16511   2.28465
H    0.81411 -2.76174   3.09926
H    1.57304 -2.83825   1.47456
H    2.12531 -1.61074   2.67754
C   -1.45564 -2.18255   1.44768
H   -1.80110 -2.51646   2.44049
H   -2.28979 -1.75343   0.87698
H   -1.06825 -3.04665   0.88523
C   -0.39133 -0.06590   3.25870
H   -1.29507   0.55576   3.18500
H   -0.52300 -0.79438   4.07695
H    0.47151   0.58153   3.48608
C    3.54733 -1.58168   0.03971
H    4.54049 -1.51945 -0.43671
H    3.68340 -1.70422   1.12325
H    3.00134 -2.44396 -0.36919
C    3.72149   1.23278   0.56159
H    3.59640   1.09608   1.64831
H    4.77716   1.05782   0.29417
H    3.42457   2.25472   0.28630
C    3.10680   0.22382 -2.13137
H    2.73858   1.19232 -2.49496
H    4.20460   0.17202 -2.22632
H    2.65043 -0.59165 -2.71407
C   -2.39717   2.05685 -1.38266
H   -3.28197   2.69250 -1.20898
H   -1.63447   2.60991 -1.94738
H   -2.70563   1.15454 -1.93579
C   -1.57971   3.09118   1.25843
H   -2.56456   3.58738   1.27460
H   -1.27664   2.85187   2.29025
H   -0.82831   3.75096   0.80179
C   -3.22913   0.71639   0.97823
H   -3.06698   0.34106   1.99904
H   -4.02563   1.48024   1.00300
H   -3.54292 -0.10700   0.31044
C   -0.35057 -0.64101 -1.33664
H   -1.41502 -0.90146 -1.20292
H   -0.15942 -0.05336 -2.25450
Cl   0.45451 -2.27251 -1.62454
Cl -3.88709 -1.82238 -1.59570
```

$^{3}2^{+}.Cl^{-}$

```
SCF (BP86) Energy =-609.430740909
Enthalpy 0K =     -609.066745
Enthalpy 298K =   -609.034507
Free Energy 298K =-609.131491

Co -0.29696 -0.03137 -0.38242
Cl -1.37165 -0.09493 -2.37647
P   0.96960   0.07113   1.48229
P  -1.01332   2.29429 -0.18685
P  -1.92429 -1.58064   0.51885
C   2.33715   1.33128   1.46625
H   2.66661   1.49836   2.50568
H   3.19160   0.95084   0.87463
H   1.99354   2.28460   1.03710
C   1.86542 -1.49439   1.92506
H   2.37327 -1.34730   2.89319
H   1.15482 -2.33128   2.00548
H   2.61437 -1.72726   1.15302
C   0.05418   0.45179   3.06051
H  -0.54549 -0.41641   3.36415
H   0.79710   0.66623   3.84737
H  -0.60542   1.32093   2.93544
C  -0.85739   3.44126   1.28120
H  -1.13636   4.46043   0.96339
H  -1.54473   3.11961   2.08029
H   0.17125   3.46001   1.67232
C  -2.79551   2.58220 -0.64445
H  -3.44541   2.21284   0.16449
H  -2.96573   3.66348 -0.78266
H  -3.02209   2.03964 -1.57312
C  -0.08069   3.21810 -1.50865
H  -0.23852   2.71012 -2.47226
H  -0.44352   4.25828 -1.56655
H   0.99605   3.21759 -1.27308
C  -1.88980 -3.13857 -0.49792
H  -2.76336 -3.76258 -0.24332
H  -1.90837 -2.87035 -1.56418
H  -0.96162 -3.69010 -0.28194
C  -3.65493 -0.94215   0.26621
H  -4.37764 -1.74723   0.48285
H  -3.83803 -0.09675   0.94844
H  -3.76569 -0.60548 -0.77481
C  -2.05142 -2.27296   2.24811
H  -2.34415 -1.48099   2.95499
H  -2.82774 -3.05708   2.25425
H  -1.09534 -2.71801   2.56616
C   1.50726 -0.42640 -1.16850
H   1.44243   0.18562 -2.08873
H   2.47954 -0.29152 -0.67138
Cl  1.42476 -2.17214 -1.65008
Cl  5.17520   0.07107 -0.49506
```

$^{1}TS(2^{+}-4)$

```
SCF (BP86) Energy = -609.448505432
Enthalpy 0K = -609.083111
Enthalpy 298K = -609.052533
Free Energy 298K = -609.142126

Co   0.05637 -0.28359 -0.08779
```

Cl	-0.03117	-2.59853	-0.19328
Cl	0.20325	-0.48411	3.02215
P	0.35806	1.89132	0.49470
P	2.32893	-0.65790	-0.42366
P	-2.27457	-0.56497	0.18752
C	1.68084	2.23184	1.76673
C	-1.05449	2.80956	1.28307
C	0.81643	3.08090	-0.86909
C	3.49518	0.69905	-0.97511
C	2.70346	-1.87837	-1.78293
C	3.17931	-1.38459	1.05641
C	-3.51389	0.82881	0.32793
C	-2.74248	-1.58027	1.67327
C	-3.04624	-1.54822	-1.20046
C	-0.07547	0.06819	-1.97945
Cl	-1.44430	1.16930	-2.62730
H	2.64487	1.77998	1.49726
H	1.80231	3.32497	1.85445
H	1.34283	1.78817	2.71413
H	-0.68293	3.79343	1.61655
H	-1.86629	2.95680	0.55764
H	-1.41526	2.23955	2.15242
H	-0.00924	3.14421	-1.59219
H	0.99510	4.07228	-0.42017
H	1.72685	2.75377	-1.39082
H	4.50479	0.26534	-1.07172
H	3.17913	1.07068	-1.96382
H	3.53924	1.54027	-0.26994
H	2.28852	-1.50799	-2.73422
H	3.79800	-1.97479	-1.87766
H	2.25009	-2.84867	-1.54345
H	2.65262	-2.31065	1.33102
H	4.23366	-1.59760	0.81242
H	3.10975	-0.68424	1.90186
H	-3.40654	1.33839	1.29613
H	-3.37941	1.54762	-0.49350
H	-4.52483	0.39127	0.26552
H	-3.83519	-1.73330	1.67018
H	-2.21880	-2.54515	1.62282
H	-2.41768	-1.05381	2.58201
H	-2.47635	-2.47652	-1.34440
H	-4.08718	-1.78476	-0.92253
H	-3.03891	-0.95562	-2.12652
H	0.82014	0.56506	-2.39127
H	-0.26575	-0.90295	-2.46899

^{3}TS(1-3)

SCF (BP86) Energy =-609.412496374
Enthalpy 0K = -609.051964
Enthalpy 298K = -609.019146
Free Energy 298K =-609.119477

Co	-0.47732	0.07860	-0.29678
Cl	-2.18262	0.71955	-1.91480
P	-1.37383	0.60299	1.76122
P	-1.25883	-2.06661	-0.48253
P	0.56478	2.06439	-0.76222
C	-1.59131	-0.76347	3.02562
H	-2.01184	-0.36200	3.96358
H	-2.26906	-1.53866	2.63471
H	-0.61035	-1.22093	3.23439
C	-3.09740	1.32102	1.69818
H	-3.46964	1.54995	2.71120
H	-3.07927	2.23837	1.08921
H	-3.76804	0.59879	1.20699
C	-0.49517	1.85326	2.84577
H	-0.43136	2.82469	2.33056
H	-1.03499	1.98929	3.79858
H	0.52602	1.49483	3.05504
C	-0.56642	-3.42710	0.59517
H	-0.98985	-4.40172	0.29878
H	0.52787	-3.44612	0.47950
H	-0.80876	-3.23143	1.65091
C	-0.93837	-2.74953	-2.19003
H	0.14852	-2.76601	-2.36687
H	-1.34821	-3.76949	-2.28623
H	-1.41341	-2.08267	-2.92611
C	-3.09775	-2.33658	-0.31099
H	-3.61078	-1.63082	-0.98176
H	-3.36139	-3.37425	-0.57694
H	-3.41410	-2.13870	0.72585
C	-0.47625	3.61330	-0.72668
H	0.10034	4.47259	-1.10901
H	-1.36526	3.44376	-1.35281
H	-0.80102	3.82670	0.30429
C	1.21023	2.08949	-2.51399
H	1.66887	3.06586	-2.74591
H	1.95871	1.28973	-2.62759
H	0.36906	1.89755	-3.19799
C	2.07654	2.59138	0.19895
H	2.82010	1.78083	0.16176
H	2.50371	3.51060	-0.23641
H	1.80686	2.77852	1.24976
C	3.76685	-1.87459	0.19557
H	3.44655	-2.56388	0.98685
H	4.06281	-2.28459	-0.77862
Cl	4.95286	-0.70031	0.79749
Cl	1.75965	-0.90087	-0.37299

^{2}3.^{2}CH$_2$Cl

SCF (BP86) Energy =-609.420810951
Enthalpy 0K = -609.061265
Enthalpy 298K = -609.027886
Free Energy 298K =-609.130596

Co	-0.70772	0.02078	-0.29072
Cl	-2.53251	0.28901	-1.80918
P	-1.55825	0.24555	1.78437
P	-1.03152	-2.21595	-0.47005
P	-0.23910	2.21076	-0.64381
C	-1.35071	-1.15373	3.01139
H	-1.78933	-0.87146	3.98376
H	-1.85071	-2.06533	2.64977
H	-0.27630	-1.36108	3.14262
C	-3.41069	0.48489	1.79804
H	-3.78617	0.58750	2.83028
H	-3.65940	1.38613	1.21646
H	-3.88917	-0.37888	1.30968
C	-0.98997	1.65047	2.88346
H	-1.19388	2.62316	2.41045

H	-1.51979	1.60790	3.85030
H	0.09363	1.55557	3.06017
C	0.03224	-3.39276	0.51004
H	-0.16353	-4.42829	0.18437
H	1.08698	-3.13481	0.33127
H	-0.18235	-3.30307	1.58510
C	-0.64724	-2.73192	-2.21819
H	0.39506	-2.45727	-2.44212
H	-0.78335	-3.82051	-2.33259
H	-1.32124	-2.19176	-2.89998
C	-2.74550	-2.90804	-0.22696
H	-3.44281	-2.32313	-0.84568
H	-2.77168	-3.96909	-0.52757
H	-3.04504	-2.82683	0.82991
C	-1.60986	3.46706	-0.50749
H	-1.26396	4.44487	-0.88274
H	-2.46296	3.11258	-1.10553
H	-1.92909	3.57802	0.54108
C	0.31218	2.42664	-2.41078
H	0.54691	3.48600	-2.60992
H	1.20615	1.80580	-2.57590
H	-0.49627	2.08696	-3.07580
C	1.15720	3.01822	0.29120
H	2.04561	2.37390	0.21103
H	1.36983	4.01049	-0.14113
H	0.89129	3.13401	1.35226
C	5.68326	-1.07504	-0.20194
H	5.15975	-1.80383	0.42342
H	5.40060	-0.77558	-1.21571
Cl	6.84305	-0.06088	0.61161
Cl	1.60636	-0.40243	-0.51056

^{1}4$_{mer,cis}$

SCF (BP86) Energy =-609.455915445
Enthalpy 0K = -609.088982
Enthalpy 298K = -609.058378
Free Energy 298K =-609.147129

Co	-0.11380	-0.25905	-0.10320
Cl	-0.00688	-2.56533	-0.52712
Cl	-0.61317	0.17601	-2.42993
P	-0.03707	1.98994	0.13953
P	-2.45285	-0.50555	0.17169
P	2.20602	-0.39473	-0.53321
C	-1.62716	2.97100	0.13401
C	0.85118	2.95588	-1.18874
C	0.71628	2.63987	1.71913
C	-3.20271	-0.07372	1.83364
C	-3.07804	-2.25302	0.00870
C	-3.62914	0.34801	-0.99937
C	3.43421	0.82440	0.19623
C	2.62195	-0.30024	-2.34506
C	3.07920	-1.97887	-0.07119
C	-0.04883	-0.58148	1.82736
Cl	1.57447	-0.65577	2.78964
H	-2.32474	2.61530	0.90625
H	-1.37855	4.02578	0.34097
H	-2.09669	2.90343	-0.85850
H	0.86900	4.01998	-0.89876
H	1.88010	2.60609	-1.34264
H	0.29251	2.82250	-2.12635
H	1.72461	2.23496	1.87630
H	0.75851	3.74078	1.66949
H	0.08472	2.34195	2.57103
H	-4.29223	-0.23576	1.78310
H	-2.78039	-0.72653	2.61340
H	-3.00816	0.97536	2.10613
H	-2.57049	-2.90377	0.73502
H	-4.16567	-2.24735	0.19455
H	-2.86494	-2.62517	-1.00354
H	-3.35358	0.07644	-2.02801
H	-4.65236	0.00559	-0.77046
H	-3.57936	1.43940	-0.89340
H	4.43061	0.59331	-0.21654
H	3.19134	1.86907	-0.04275
H	3.45556	0.69649	1.28843
H	3.70863	-0.44432	-2.47128
H	2.06734	-1.09162	-2.87024
H	2.31483	0.66949	-2.76141
H	2.71184	-2.79134	-0.71117
H	4.16193	-1.82895	-0.22179
H	2.87511	-2.22189	0.98023
H	-0.59701	0.17469	2.41188
H	-0.45835	-1.58904	2.01386

^{3}4$_{mer,cis}$

SCF (BP86) Energy =-609.424758099
Enthalpy 0K = -609.061569
Enthalpy 298K = -609.030070
Free Energy 298K =-609.123722

Co	-0.09426	-0.45246	-0.08614
Cl	0.04259	-2.96293	-0.21646
Cl	-0.45692	-0.07665	-2.37002
P	-0.07547	2.37057	-0.17387
P	-2.47343	-0.66124	0.23759
P	2.24675	-0.66077	-0.39315
C	-1.76390	3.18001	-0.28635
C	0.70082	3.16569	-1.68186
C	0.66981	3.39067	1.21201
C	-3.27082	0.21504	1.68503
C	-3.06937	-2.39683	0.54508
C	-3.55847	-0.14988	-1.18490
C	3.35529	0.82881	-0.19708
C	2.68767	-1.22410	-2.11102
C	3.14173	-1.92379	0.64492
C	-0.03403	-0.25898	1.89020
Cl	1.49867	0.21046	2.82402
H	-2.35233	2.97333	0.62158
H	-1.65167	4.27313	-0.39403
H	-2.30124	2.78838	-1.16459
H	0.59437	4.26284	-1.62523
H	1.76867	2.91090	-1.75957
H	0.18651	2.78209	-2.57618
H	1.74251	3.16187	1.30793
H	0.53852	4.46889	1.01492
H	0.17530	3.12946	2.16166
H	-4.36196	0.06121	1.64146
H	-2.89000	-0.20547	2.62955
H	-3.05686	1.29415	1.66191

H	-2.55605	-2.81032	1.42619
H	-4.15947	-2.37904	0.71493
H	-2.82375	-3.02411	-0.32331
H	-3.28494	-0.74766	-2.06660
H	-4.61465	-0.32326	-0.91819
H	-3.40274	0.91201	-1.42296
H	4.40046	0.52833	-0.38451
H	3.07497	1.60559	-0.92334
H	3.26849	1.22911	0.82367
H	3.77708	-1.38596	-2.17323
H	2.14920	-2.15968	-2.32222
H	2.37216	-0.46031	-2.83634
H	2.66485	-2.90120	0.48649
H	4.19809	-1.95500	0.32814
H	3.07891	-1.64929	1.70701
H	-0.74916	0.50542	2.22273
H	-0.29423	-1.26224	2.27498

$^{1}4_{fac}$

SCF (BP86) Energy =-609.446921795
Enthalpy 0K = -609.079819
Enthalpy 298K = -609.049426
Free Energy 298K =-609.137192

Co	-0.19869	0.04824	-0.33270
Cl	0.43299	0.91540	-2.43578
Cl	-1.04720	-1.81608	-1.45411
P	-0.98201	-1.05061	1.48503
P	0.55809	1.92399	0.74001
P	1.99217	-0.97083	-0.36763
C	-0.34169	-0.59618	3.18353
H	-0.52666	0.46444	3.40945
H	-0.85951	-1.21332	3.93703
H	0.73950	-0.79752	3.23748
C	-0.74941	-2.90303	1.55011
H	-0.99951	-3.24821	2.56766
H	-1.41493	-3.36886	0.81134
H	0.28628	-3.18351	1.31221
C	-2.82251	-0.93944	1.74703
H	-3.32943	-1.19672	0.80498
H	-3.11114	-1.64946	2.53980
H	-3.11117	0.07900	2.05036
C	-0.69106	2.90229	1.73480
H	-0.15847	3.71210	2.26082
H	-1.44067	3.34522	1.06175
H	-1.20619	2.27109	2.47513
C	1.19361	3.27102	-0.37492
H	0.40996	3.54110	-1.09768
H	1.46026	4.14373	0.24523
H	2.07022	2.91511	-0.93389
C	1.94567	1.81448	1.99016
H	2.82801	1.32221	1.55771
H	2.22293	2.84062	2.28495
H	1.62757	1.26110	2.88497
C	2.81767	-1.69663	1.15744
H	3.82160	-2.06697	0.88913
H	2.92030	-0.93444	1.94565
H	2.23040	-2.53781	1.55674
C	3.38982	0.10905	-0.99425
H	4.31429	-0.49034	-1.04553
H	3.11655	0.47289	-1.99529
H	3.56475	0.97583	-0.33849
C	2.15712	-2.39393	-1.55850
H	1.79009	-2.06454	-2.54170
H	3.21544	-2.69798	-1.62442
H	1.53742	-3.23690	-1.22008
C	-1.88149	1.12796	-0.50436
Cl	-3.28372	0.54318	-1.57818
H	-2.39079	1.32688	0.45041
H	-1.60800	2.07862	-0.99301

$^{3}4_{fac}$

SCF (BP86) Energy = -609.420565215
Enthalpy 0K = -609.056894
Enthalpy 298K = -609.026540
Free Energy 298K = -609.116674

Co	0.33313	0.10720	-0.41401
Cl	-0.59532	0.50879	-2.50905
Cl	2.28604	1.64934	-0.57273
P	1.45245	-0.48996	1.54948
P	-2.04191	-1.52634	0.21877
P	-0.93784	2.12035	0.21545
C	0.67793	-1.80279	2.62326
H	0.56246	-2.73718	2.05355
H	1.32955	-1.99047	3.49333
H	-0.30848	-1.46428	2.97635
C	1.75617	0.85117	2.80308
H	2.45493	0.47291	3.56849
H	2.18918	1.72612	2.29753
H	0.80778	1.12622	3.28676
C	3.16254	-1.17525	1.29287
H	3.75957	-0.43296	0.74455
H	3.61484	-1.38193	2.27720
H	3.11739	-2.10460	0.70595
C	-1.77204	-3.38537	0.25350
H	-2.74588	-3.90554	0.27422
H	-1.21651	-3.69768	-0.64594
H	-1.19425	-3.67407	1.14600
C	-3.29806	-1.44006	-1.16527
H	-2.79549	-1.69147	-2.11301
H	-4.12159	-2.15113	-0.97696
H	-3.70182	-0.42020	-1.25033
C	-3.14590	-1.34887	1.72892
H	-3.51548	-0.31433	1.81809
H	-4.00807	-2.03496	1.65640
H	-2.57011	-1.59133	2.63778
C	-0.95344	2.82492	1.94923
H	-1.60902	3.71200	1.98140
H	-1.32970	2.07333	2.66187
H	0.06592	3.12198	2.23850
C	-2.76880	2.08245	-0.14707
H	-3.18473	3.09673	-0.02480
H	-2.91808	1.74247	-1.18265
H	-3.28668	1.40087	0.54417
C	-0.43164	3.61709	-0.77142
H	-0.47119	3.36004	-1.84035
H	-1.12091	4.45031	-0.55294
H	0.60088	3.88824	-0.51003
C	0.91027	-1.71406	-1.07237

Cl 2.39638 -1.66259 -2.13914
H 1.11545 -2.48820 -0.31418
H 0.09229 -2.02560 -1.74123

^{1}4$_{mer,trans}$
SCF (BP86) Energy =-609.455118362
Enthalpy 0K = -609.089089
Enthalpy 298K = -609.058127
Free Energy 298K =-609.147006

Co 0.00999 -0.23120 0.03021
Cl -0.12405 -0.13972 2.34871
Cl 0.04179 -0.27683 -2.27227
P -0.76178 2.00057 -0.33709
P -2.15990 -1.07244 0.21225
P 2.18942 0.44333 0.38230
C -2.30589 2.21121 -1.37826
C 0.33693 3.10532 -1.37807
C -1.14609 3.09187 1.13081
C -3.39571 -0.09982 1.22248
C -2.29895 -2.70526 1.11431
C -3.08740 -1.44459 -1.36006
C 2.44007 2.00771 1.37801
C 3.27593 0.71966 -1.10324
C 3.21196 -0.69566 1.45036
C 0.59022 -2.13827 0.04246
Cl 2.06505 -2.71087 -0.98767
H -3.19990 1.81517 -0.87692
H -2.46170 3.28399 -1.58182
H -2.15409 1.67454 -2.32744
H -0.16075 4.07877 -1.52374
H 1.31826 3.27502 -0.91393
H 0.48093 2.61320 -2.35207
H -0.24102 3.21810 1.74406
H -1.50925 4.07848 0.79750
H -1.91233 2.60415 1.75257
H -4.34852 -0.65446 1.25568
H -2.99253 0.00957 2.24048
H -3.57931 0.89863 0.80227
H -1.76080 -2.63385 2.07186
H -3.36522 -2.91295 1.30258
H -1.87628 -3.52630 0.51654
H -2.47749 -2.12001 -1.97989
H -4.05308 -1.92136 -1.12165
H -3.25871 -0.51753 -1.92592
H 3.51716 2.12853 1.58319
H 2.07886 2.90112 0.85073
H 1.89317 1.89946 2.32707
H 4.29206 0.99907 -0.77774
H 3.30637 -0.20996 -1.68967
H 2.85142 1.51860 -1.72896
H 3.32975 -1.67311 0.96480
H 4.20145 -0.23490 1.60855
H 2.69871 -0.81409 2.41643
H 0.84397 -2.46873 1.06460
H -0.18077 -2.78554 -0.39883

^{3}4$_{mer,trans}$
SCF (BP86) Energy =-609.433601060
Enthalpy 0K = -609.069633
Enthalpy 298K = -609.037434
Free Energy 298K =-609.131982

Co 0.02663 -0.21717 -0.22621
Cl -0.18948 -0.15694 2.63981
Cl 0.02446 -0.17117 -2.57136
P -0.81617 1.99831 -0.41337
P -2.09324 -1.16019 0.32979
P 2.14858 0.46468 0.58572
C -2.35148 2.17826 -1.46502
C 0.29017 3.18216 -1.34470
C -1.26645 2.97900 1.10752
C -3.37319 -0.19790 1.28156
C -2.07694 -2.75627 1.28970
C -3.00728 -1.64972 -1.22260
C 2.31425 2.00117 1.62776
C 3.31859 0.81924 -0.82353
C 3.08646 -0.75925 1.62628
C 0.63579 -2.11355 -0.23653
Cl 2.17773 -2.55808 -1.18887
H -3.20645 1.64438 -1.02495
H -2.60805 3.24705 -1.55728
H -2.13898 1.75809 -2.45984
H -0.23333 4.14254 -1.48747
H 1.22857 3.36653 -0.80100
H 0.52238 2.73553 -2.32376
H -0.37700 3.10418 1.74251
H -1.66192 3.96748 0.81838
H -2.02081 2.42758 1.68805
H -4.27731 -0.82109 1.38803
H -2.95618 0.03853 2.27137
H -3.64139 0.73378 0.76224
H -1.60470 -2.56784 2.26472
H -3.11777 -3.09395 1.42666
H -1.51420 -3.53105 0.74789
H -2.37557 -2.33306 -1.81152
H -3.95420 -2.15053 -0.95886
H -3.21288 -0.75672 -1.83144
H 3.37835 2.13086 1.88902
H 1.97315 2.89289 1.08198
H 1.71356 1.87161 2.53989
H 4.32417 1.03839 -0.42583
H 3.35598 -0.05899 -1.48395
H 2.95152 1.68405 -1.39719
H 3.23313 -1.69209 1.06425
H 4.06584 -0.32388 1.88725
H 2.50041 -0.95223 2.53662
H 0.82472 -2.47734 0.78824
H -0.11277 -2.73665 -0.75390

TS from **4$_{mer,cis}$** to **5$_{Cax,trans}$**
SCF (BP86) Energy =-609.428605733
Enthalpy 0K = -609.066097
Enthalpy 298K = -609.034408
Free Energy 298K =-609.129026

Co -0.74144 0.22293 0.02909
Cl -2.86416 0.89985 0.35930
Cl -0.33695 0.34649 -2.29520
P 2.92069 -0.51647 -0.22348

P	-0.14922	2.45804	0.14222
P	-1.58591	-1.88720	-0.34593
C	3.86494	0.09039	-1.73261
C	3.29543	-2.35369	-0.34587
C	4.13597	-0.04472	1.13354
C	1.61450	2.92671	-0.21850
C	-0.47217	3.32739	1.75928
C	-1.09074	3.51621	-1.06246
C	-0.36434	-3.17962	-0.88875
C	-2.86153	-1.93624	-1.69661
C	-2.48540	-2.70591	1.06361
C	-0.59314	-0.06438	1.94132
Cl	0.59020	-1.44383	2.37089
H	3.91431	1.19212	-1.71844
H	4.89121	-0.31740	-1.75948
H	3.32396	-0.21971	-2.64273
H	4.38253	-2.53395	-0.42449
H	2.90478	-2.86566	0.54922
H	2.79420	-2.76985	-1.23545
H	3.78707	-0.46812	2.09026
H	5.15094	-0.42193	0.91428
H	4.17408	1.05363	1.23239
H	1.72205	4.02474	-0.20186
H	2.27660	2.47869	0.53810
H	1.88457	2.53925	-1.21254
H	0.20816	2.94927	2.53932
H	-0.30885	4.41091	1.63571
H	-1.51386	3.14279	2.06529
H	-2.16593	3.43346	-0.84533
H	-0.76306	4.56498	-0.96780
H	-0.89811	3.14438	-2.07962
H	-0.88723	-4.12648	-1.10612
H	0.14686	-2.81932	-1.79486
H	0.37595	-3.33674	-0.09049
H	-3.21840	-2.97146	-1.82857
H	-3.69996	-1.28037	-1.41811
H	-2.40615	-1.56560	-2.62644
H	-3.29301	-2.03965	1.40543
H	-2.91748	-3.66052	0.71975
H	-1.78740	-2.89404	1.89309
H	-0.16954	0.79514	2.48292
H	-1.54823	-0.37273	2.39649

TS from $\mathbf{4}_{mer,cis}$ to $\mathbf{5}_{Pax,cis}$
SCF (BP86) Energy =-609.438760572
Enthalpy 0K = -609.075590
Enthalpy 298K = -609.044337
Free Energy 298K =-609.136923

Co	0.28639	-0.24101	-0.18671
Cl	-0.37309	-2.43410	-0.37017
Cl	-0.10021	0.03847	-2.49914
P	0.51038	2.02252	-0.22442
P	-3.36501	-0.16487	0.25954
P	2.36550	-0.91908	-0.22046
C	-1.12984	2.78913	-0.66500
C	1.65765	2.77459	-1.48592
C	0.95091	3.00234	1.29763
C	-4.73570	1.06321	0.66332
C	-3.83350	-1.56200	1.42474
C	-4.01917	-0.85414	-1.35895
C	3.70604	0.30655	0.17006
C	2.85842	-1.56348	-1.88787
C	2.76032	-2.32752	0.92260
C	0.12886	-0.39711	1.74083
Cl	1.40011	0.21258	2.97850
H	-1.87624	2.50428	0.09126
H	-1.01425	3.88615	-0.69183
H	-1.44454	2.40822	-1.64688
H	1.35622	3.82235	-1.65418
H	2.69257	2.76144	-1.11226
H	1.58276	2.20580	-2.42309
H	1.96570	2.75477	1.63899
H	0.89760	4.07438	1.04083
H	0.24052	2.78109	2.10801
H	-5.73413	0.59281	0.61462
H	-4.57795	1.46995	1.67690
H	-4.69719	1.89968	-0.05532
H	-3.66722	-1.24199	2.46750
H	-4.89103	-1.85521	1.29897
H	-3.18440	-2.42875	1.21687
H	-3.37614	-1.69287	-1.67307
H	-5.06252	-1.20274	-1.25842
H	-3.96802	-0.07061	-2.13385
H	4.65905	-0.24344	0.25529
H	3.79011	1.04183	-0.64303
H	3.49189	0.81137	1.12362
H	3.89344	-1.94215	-1.82940
H	2.16696	-2.37090	-2.16999
H	2.78520	-0.75373	-2.62801
H	2.08970	-3.16728	0.69425
H	3.81243	-2.61648	0.75863
H	2.62130	-2.00818	1.96563
H	-0.77853	0.18698	1.98629
H	0.01136	-1.45565	2.01798

TS from $\mathbf{4}_{fac}$ to $\mathbf{5}_{Pax,trans}.\mathbf{PMe}_3$
SCF (BP86) Energy =-609.414570235
Enthalpy 0K = -609.051900
Enthalpy 298K = -609.020418
Free Energy 298K =-609.114126

Co	0.60142	0.46982	-0.12373
Cl	2.63583	1.37270	0.10024
Cl	-0.19292	0.63609	-2.26250
P	-3.10572	-0.62114	-0.00327
P	0.51996	-0.19431	2.01691
P	1.64001	-1.53786	-0.91162
C	-4.47414	-1.29952	1.09675
H	-4.54525	-0.68721	2.01175
H	-5.45026	-1.29202	0.57979
H	-4.22865	-2.33414	1.39087
C	-3.37739	-1.65709	-1.54415
H	-4.42619	-1.59912	-1.88618
H	-2.71018	-1.28848	-2.34096
H	-3.12256	-2.70855	-1.32906
C	-3.88936	0.99387	-0.54865
H	-3.24182	1.46740	-1.30554
H	-4.89468	0.82779	-0.97537
H	-3.97129	1.67327	0.31700

C	-0.63154	0.75351	3.13468
H	-0.64614	0.25505	4.11853
H	-0.28625	1.79076	3.25876
H	-1.64433	0.75038	2.70362
C	2.09811	-0.17792	2.99443
H	2.45795	0.85888	3.07224
H	1.89838	-0.58671	3.99928
H	2.86606	-0.78010	2.48904
C	-0.13200	-1.92358	2.24685
H	0.53491	-2.66438	1.78282
H	-0.21264	-2.13607	3.32675
H	-1.12507	-1.97764	1.77494
C	0.53518	-2.94554	-1.43944
H	1.12730	-3.74583	-1.91446
H	0.00235	-3.35455	-0.56658
H	-0.20325	-2.55414	-2.15625
C	2.94815	-2.40768	0.10659
H	3.40341	-3.21829	-0.48703
H	3.72641	-1.67433	0.37312
H	2.52821	-2.83867	1.02883
C	2.62717	-1.20702	-2.45747
H	3.37363	-0.42887	-2.23465
H	3.13253	-2.13106	-2.78475
H	1.95041	-0.84091	-3.24243
C	-0.21154	2.17798	0.40329
Cl	-0.10462	3.60213	-0.77873
H	-1.29598	2.00755	0.53190
H	0.24400	2.59673	1.31407

TS from $\mathbf{4}_{fac}$ to $\mathbf{5}_{Pax,cis}.\mathbf{PMe_3}$
SCF (BP86) Energy =-609.436093147
Enthalpy 0K = -609.072822
Enthalpy 298K = -609.041522
Free Energy 298K =-609.134845

Co	-0.55522	0.02023	-0.40003
Cl	0.22889	0.80069	-2.42059
Cl	-0.39634	-2.13955	-1.21053
P	-1.24627	-1.03174	1.47639
P	-0.07575	2.01340	0.57273
P	3.03426	-0.54300	-0.01083
C	-1.95358	-0.06401	2.91147
H	-2.86364	0.46635	2.58678
H	-2.22902	-0.77593	3.70790
H	-1.23532	0.66066	3.32131
C	0.08301	-2.04247	2.29437
H	-0.33848	-2.57148	3.16584
H	0.46816	-2.76343	1.55850
H	0.90339	-1.38346	2.61762
C	-2.63520	-2.24380	1.22942
H	-2.32362	-3.00410	0.50122
H	-2.88134	-2.70664	2.19979
H	-3.51528	-1.71095	0.83746
C	-1.49590	3.04224	1.21342
H	-1.08766	3.96282	1.66283
H	-2.15564	3.31467	0.37446
H	-2.08013	2.49970	1.96933
C	0.79103	3.27416	-0.48307
H	0.15322	3.53592	-1.33954
H	0.98893	4.16713	0.13444
H	1.73271	2.85407	-0.86252
C	1.07593	1.93926	2.03892
H	2.04487	1.55129	1.69134
H	1.19995	2.95520	2.45093
H	0.69397	1.27229	2.82544
C	4.14822	-1.13593	1.38852
H	5.17082	-1.35229	1.03104
H	4.19736	-0.36325	2.17483
H	3.71931	-2.05173	1.82992
C	4.12415	0.81550	-0.72312
H	5.14405	0.44744	-0.93422
H	3.66969	1.18230	-1.65934
H	4.18501	1.65593	-0.01032
C	3.35767	-1.89475	-1.26867
H	2.86564	-1.62383	-2.21724
H	4.44025	-2.03655	-1.43570
H	2.91101	-2.83686	-0.91022
C	-2.33275	0.69084	-0.75742
Cl	-3.37817	-0.38007	-1.83495
H	-2.94232	0.84030	0.15081
H	-2.22832	1.62377	-1.33631

TS from $\mathbf{4}_{mer,trans}$ to $\mathbf{5}_{Cax,trans}.\mathbf{PMe_3}$
SCF (BP86) Energy =-609.442686447
Enthalpy 0K = -609.079463
Enthalpy 298K = -609.048183
Free Energy 298K =-609.140549

Co	-0.53806	0.29311	0.08205
Cl	-0.74005	0.49284	2.34621
Cl	0.02209	-0.03535	-2.07703
P	2.80954	-0.98727	-0.03857
P	0.40843	2.40269	0.14877
P	-1.32611	-1.86332	0.38309
C	3.83897	0.09684	-1.18155
C	2.77162	-2.54328	-1.09574
C	4.13568	-1.49125	1.20042
C	1.91227	2.54787	1.23480
C	-0.69641	3.72637	0.85593
C	0.96192	3.15833	-1.45692
C	-0.19738	-2.88436	1.46151
C	-1.54904	-2.95391	-1.10559
C	-2.93560	-2.04480	1.30314
C	-2.19865	1.14051	-0.38665
Cl	-3.49395	0.16716	-1.30174
H	4.15384	1.01405	-0.65522
H	4.73867	-0.43804	-1.53486
H	3.21927	0.38250	-2.04780
H	3.78351	-2.80256	-1.45517
H	2.37612	-3.38995	-0.50911
H	2.10701	-2.37208	-1.95856
H	3.72691	-2.26611	1.87112
H	5.03677	-1.88541	0.69757
H	4.41505	-0.61792	1.81402
H	2.25709	3.59539	1.25713
H	1.64540	2.21587	2.24937
H	2.71111	1.90116	0.84466
H	-1.03386	3.41006	1.85465
H	-0.13805	4.67434	0.93102
H	-1.57298	3.87381	0.20548

H	0.10521	3.21358	-2.14692
H	1.36239	4.17044	-1.27848
H	1.73310	2.51916	-1.91136
H	-0.63215	-3.88818	1.60552
H	0.79120	-2.97397	0.98942
H	-0.08743	-2.37900	2.43263
H	-1.91976	-3.94414	-0.79153
H	-2.26476	-2.48238	-1.79486
H	-0.58096	-3.05897	-1.61819
H	-3.75486	-1.62676	0.70151
H	-3.12307	-3.11298	1.50408
H	-2.85767	-1.49370	2.25255
H	-2.69700	1.46422	0.54269
H	-2.00800	1.96921	-1.08834

TS from $\mathbf{4}_{mer,trans}$ to $\mathbf{5}_{Pax,trans}$
SCF (BP86) Energy =-609.436433227
Enthalpy 0K = -609.073824
Enthalpy 298K = -609.042357
Free Energy 298K =-609.136149

Co	0.35840	-0.13210	0.00062
Cl	-0.07655	0.08861	2.21478
Cl	0.38055	-0.26568	-2.24830
P	0.08682	2.21250	-0.34248
P	-3.25049	-0.48707	0.09931
P	2.49027	-0.23053	0.43475
C	-1.53815	2.63254	-1.15638
C	1.27566	3.05764	-1.51070
C	0.07300	3.37645	1.11612
C	-4.19825	0.62144	1.28739
C	-3.61499	-2.15551	0.88471
C	-4.45798	-0.53533	-1.34227
C	3.18643	1.26210	1.29597
C	3.56747	-0.43249	-1.05847
C	3.03177	-1.59340	1.57205
C	0.19623	-2.07334	0.20336
Cl	1.11413	-3.28669	-0.87009
H	-2.36153	2.35621	-0.48092
H	-1.58392	3.71279	-1.37616
H	-1.62769	2.05321	-2.08783
H	0.95722	4.09967	-1.68219
H	2.29645	3.06069	-1.09671
H	1.27872	2.50559	-2.46279
H	1.04248	3.34190	1.63603
H	-0.12717	4.40726	0.77864
H	-0.70931	3.05346	1.81978
H	-5.22838	0.25612	1.44697
H	-3.66637	0.64794	2.25357
H	-4.23950	1.64834	0.88541
H	-3.06993	-2.23131	1.84093
H	-4.69612	-2.28646	1.06923
H	-3.26224	-2.96081	0.21782
H	-4.10809	-1.27804	-2.07947
H	-5.47932	-0.79998	-1.01522
H	-4.47832	0.45303	-1.83210
H	4.25195	1.07533	1.51484
H	3.10325	2.15598	0.66102
H	2.63319	1.41941	2.23393
H	4.62005	-0.50256	-0.73467
H	3.26751	-1.34838	-1.58809
H	3.43100	0.43057	-1.72669
H	2.84376	-2.56887	1.10086
H	4.11106	-1.47573	1.76689
H	2.46911	-1.51524	2.51437
H	0.38107	-2.42699	1.22976
H	-0.85988	-2.21644	-0.08669

$\mathbf{5}_{Cax,trans}\cdot\mathbf{PMe}_3$
SCF (BP86) Energy = -609.449745277
Enthalpy 0K = -609.087911
Enthalpy 298K = -609.054767
Free Energy 298K = -609.159262

Co	1.91486	0.05537	0.07167
Cl	3.55713	1.08130	-1.08025
Cl	0.63590	-0.78756	1.72321
P	-7.27919	0.05823	0.16251
P	1.01521	2.14351	0.52206
P	3.14675	-1.87794	0.06999
C	-7.50370	-1.22359	1.52352
C	-5.71218	-0.61520	-0.63534
C	-8.54977	-0.58197	-1.07103
C	-0.74986	2.27842	1.08868
C	1.14965	3.49199	-0.75001
C	1.96804	2.84111	1.96706
C	2.26605	-3.48394	0.38696
C	4.39475	-1.77639	1.44550
C	4.16887	-2.27091	-1.43188
C	0.93043	-0.61465	-1.41322
Cl	-0.42057	0.47029	-2.06861
H	-8.48087	-1.06980	2.01227
H	-7.45497	-2.25386	1.12808
H	-6.71463	-1.09019	2.28317
H	-5.79799	-1.69310	-0.86124
H	-5.51535	-0.06304	-1.57031
H	-4.85922	-0.45404	0.04592
H	-8.45229	-0.02355	-2.01763
H	-8.42037	-1.66042	-1.27194
H	-9.56376	-0.40769	-0.67242
H	-0.97157	3.32306	1.36447
H	-1.41315	1.95769	0.27132
H	-0.90047	1.61737	1.95442
H	0.53408	3.22383	-1.62181
H	0.79585	4.44331	-0.31867
H	2.19911	3.58487	-1.06507
H	3.03154	2.92397	1.69196
H	1.57633	3.83712	2.23429
H	1.86698	2.16223	2.82885
H	2.99926	-4.30622	0.43454
H	1.71032	-3.41230	1.33312
H	1.55427	-3.67604	-0.43251
H	5.00444	-2.69508	1.47545
H	5.04491	-0.90385	1.27369
H	3.86282	-1.65185	2.40205
H	4.83988	-1.42640	-1.64562
H	4.75400	-3.18862	-1.25469
H	3.50090	-2.42407	-2.29515
H	1.61213	-0.74347	-2.27072
H	0.40954	-1.53971	-1.11460

$5_{Pax,cis}.PMe_3$

SCF (BP86) Energy = -609.448682032
Enthalpy 0K = -609.084942
Enthalpy 298K = -609.052632
Free Energy 298K = -609.154431

Co	1.49667	-0.28620	-0.40006
Cl	1.34227	-2.23421	-1.59998
Cl	-0.25034	0.64160	-1.63538
P	1.74960	1.81947	0.39325
P	0.49142	-1.28135	1.25362
P	-5.52081	0.07701	0.24504
C	3.05118	2.14107	1.68857
H	4.03866	1.84077	1.30475
H	3.06534	3.21886	1.92147
H	2.83129	1.57633	2.60835
C	0.27895	2.73577	1.07167
H	0.50253	3.81576	1.05720
H	-0.59505	2.52418	0.43918
H	0.07883	2.42871	2.10883
C	2.30014	2.92525	-0.99992
H	1.49797	2.97002	-1.75083
H	2.50708	3.93215	-0.59902
H	3.21024	2.51096	-1.45828
C	1.33767	-2.81289	1.87062
H	0.68082	-3.30039	2.61076
H	1.52489	-3.48815	1.02339
H	2.29140	-2.54447	2.35180
C	-1.20937	-1.84112	0.77909
H	-1.13011	-2.50862	-0.09064
H	-1.66516	-2.36649	1.63569
H	-1.80991	-0.96044	0.50740
C	0.18818	-0.34754	2.83165
H	-0.54463	0.45410	2.65851
H	-0.22453	-1.05566	3.57096
H	1.12527	0.07547	3.22562
C	-7.37777	0.31991	0.43945
H	-7.85424	0.61715	-0.51185
H	-7.83303	-0.62101	0.79292
H	-7.56667	1.09902	1.19758
C	-5.51354	-1.06152	-1.25358
H	-6.12939	-0.65646	-2.07644
H	-4.47588	-1.18859	-1.60659
H	-5.90384	-2.05179	-0.96302
C	-5.08410	1.69929	-0.60487
H	-4.03276	1.65960	-0.93873
H	-5.73486	1.89014	-1.47701
H	-5.18879	2.52968	0.11435
C	3.21425	-0.84613	0.24676
Cl	4.32238	-0.11273	-1.05982
H	3.58927	-0.44928	1.20546
H	3.37546	-1.93287	0.16258

$5_{Pax,trans}.PMe_3$

SCF (BP86) Energy = -609.446239811
Enthalpy 0K = -609.083262
Enthalpy 298K = -609.050844
Free Energy 298K = -609.151973

Co	1.36285	-0.17781	0.45672
Cl	3.34281	-1.28683	0.65367
Cl	-0.52424	1.09254	0.32646
P	-5.81341	-0.14208	-0.38792
P	0.78908	-1.58749	-1.10046
P	2.46342	1.62067	-0.59178
C	-7.62929	-0.02026	0.09370
H	-7.93838	-0.95573	0.59037
H	-7.81598	0.82978	0.77404
H	-8.24049	0.10387	-0.81648
C	-5.51952	1.63536	-0.93393
H	-5.86859	2.35917	-0.17565
H	-4.44026	1.78518	-1.10856
H	-6.05228	1.81905	-1.88247
C	-5.03552	-0.06731	1.32481
H	-3.94251	0.04379	1.22128
H	-5.43141	0.77844	1.91522
H	-5.23953	-1.01059	1.85963
C	0.74184	-3.36555	-0.57075
H	0.53011	-3.99909	-1.44857
H	1.71270	-3.63919	-0.13196
H	-0.05450	-3.50247	0.17792
C	1.93283	-1.60299	-2.56421
H	2.95074	-1.84147	-2.22252
H	1.58569	-2.36225	-3.28609
H	1.92726	-0.61365	-3.04799
C	-0.88013	-1.33791	-1.86711
H	-0.92462	-0.34515	-2.33772
H	-1.04191	-2.12621	-2.62217
H	-1.65432	-1.39599	-1.08807
C	1.63339	2.46926	-2.02976
H	2.18913	3.38091	-2.30678
H	1.60562	1.78592	-2.89429
H	0.60265	2.72638	-1.74406
C	4.20672	1.41998	-1.21761
H	4.58830	2.38501	-1.59146
H	4.84321	1.05368	-0.39848
H	4.22309	0.67682	-2.03034
C	2.64905	3.00747	0.64118
H	3.25753	2.65137	1.48811
H	3.13707	3.88075	0.17648
H	1.65021	3.28797	1.01007
C	0.58156	-1.24864	1.84319
Cl	1.22950	0.00585	3.04522
H	-0.51647	-1.25221	1.94718
H	1.07200	-2.20277	2.09626

TS from **$5_{Cax,trans}$** to **$8_{Cax,trans}.Cl$**

SCF (BP86) Energy =-609.423930883
Enthalpy 0K = -609.063500
Enthalpy 298K = -609.031264
Free Energy 298K =-609.127330

Co	-0.97306	0.57403	0.01087
Cl	-1.35556	0.86770	-2.17720
Cl	-1.11258	0.82380	2.23400
P	-2.72312	-0.91576	0.11079
P	0.49361	2.34828	-0.07923
C	-3.01957	-1.96703	-1.37934
H	-2.14627	-2.62892	-1.49628

H	-3.93065	-2.56656	-1.21316
H	-3.13660	-1.32935	-2.26676
C	-4.29105	0.05862	0.32779
H	-5.14413	-0.63981	0.37089
H	-4.23472	0.63724	1.26287
H	-4.41700	0.74458	-0.52481
C	-2.70497	-2.11713	1.51489
H	-2.59963	-1.57463	2.46506
H	-3.64655	-2.69174	1.50318
H	-1.84752	-2.79179	1.35925
C	1.60394	2.42717	-1.55892
H	2.22546	3.33608	-1.49782
H	2.24720	1.53390	-1.56812
H	0.98982	2.44425	-2.47059
C	1.63781	2.56774	1.35942
H	2.24509	1.65624	1.46751
H	2.29126	3.43633	1.17311
H	1.04798	2.72135	2.27429
C	-0.46845	3.93672	-0.14564
H	-1.10543	4.01431	0.74973
H	0.23505	4.78598	-0.17622
H	-1.09891	3.94011	-1.04833
C	0.25569	-0.67351	-0.06373
Cl	0.11462	-3.52008	-0.33735
P	3.34556	-0.79733	0.06542
C	4.85044	0.32586	0.12435
H	4.86296	0.97065	-0.77043
H	4.79717	0.96821	1.01950
H	5.78219	-0.26649	0.15746
C	3.78956	-1.91176	-1.37201
H	3.04174	-2.71967	-1.43572
H	3.76135	-1.32926	-2.30835
H	4.79616	-2.34700	-1.24179
C	3.68572	-1.92600	1.52082
H	3.59391	-1.35219	2.45839
H	2.93571	-2.73485	1.52675
H	4.69782	-2.36320	1.45652
H	0.64816	-0.98978	-1.03794
H	0.61521	-1.12874	0.86698

$8_{Cax,trans}$.Cl

eight_Caxtrans_cl_s.log
SCF (BP86) Energy =-609.483364389
Enthalpy 0K = -609.118986
Enthalpy 298K = -609.086861
Free Energy 298K =-609.183317

Co	0.70606	0.56964	0.00111
Cl	1.55608	1.12627	-2.00479
Cl	0.31529	0.36243	2.18825
P	-0.58125	2.45207	-0.08353
P	2.60767	-0.80260	0.29977
C	-1.41848	2.83799	-1.69383
H	-2.16595	2.05815	-1.91139
H	-1.92620	3.81377	-1.61485
H	-0.66877	2.86200	-2.49779
C	0.51411	3.91841	0.23546
H	-0.08799	4.84245	0.21244
H	0.98492	3.80999	1.22575
H	1.29456	3.95921	-0.54000
C	-1.94938	2.62321	1.15612
H	-1.53081	2.57905	2.17173
H	-2.46491	3.58492	0.99577
H	-2.66927	1.79774	1.02863
C	3.53233	-1.52675	-1.14692
H	4.48031	-1.96661	-0.79468
H	2.92998	-2.30396	-1.64119
H	3.73379	-0.72576	-1.87299
C	2.67644	-2.16720	1.56878
H	2.12983	-3.05837	1.22071
H	3.72869	-2.44535	1.74867
H	2.21987	-1.80684	2.50285
C	3.85419	0.40403	0.98953
H	3.48499	0.79292	1.95125
H	4.81918	-0.10868	1.14116
H	3.98748	1.23843	0.28286
C	-0.84863	-0.42224	-0.65702
Cl	-5.14839	-0.38001	0.42979
P	-1.11520	-2.22030	-0.45631
C	0.15073	-3.26321	-1.28024
H	0.31016	-2.89359	-2.30605
H	1.09800	-3.24351	-0.72502
H	-0.22318	-4.29969	-1.31468
C	-2.71591	-2.60140	-1.27336
H	-3.50770	-1.99509	-0.79430
H	-2.64344	-2.34934	-2.34371
H	-2.93407	-3.67580	-1.15497
C	-1.26755	-2.71513	1.29926
H	-0.35847	-2.42977	1.84742
H	-2.13035	-2.17980	1.72855
H	-1.43554	-3.80297	1.35451
H	-0.87886	-0.23952	-1.74774
H	-1.76576	-0.00565	-0.19389

TS from **$8_{Cax,trans}$.Cl** to **$9_{mer,trans}$**
SCF (BP86) Energy =-609.479648455
Enthalpy 0K = -609.114279
Enthalpy 298K = -609.083834
Free Energy 298K =-609.172582

Co	-0.40205	0.05278	0.14801
Cl	-1.18653	0.16518	2.27960
Cl	0.17244	-0.03013	-2.02349
P	-0.93679	-2.21935	0.19078
P	2.94088	-0.29458	-0.07647
P	-0.40691	2.38067	0.15362
C	0.10935	-3.31552	1.27799
C	-0.95304	-3.12180	-1.43405
C	-2.64359	-2.55550	0.84423
C	4.32265	-0.42476	1.13876
C	3.31711	1.16142	-1.12517
C	3.03607	-1.80447	-1.11260
C	0.67702	3.22423	1.41258
C	-2.08901	3.04933	0.56825
C	-0.00304	3.28146	-1.42253
C	1.40360	-0.13578	0.90462
Cl	-3.52073	0.23561	-1.28692
H	0.12269	-2.90432	2.30048
H	-0.32552	-4.32870	1.29972
H	1.14095	-3.37961	0.89762

H	-1.28213	-4.16251	-1.27437
H	-1.65191	-2.60438	-2.10924
H	0.04859	-3.11019	-1.88886
H	-3.35635	-1.96089	0.25173
H	-2.86108	-3.63326	0.75368
H	-2.69506	-2.24049	1.89651
H	5.27646	-0.53682	0.59729
H	4.35323	0.48649	1.75723
H	4.15858	-1.30180	1.78507
H	3.35280	2.06447	-0.49465
H	4.29996	1.00954	-1.60096
H	2.53040	1.25275	-1.88776
H	2.24112	-1.76866	-1.87159
H	4.02692	-1.83312	-1.59533
H	2.91909	-2.69317	-0.47203
H	0.44134	4.30140	1.43423
H	0.48200	2.78504	2.40384
H	1.74175	3.09791	1.15854
H	-2.07624	4.14953	0.48879
H	-2.81657	2.61279	-0.13391
H	-2.35092	2.74108	1.59108
H	-0.69297	2.93910	-2.20886
H	-0.12121	4.36676	-1.26400
H	1.02738	3.06415	-1.74018
H	1.40378	-1.02555	1.56022
H	1.58960	0.73350	1.56157

TS from **5*Pax,cis*.Cl** to **9*fac***
SCF (BP86) Energy =-609.429827202
Enthalpy 0K = -609.067933
Enthalpy 298K = -609.037051
Free Energy 298K =-609.128113

Co	0.81973	0.12869	-0.57699
Cl	0.24380	1.62818	-2.28522
Cl	3.05300	0.88674	-0.67584
P	1.67534	-1.30032	0.97518
P	0.05648	1.63228	0.87594
P	-3.29058	-0.50659	0.07958
C	0.47822	-2.46738	1.80037
H	0.03199	-3.12794	1.03981
H	1.02152	-3.08463	2.53530
H	-0.32287	-1.91121	2.30950
C	2.61770	-0.57974	2.41328
H	3.02092	-1.41153	3.01512
H	3.44145	0.02704	2.00935
H	1.98356	0.04762	3.05594
C	2.94376	-2.47924	0.29824
H	3.73213	-1.89658	-0.19956
H	3.36546	-3.06085	1.13544
H	2.46908	-3.14897	-0.43189
C	-1.28794	2.76333	0.27136
H	-1.69470	3.31382	1.13669
H	-0.86462	3.45982	-0.46485
H	-2.07751	2.17515	-0.21546
C	1.32807	2.84321	1.47758
H	1.74001	3.37356	0.60615
H	0.84443	3.55582	2.16743
H	2.14728	2.31725	1.98762
C	-0.70620	0.98729	2.44841
H	0.02772	0.45621	3.07065
H	-1.10783	1.83891	3.02271
H	-1.52579	0.30223	2.18567
C	-4.32041	0.30808	1.41993
H	-5.38985	0.06942	1.28357
H	-3.99134	-0.05159	2.40928
H	-4.18366	1.40142	1.37793
C	-3.83068	-2.29064	0.24212
H	-4.92926	-2.38022	0.18147
H	-3.37322	-2.88447	-0.56751
H	-3.48455	-2.68978	1.21033
C	-4.20532	0.02000	-1.46347
H	-3.81402	-0.54559	-2.32611
H	-5.28967	-0.16373	-1.36929
H	-4.03032	1.09439	-1.64345
C	-0.74661	-0.83452	-0.88719
Cl	0.95161	-1.64421	-2.20559
H	-0.98150	-1.81325	-0.44714
H	-1.36265	-0.54221	-1.74725

TS from **5*Pax,trans*.Cl** to **9*mer,cis***
SCF (BP86) Energy =-609.429226180
Enthalpy 0K = -609.067646
Enthalpy 298K = -609.035948
Free Energy 298K =-609.130156

Co	0.59495	-0.34155	-0.14125
Cl	0.93124	0.07501	-2.38109
Cl	0.39019	-0.70680	2.11670
P	-3.62162	-0.26995	0.03381
P	-0.08068	1.76985	-0.01428
P	2.92386	-0.12209	0.26191
C	-4.49304	-1.62800	-0.91395
H	-3.96963	-2.58386	-0.74288
H	-5.54558	-1.72585	-0.59567
H	-4.45716	-1.39733	-1.99213
C	-4.79177	1.17128	-0.24652
H	-5.82534	0.89758	0.02962
H	-4.46737	2.03111	0.36312
H	-4.76451	1.46339	-1.30982
C	-4.03335	-0.73328	1.80047
H	-3.69696	0.06987	2.47778
H	-5.11887	-0.88926	1.92816
H	-3.49603	-1.65928	2.06638
C	-1.28642	2.30890	-1.31966
H	-1.66207	3.31403	-1.06441
H	-0.77221	2.32613	-2.29073
H	-2.11798	1.59201	-1.35917
C	1.24156	3.06398	-0.20672
H	1.76932	2.89788	-1.15813
H	0.76599	4.05972	-0.21881
H	1.95407	3.01784	0.62998
C	-0.90735	2.27153	1.57013
H	-0.19681	2.16344	2.40225
H	-1.24261	3.31899	1.48397
H	-1.76772	1.61208	1.75568
C	3.51433	0.76268	1.79639
H	4.59908	0.60481	1.91876
H	3.31663	1.84339	1.72251
H	2.97370	0.35900	2.66520

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C    4.03522   0.59616 -1.05157
H    5.08840   0.51937 -0.73281
H    3.88316   0.04183 -1.98966
H    3.78028   1.65280 -1.22542
C    3.68863 -1.80248   0.51185
H    3.56405 -2.39628 -0.40630
H    4.76059 -1.69612   0.74945
H    3.16756 -2.31177   1.33684
C   -1.07137 -1.17993 -0.43915
Cl   0.60458 -2.69106 -0.60471
H   -1.54660 -1.75448   0.36842
H   -1.48330 -1.31298 -1.45283
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9*fac*

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SCF (BP86) Energy =-609.485425305
Enthalpy 0K =     -609.119083
Enthalpy 298K =   -609.088347
Free Energy 298K =-609.177064

Co   0.31289 -0.10747 -0.44722
Cl  -1.05511   0.99131 -2.02775
Cl   2.15444   0.01243 -1.98314
P    1.83964 -1.22343   0.82314
P    0.79934   1.93759   0.42140
P   -2.94337 -0.31195   0.50521
C    1.30640 -1.70592   2.54921
H    0.49160 -2.44483   2.48595
H    2.15971 -2.15926   3.08082
H    0.94949 -0.82907   3.11059
C    3.49401 -0.41213   1.13168
H    4.11015 -1.09565   1.73971
H    3.97055 -0.24412   0.15472
H    3.40120   0.54693   1.65973
C    2.42386 -2.85986   0.15871
H    2.78281 -2.71139 -0.86974
H    3.23986 -3.22742   0.80407
H    1.58811 -3.57210   0.14665
C   -0.48465   3.27251   0.22715
H   -0.09658   4.19726   0.68657
H   -0.69129   3.42595 -0.84049
H   -1.41417   2.97824   0.73445
C    2.29495   2.80687 -0.26089
H    2.13864   2.95977 -1.33917
H    2.41118   3.77694   0.25151
H    3.19547   2.19228 -0.12778
C    1.06040   2.06596   2.27272
H    1.88928   1.43363   2.62085
H    1.28608   3.11580   2.52497
H    0.14012   1.76703   2.80013
C   -3.63889   1.37821   0.31334
H   -4.72896   1.29290   0.17126
H   -3.43791   1.96286   1.22557
H   -3.17306   1.85266 -0.56192
C   -3.82265 -1.01833   1.97121
H   -4.91160 -0.98539   1.80241
H   -3.50428 -2.06344   2.11462
H   -3.57211 -0.43314   2.87055
C   -3.50820 -1.30941 -0.92410
H   -3.25568 -2.36496 -0.74793
H   -4.60035 -1.18375 -1.01328
H   -2.98785 -0.95547 -1.82444
C   -1.15387 -0.36457   0.89735
Cl  -0.33289 -2.20219 -1.33587
H   -1.08035   0.29338   1.78693
H   -1.03972 -1.40321   1.25793
```

9*mer,cis*

```
SCF (BP86) Energy =-609.487441157
Enthalpy 0K =     -609.121868
Enthalpy 298K =   -609.090775
Free Energy 298K =-609.181075

Co  -0.22952 -0.19088   0.28277
Cl  -0.83136   0.31664   2.46309
Cl   0.28051 -0.59696 -1.94257
P    3.16784 -0.26493 -0.06391
P   -0.55613   2.01505 -0.10110
P   -2.41803 -0.83867 -0.33519
C    4.66398 -0.05744   1.00278
H    4.60636 -0.76859   1.84244
H    5.57561 -0.25319   0.41422
H    4.69272   0.97068   1.39761
C    3.41533   0.89448 -1.46983
H    4.34281   0.62802 -2.00221
H    2.54933   0.81330 -2.14289
H    3.50210   1.92181 -1.07999
C    3.25966 -1.98215 -0.70003
H    2.39393 -2.16008 -1.35283
H    4.20619 -2.10891 -1.25053
H    3.22018 -2.67420   0.15518
C    0.67745   3.19171   0.65675
H    0.33985   4.22459   0.46789
H    0.73306   3.01762   1.74261
H    1.67274   3.05345   0.20781
C   -2.12863   2.76290   0.57267
H   -2.09893   2.69400   1.66955
H   -2.18790   3.81804   0.25681
H   -3.01622   2.22648   0.20964
C   -0.55446   2.60049 -1.86967
H   -1.32125   2.06576 -2.44695
H   -0.75387   3.68516 -1.89009
H    0.42665   2.38916 -2.31953
C   -3.30304   0.07891 -1.70929
H   -4.27433 -0.40515 -1.90660
H   -3.48160   1.13422 -1.45536
H   -2.68104   0.02686 -2.61719
C   -3.70172 -0.87669   1.01485
H   -4.65232 -1.27829   0.62522
H   -3.32741 -1.51669   1.82868
H   -3.85895   0.13610   1.41602
C   -2.55239 -2.56496 -1.02704
H   -2.30236 -3.29082 -0.24157
H   -3.57872 -2.73013 -1.39607
H   -1.82969 -2.66910 -1.85018
C    1.68678   0.09187   0.91964
Cl   0.08075 -2.47165   0.90026
H    1.74628 -0.62145   1.76071
H    1.86265   1.10210   1.32778
```

9*mer,trans*

SCF (BP86) Energy =-609.489261518
Enthalpy 0K = -609.124203
Enthalpy 298K = -609.092927
Free Energy 298K =-609.183707

Co	0.55209	0.05364	0.02330
Cl	1.40614	0.17680	2.18232
Cl	-0.37809	-0.06824	-2.08629
P	0.51637	2.37243	0.04460
P	-2.86350	-0.28968	0.15866
P	1.02371	-2.21469	0.06379
C	-0.64313	3.21056	1.24744
C	0.12842	3.23627	-1.55861
C	2.12588	3.17319	0.52519
C	-4.12978	-0.38982	1.50100
C	-3.10268	-1.81340	-0.84008
C	-3.36749	1.14754	-0.86765
C	-0.02869	-3.31606	1.14768
C	2.71827	-2.65867	0.69280
C	0.97781	-3.10372	-1.56934
C	-1.22505	-0.13828	0.94802
Cl	2.70951	0.26620	-1.02610
H	-0.44104	2.82821	2.26110
H	-0.46996	4.29952	1.22836
H	-1.69516	3.01412	0.98933
H	0.22914	4.32735	-1.43104
H	0.83325	2.87911	-2.32504
H	-0.89330	2.99011	-1.88357
H	2.88984	2.90203	-0.21678
H	1.99302	4.26726	0.56564
H	2.43242	2.78739	1.50870
H	-5.13518	-0.48875	1.05956
H	-3.91872	-1.26371	2.13799
H	-4.08370	0.52548	2.11250
H	-3.00158	-2.69522	-0.18727
H	-4.11824	-1.79652	-1.26883
H	-2.34849	-1.83491	-1.63968
H	-2.64882	1.25586	-1.69220
H	-4.38184	0.96435	-1.25854
H	-3.37901	2.05492	-0.24269
H	0.36535	-4.34573	1.11875
H	0.00575	-2.94567	2.18533
H	-1.07342	-3.32695	0.80192
H	2.84392	-3.75412	0.66222
H	3.46841	-2.16519	0.05879
H	2.82329	-2.28991	1.72374
H	1.63135	-2.56518	-2.27230
H	1.33012	-4.14096	-1.44042
H	-0.04623	-3.09984	-1.97091
H	-1.34973	0.72058	1.63286
H	-1.17661	-1.02954	1.60013

TS from $\mathbf{4}_{mer,cis}$ to $\mathbf{6}_{Pax,cis}$.Cl
SCF (BP86) Energy =-609.434297008
Enthalpy 0K = -609.069980
Enthalpy 298K = -609.039108
Free Energy 298K =-609.129343

Co	-0.05829	0.04858	-0.39136
Cl	-0.34869	-1.41457	-2.18777
Cl	-0.42630	1.84890	-1.89342
P	0.14220	1.75119	1.08832
P	-2.51880	-0.66925	0.10452
P	2.13649	-0.26310	-0.72935
C	-1.40565	2.75187	1.35765
C	1.32061	3.12780	0.65379
C	0.60529	1.28833	2.83138
C	-3.32352	-0.59045	1.78108
C	-3.07202	-2.33234	-0.50033
C	-3.49266	0.51842	-0.94270
C	3.30313	0.11383	0.66820
C	2.79363	0.68157	-2.18210
C	2.61331	-2.02228	-1.06282
C	-0.33094	-1.22824	0.85458
Cl	1.59799	-2.51155	2.41899
H	-2.18940	2.14979	1.84024
H	-1.15809	3.59959	2.01924
H	-1.75988	3.12684	0.38627
H	1.42295	3.78662	1.53252
H	2.31137	2.75552	0.36179
H	0.89002	3.68160	-0.19246
H	1.51121	0.66582	2.84022
H	0.76627	2.20597	3.42122
H	-0.21454	0.70926	3.28598
H	-4.41610	-0.66927	1.65342
H	-2.96493	-1.43416	2.39209
H	-3.08742	0.35181	2.29761
H	-2.63820	-3.12282	0.13138
H	-4.17274	-2.36680	-0.43399
H	-2.74275	-2.46931	-1.53900
H	-3.10652	0.47276	-1.97113
H	-4.55177	0.20955	-0.90379
H	-3.37877	1.54279	-0.56147
H	4.32327	-0.11391	0.31346
H	3.26774	1.16089	0.99656
H	3.04341	-0.56248	1.50049
H	3.85530	0.41636	-2.32478
H	2.20604	0.40725	-3.07065
H	2.68924	1.76215	-2.00669
H	2.14941	-2.36804	-1.99482
H	3.71383	-2.06250	-1.13270
H	2.27215	-2.62997	-0.20994
H	-0.50690	-1.05000	1.92415
H	-0.41678	-2.28787	0.56410

TS from $\mathbf{4}_{mer,cis}$ to $\mathbf{6}_{Cax,trans}$.Cl
SCF (BP86) Energy = -609.417509607
Enthalpy 0K = -609.052007
Enthalpy 298K = -609.021566
Free Energy 298K = -609.110629

Co	0.03393	-0.19756	-0.11176
Cl	0.14689	-2.51200	0.22147
Cl	0.21161	-0.36137	-2.49602
P	-0.04110	1.96936	0.18981
P	-2.24733	-0.45163	-0.47109
P	2.35313	-0.41391	-0.17494
C	-1.61341	2.88656	0.63657
C	0.29847	2.84388	-1.44605
C	1.15562	2.91982	1.28910

C	-3.40266	-0.19856	0.97301
C	-2.74437	-2.14796	-1.04693
C	-3.02853	0.56760	-1.82887
C	3.36413	0.93730	-0.98096
C	3.00569	-1.88391	-1.10985
C	3.17924	-0.61439	1.48472
C	-0.04235	0.45581	1.64554
Cl	-0.57550	-0.93825	3.12764
H	-1.98571	2.62754	1.64059
H	-1.36106	3.96051	0.62152
H	-2.40255	2.70837	-0.10695
H	0.22271	3.93494	-1.29758
H	1.29972	2.57995	-1.81259
H	-0.43996	2.50041	-2.18523
H	2.16314	2.47778	1.27811
H	1.20694	3.94575	0.88772
H	0.78839	2.95346	2.32673
H	-4.42518	-0.48783	0.67753
H	-3.05728	-0.82737	1.80790
H	-3.40548	0.85296	1.29584
H	-2.58571	-2.87322	-0.23751
H	-3.80793	-2.11994	-1.33951
H	-2.11766	-2.42707	-1.90649
H	-2.55898	0.27300	-2.77915
H	-4.11035	0.35484	-1.85923
H	-2.87778	1.64720	-1.68572
H	4.43065	0.65802	-0.94385
H	3.04719	1.02596	-2.03224
H	3.23443	1.90724	-0.47891
H	4.10112	-1.78474	-1.19383
H	2.73964	-2.80293	-0.57173
H	2.54173	-1.89795	-2.10634
H	2.66654	-1.41986	2.03359
H	4.24041	-0.87637	1.33943
H	3.11997	0.31666	2.07114
H	0.91714	0.65527	2.14055
H	-0.81281	1.11478	2.07696

TS from $\mathbf{4}_{mer,trans}$ to $\mathbf{6}_{Pax,trans}$.**Cl**
SCF (BP86) Energy = -609.428839660
Enthalpy 0K = -609.065799
Enthalpy 298K = -609.035306
Free Energy 298K = -609.125076

Co	0.01262	0.01321	0.05459
Cl	0.29809	-0.05158	2.33438
Cl	-0.13029	0.05869	-2.22268
P	1.93146	-1.35955	-0.36367
P	0.98314	2.33268	0.18229
P	-1.47704	-1.64339	0.37550
C	3.29004	-0.53845	-1.34881
C	1.66893	-2.85563	-1.45141
C	2.87110	-2.06125	1.08416
C	2.55609	2.24975	1.17369
C	0.15228	3.77767	1.02011
C	1.44131	2.99771	-1.48070
C	-0.87322	-3.14828	1.28484
C	-2.26284	-2.29453	-1.16785
C	-2.90996	-1.11596	1.41820
C	-1.16479	1.37263	0.15771
Cl	-4.05885	1.47732	-0.72809
H	3.74454	0.28999	-0.78563
H	4.07459	-1.27790	-1.58232
H	2.85979	-0.15040	-2.28517
H	2.63366	-3.36480	-1.61387
H	0.96251	-3.56571	-0.99656
H	1.26231	-2.51490	-2.41592
H	2.20442	-2.70360	1.67923
H	3.73699	-2.64708	0.73326
H	3.21378	-1.23462	1.72588
H	3.00301	3.25891	1.17938
H	2.30187	1.93429	2.19611
H	3.26225	1.53245	0.73458
H	-0.11553	3.49632	2.05069
H	0.87592	4.61039	1.03984
H	-0.75105	4.08538	0.47206
H	0.52308	3.15436	-2.06746
H	1.97395	3.95447	-1.34722
H	2.07937	2.27456	-2.00836
H	-1.74309	-3.80286	1.46563
H	-0.12173	-3.70518	0.70698
H	-0.44243	-2.82732	2.24456
H	-2.98633	-3.08088	-0.89179
H	-2.78145	-1.46147	-1.66629
H	-1.49694	-2.70088	-1.84381
H	-3.44434	-0.30606	0.89154
H	-3.57514	-1.98403	1.56529
H	-2.53204	-0.76023	2.38817
H	-1.58061	1.73117	1.11444
H	-1.51160	1.92553	-0.72983

TS from $\mathbf{4}_{fac}$ to $\mathbf{6}_{Pax,trans}$.**Cl**
SCF (BP86) Energy = -609.413823902
Enthalpy 0K = -609.050827
Enthalpy 298K = -609.019741
Free Energy 298K = -609.111192

Co	-0.01472	-0.07510	-0.37191
Cl	0.17971	1.20843	-2.31921
Cl	-0.14597	-1.93444	-1.65099
P	-0.12744	-1.56987	1.35401
P	-0.70235	2.13689	0.79633
P	2.43340	-0.03560	-0.37686
C	0.28751	-0.98583	3.08022
H	-0.37207	-0.15419	3.37559
H	0.13293	-1.82436	3.78041
H	1.33603	-0.65700	3.13741
C	0.93708	-3.08971	1.20879
H	0.88350	-3.63791	2.16456
H	0.55156	-3.71260	0.39015
H	1.98306	-2.82882	0.99564
C	-1.80802	-2.32484	1.58364
H	-2.17901	-2.67815	0.60961
H	-1.72402	-3.16741	2.29009
H	-2.51180	-1.58122	1.98882
C	-2.08973	2.28331	2.02979
H	-1.97818	3.25279	2.54603
H	-3.05953	2.24655	1.50802
H	-2.03667	1.46396	2.76485
C	-0.94966	3.57919	-0.32709

H	-1.83962	3.41461	-0.95420
H	-1.09340	4.46787	0.31288
H	-0.06678	3.69986	-0.97081
C	0.78033	2.62127	1.82404
H	1.64948	2.77776	1.16950
H	0.51797	3.56842	2.32884
H	1.00016	1.84760	2.57340
C	3.43748	-0.24277	1.19310
H	4.51314	-0.18394	0.95610
H	3.18580	0.56171	1.90299
H	3.23647	-1.21347	1.67159
C	3.24075	1.50644	-1.05448
H	4.33470	1.36555	-1.06045
H	2.87002	1.68159	-2.07380
H	2.99328	2.38225	-0.43419
C	3.17799	-1.32820	-1.49046
H	2.76787	-1.19144	-2.50273
H	4.27504	-1.21822	-1.50789
H	2.90684	-2.33540	-1.14044
C	-1.75663	0.39438	-0.22184
Cl	-4.31519	-0.91446	-1.25992
H	-2.45950	0.08846	0.57067
H	-2.23175	1.02990	-0.99557

$6_{Cax,trans}$.Cl

SCF (BP86) Energy =-609.483364389
Enthalpy 0K = -609.118986
Enthalpy 298K = -609.086861
Free Energy 298K =-609.183317

Co	0.70606	0.56964	0.00111
Cl	1.55608	1.12627	-2.00479
Cl	0.31529	0.36243	2.18825
P	-0.58125	2.45207	-0.08353
P	2.60767	-0.80260	0.29977
C	-1.41848	2.83799	-1.69383
H	-2.16595	2.05815	-1.91139
H	-1.92620	3.81377	-1.61485
H	-0.66877	2.86200	-2.49779
C	0.51411	3.91841	0.23546
H	-0.08799	4.84245	0.21244
H	0.98492	3.80999	1.22575
H	1.29456	3.95921	-0.54000
C	-1.94938	2.62321	1.15612
H	-1.53081	2.57905	2.17173
H	-2.46491	3.58492	0.99577
H	-2.66927	1.79774	1.02863
C	3.53233	-1.52675	-1.14692
H	4.48031	-1.96661	-0.79468
H	2.92998	-2.30396	-1.64119
H	3.73379	-0.72576	-1.87299
C	2.67644	-2.16720	1.56878
H	2.12983	-3.05837	1.22071
H	3.72869	-2.44535	1.74867
H	2.21987	-1.80684	2.50285
C	3.85419	0.40403	0.98953
H	3.48499	0.79292	1.95125
H	4.81918	-0.10868	1.14116
H	3.98748	1.23843	0.28286
C	-0.84863	-0.42224	-0.65702
Cl	-5.14839	-0.38001	0.42979
P	-1.11520	-2.22030	-0.45631
C	0.15073	-3.26321	-1.28024
H	0.31016	-2.89359	-2.30605
H	1.09800	-3.24351	-0.72502
H	-0.22318	-4.29969	-1.31468
C	-2.71591	-2.60140	-1.27336
H	-3.50770	-1.99509	-0.79430
H	-2.64344	-2.34934	-2.34371
H	-2.93407	-3.67580	-1.15497
C	-1.26755	-2.71513	1.29926
H	-0.35847	-2.42977	1.84742
H	-2.13035	-2.17980	1.72855
H	-1.43554	-3.80297	1.35451
H	-0.87886	-0.23952	-1.74774
H	-1.76576	-0.00565	-0.19389

$6_{Pax,cis}$.Cl

SCF (BP86) Energy =-609.488384905
Enthalpy 0K = -609.122745
Enthalpy 298K = -609.093097
Free Energy 298K =-609.181037

Co	-0.75658	-0.48112	-0.32692
Cl	-0.21226	-1.40684	-2.33385
Cl	-2.87033	-1.39544	-0.48786
P	-1.31999	-0.11585	1.83318
P	2.37561	-1.42551	-0.02839
P	-1.10048	1.54872	-1.05515
C	-1.56596	-1.75614	2.67624
C	-2.91087	0.77454	2.19367
C	-0.11356	0.72289	2.97929
C	3.64493	-1.08247	1.25868
C	3.26525	-1.54571	-1.62907
C	1.68685	-3.08784	0.34727
C	-0.52376	2.94329	0.01894
C	-2.88439	1.90330	-1.40375
C	-0.27806	1.90756	-2.67721
C	1.16418	-0.03830	-0.04282
Cl	3.55487	3.06513	0.64504
H	-0.64620	-2.35789	2.60221
H	-1.79859	-1.58095	3.74051
H	-2.39152	-2.28867	2.18319
H	-3.12507	0.69252	3.27247
H	-2.82749	1.84075	1.92918
H	-3.71676	0.30568	1.61075
H	0.17138	1.71934	2.60837
H	-0.58603	0.82578	3.97054
H	0.79558	0.10917	3.08014
H	4.42719	-1.85822	1.22097
H	4.08216	-0.08852	1.06674
H	3.16848	-1.08385	2.25250
H	3.76167	-0.58193	-1.82776
H	4.01790	-2.34841	-1.56248
H	2.53546	-1.76298	-2.42274
H	0.92349	-3.34343	-0.40328
H	2.51068	-3.81980	0.31431
H	1.24162	-3.08773	1.35509
H	-0.75006	3.88868	-0.50410
H	-1.04433	2.94004	0.98820

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H    0.56527   2.87010   0.17742
H   -2.95957   2.92862  -1.80580
H   -3.24602   1.17294  -2.14254
H   -3.48428   1.81347  -0.48751
H   -0.68582   1.23278  -3.44279
H   -0.48493   2.96020  -2.93689
H    0.80839   1.75387  -2.59668
H    1.35750   0.52198   0.88764
H    1.54434   0.59112  -0.86954
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$6_{Pax,trans}$.Cl

```
SCF (BP86) Energy =-609.485591078
Enthalpy 0K =     -609.121169
Enthalpy 298K =   -609.089331
Free Energy 298K =-609.183973

Co   0.76609  -0.27136   0.32911
Cl   0.52816  -1.40853  -1.58747
Cl   1.22395   0.47456   2.40517
P    0.26884   1.74218  -0.32973
P   -2.37440  -1.69251   0.17745
P    3.07325  -0.30332  -0.13436
C   -0.14127   1.87355  -2.13000
H   -1.03049   1.26889  -2.35686
H   -0.34322   2.93441  -2.35862
H    0.70696   1.50992  -2.72850
C    1.63172   2.97917  -0.10357
H    1.25705   3.96512  -0.42977
H    1.91516   3.01680   0.95836
H    2.50416   2.70718  -0.71674
C   -1.15820   2.53914   0.53865
H   -0.98666   2.50248   1.62515
H   -1.21485   3.58922   0.20407
H   -2.10527   2.03443   0.28921
C   -3.84437  -1.74686   1.28767
H   -4.63285  -2.36365   0.82577
H   -3.55410  -2.17813   2.25901
H   -4.21779  -0.71885   1.42778
C   -1.88779  -3.44239  -0.10236
H   -1.61533  -3.89266   0.86609
H   -2.74467  -3.98585  -0.53261
H   -1.02949  -3.47741  -0.78806
C   -2.96624  -0.96877  -1.39804
H   -2.12897  -0.90928  -2.10777
H   -3.76185  -1.61684  -1.80153
H   -3.38949   0.03014  -1.18822
C    3.67813   0.03085  -1.86408
H    4.73543  -0.27021  -1.95354
H    3.06363  -0.54009  -2.57589
H    3.59234   1.10594  -2.09220
C    3.61594  -2.06484   0.15797
H    4.69873  -2.15794  -0.03094
H    3.40240  -2.34090   1.20338
H    3.05873  -2.73223  -0.51704
C    4.28840   0.64249   0.91286
H    4.11620   0.39693   1.97106
H    5.31517   0.36378   0.62246
H    4.15110   1.72545   0.77511
C   -1.05557  -0.75838   1.02527
Cl  -5.02599   1.99515  -0.15545
H   -1.55548   0.08017   1.53999
H   -0.71486  -1.45928   1.81977
```

TS from **$6_{Pax,cis}$.Cl** to **9_{fac}**

```
SCF (BP86) Energy =-609.476476271
Enthalpy 0K =     -609.110585
Enthalpy 298K =   -609.080337
Free Energy 298K =-609.169401

C    3.53067  -0.44641   1.19448
P    1.80451  -1.11614   0.98930
C    2.16246  -2.86261   0.47508
C    1.25303  -1.33647   2.75787
Co   0.37282  -0.04554  -0.44130
P    0.98516   1.98953   0.11982
C   -0.11841   3.38731  -0.40569
C   -1.10119  -0.16592   0.88722
P   -2.88927   0.11808   0.58864
C   -3.73332  -0.37165   2.15815
Cl  -0.99333   0.71018  -2.10633
Cl  -0.97034  -3.17797  -1.00583
C    2.60467   2.52454  -0.61103
C    1.15788   2.35092   1.93844
C   -3.63763  -0.92322  -0.71892
C   -3.38848   1.86246   0.30003
H    3.54053   0.53097   1.69942
H    4.10326  -1.16483   1.80496
H    3.99212  -0.35968   0.19949
H    2.74202  -3.35378   1.27524
H    1.21029  -3.38248   0.28808
H    2.73980  -2.83425  -0.46031
H    0.33974  -1.95095   2.78512
H    2.05160  -1.85305   3.31598
H    1.04963  -0.36560   3.23490
H    1.47215   3.40255   2.04987
H    0.18707   2.21026   2.43889
H    1.90777   1.70350   2.41446
H   -1.10122   3.30379   0.07612
H    0.36524   4.32804  -0.09015
H   -0.24293   3.36296  -1.49681
H    2.49902   2.52650  -1.70607
H    2.83045   3.54065  -0.24415
H    3.41035   1.83251  -0.33600
H   -3.03390   2.49530   1.12955
H   -2.96410   2.19847  -0.65678
H   -4.48972   1.90214   0.25963
H   -3.52508  -1.43478   2.36013
H   -3.35391   0.24122   2.99125
H   -4.82071  -0.22270   2.05470
H   -3.44776  -0.46229  -1.69790
H   -3.14473  -1.91043  -0.69634
H   -4.71908  -1.00557  -0.52280
H   -0.90963   0.34394   1.85087
H   -1.09521  -1.26019   1.07843
Cl   2.04935  -0.48036  -1.99400
```

TS from **$6_{Pax,trans}$.Cl** to **$9_{mer,cis}$**

```
SCF (BP86) Energy =-609.476476271
Enthalpy 0K =     -609.110585
Enthalpy 298K =   -609.080337
```

Free Energy 298K =-609.169401

C	3.53067	-0.44641	1.19448
P	1.80451	-1.11614	0.98930
C	2.16246	-2.86261	0.47508
C	1.25303	-1.33647	2.75787
Co	0.37282	-0.04554	-0.44130
P	0.98516	1.98953	0.11982
C	-0.11841	3.38731	-0.40569
C	-1.10119	-0.16592	0.88722
P	-2.88927	0.11808	0.58864
C	-3.73332	-0.37165	2.15815
Cl	-0.99333	0.71018	-2.10633
Cl	-0.97034	-3.17797	-1.00583
C	2.60467	2.52454	-0.61103
C	1.15788	2.35092	1.93844
C	-3.63763	-0.92322	-0.71892
C	-3.38848	1.86246	0.30003
H	3.54053	0.53097	1.69942
H	4.10326	-1.16483	1.80496
H	3.99212	-0.35968	0.19949
H	2.74202	-3.35378	1.27524
H	1.21029	-3.38248	0.28808
H	2.73980	-2.83425	-0.46031
H	0.33974	-1.95095	2.78512
H	2.05160	-1.85305	3.31598
H	1.04963	-0.36560	3.23490
H	1.47215	3.40255	2.04987
H	0.18707	2.21026	2.43889
H	1.90777	1.70350	2.41446
H	-1.10122	3.30379	0.07612
H	0.36524	4.32804	-0.09015
H	-0.24293	3.36296	-1.49681
H	2.49902	2.52650	-1.70607
H	2.83045	3.54065	-0.24415
H	3.41035	1.83251	-0.33600
H	-3.03390	2.49530	1.12955
H	-2.96410	2.19847	-0.65678
H	-4.48972	1.90214	0.25963
H	-3.52508	-1.43478	2.36013
H	-3.35391	0.24122	2.99125
H	-4.82071	-0.22270	2.05470
H	-3.44776	-0.46229	-1.69790
H	-3.14473	-1.91043	-0.69634
H	-4.71908	-1.00557	-0.52280
H	-0.90963	0.34394	1.85087
H	-1.09521	-1.26019	1.07843
Cl	2.04935	-0.48036	-1.99400

TS from **6**$_{Cax,trans}$**.Cl** to **9**$_{mer,trans}$
SCF (BP86) Energy =-609.479648455
Enthalpy 0K = -609.114279
Enthalpy 298K = -609.083834
Free Energy 298K =-609.172582

Co	-0.40205	0.05278	0.14801
Cl	-1.18653	0.16518	2.27960
Cl	0.17244	-0.03013	-2.02349
P	-0.93679	-2.21935	0.19078
P	2.94088	-0.29458	-0.07647
P	-0.40691	2.38067	0.15362
C	0.10935	-3.31552	1.27799
C	-0.95304	-3.12180	-1.43405
C	-2.64359	-2.55550	0.84423
C	4.32265	-0.42476	1.13876
C	3.31711	1.16142	-1.12517
C	3.03607	-1.80447	-1.11260
C	0.67702	3.22423	1.41258
C	-2.08901	3.04933	0.56825
C	-0.00304	3.28146	-1.42253
C	1.40360	-0.13578	0.90462
Cl	-3.52073	0.23561	-1.28692
H	0.12269	-2.90432	2.30048
H	-0.32552	-4.32870	1.29972
H	1.14095	-3.37961	0.89762
H	-1.28213	-4.16251	-1.27437
H	-1.65191	-2.60438	-2.10924
H	0.04859	-3.11019	-1.88886
H	-3.35635	-1.96089	0.25173
H	-2.86108	-3.63326	0.75368
H	-2.69506	-2.24049	1.89651
H	5.27646	-0.53682	0.59729
H	4.35323	0.48649	1.75723
H	4.15858	-1.30180	1.78507
H	3.35280	2.06447	-0.49465
H	4.29996	1.00954	-1.60096
H	2.53040	1.25275	-1.88776
H	2.24112	-1.76866	-1.87159
H	4.02692	-1.83312	-1.59533
H	2.91909	-2.69317	-0.47203
H	0.44134	4.30140	1.43423
H	0.48200	2.78504	2.40384
H	1.74175	3.09791	1.15854
H	-2.07624	4.14953	0.48879
H	-2.81657	2.61279	-0.13391
H	-2.35092	2.74108	1.59108
H	-0.69297	2.93910	-2.20886
H	-0.12121	4.36676	-1.26400
H	1.02738	3.06415	-1.74018
H	1.40378	-1.02555	1.56022
H	1.58960	0.73350	1.56157

^{2}10
SCF (BP86) Energy =-428.804893445
Enthalpy 0K = -428.579711
Enthalpy 298K = -428.559068
Free Energy 298K =-428.630316

Co	0.03058	-0.68027	-0.09268
Cl	1.51062	-2.07971	-1.09358
P	-1.69904	0.67827	-0.25396
P	1.59001	0.84615	0.24890
C	-3.11636	-0.23419	-1.04416
H	-3.95841	0.45997	-1.20770
H	-2.78640	-0.64889	-2.01022
H	-3.41966	-1.05867	-0.38267
C	-1.52559	2.14566	-1.38960
H	-2.50044	2.65257	-1.49085
H	-0.78745	2.86545	-1.00280
H	-1.19654	1.79015	-2.37956

C	-2.44889	1.38132	1.29448
H	-1.74024	2.06856	1.78160
H	-3.37648	1.92404	1.04651
H	-2.67203	0.54755	1.97794
C	2.40969	1.56245	-1.25752
H	3.26191	2.19620	-0.95961
H	2.76259	0.73074	-1.88684
H	1.68450	2.16459	-1.82723
C	2.99231	0.07983	1.20087
H	3.76460	0.84115	1.40482
H	2.60425	-0.31941	2.15163
H	3.41041	-0.74641	0.60803
C	1.19530	2.33205	1.29869
H	0.77649	1.98730	2.25791
H	2.12058	2.90189	1.48903
H	0.46796	2.98984	0.79960
Cl	-1.19559	-2.12314	1.18723

^{4}10

SCF (BP86) Energy =-428.817717213
Enthalpy 0K = -428.593611
Enthalpy 298K = -428.572219
Free Energy 298K =-428.647609

Co	-0.00098	-0.62987	0.00045
Cl	0.05447	-1.86315	-1.91188
P	-1.97524	0.66461	-0.01686
P	1.96382	0.67836	0.00972
C	-3.51552	-0.33034	-0.33017
H	-4.40789	0.31780	-0.31915
H	-3.42672	-0.82614	-1.31002
H	-3.60664	-1.10211	0.45093
C	-2.06189	2.01358	-1.29573
H	-3.03084	2.53813	-1.24327
H	-1.24520	2.73215	-1.12161
H	-1.93654	1.56776	-2.29564
C	-2.34384	1.54306	1.58125
H	-1.52210	2.23875	1.81420
H	-3.29162	2.10262	1.50835
H	-2.41397	0.79525	2.38722
C	2.29908	1.61083	-1.56494
H	3.25551	2.15618	-1.49768
H	2.33820	0.89265	-2.39953
H	1.48042	2.32448	-1.74952
C	3.50784	-0.32916	0.25601
H	4.40175	0.31690	0.25119
H	3.43608	-0.86005	1.21876
H	3.58150	-1.07258	-0.55393
C	2.08130	1.98289	1.33242
H	1.97478	1.50225	2.31835
H	3.05122	2.50547	1.27831
H	1.26442	2.71041	1.20150
Cl	-0.02545	-1.83821	1.92856

^{2}11

SCF (BP86) Energy =-468.089382766
Enthalpy 0K = -467.838738
Enthalpy 298K = -467.816616
Free Energy 298K =-467.891257

Co	0.40651	0.70962	-0.27228
Cl	0.93650	1.41874	1.88594
P	-2.30789	-0.77317	0.06388
P	2.02384	-0.76903	-0.24998
C	-3.20976	0.78502	0.40958
H	-4.06919	0.55484	1.06038
H	-2.52985	1.49666	0.90056
H	-3.55849	1.21978	-0.53989
C	-1.77292	-1.46808	1.67539
H	-2.64603	-1.56805	2.34030
H	-1.31681	-2.45795	1.51502
H	-1.03180	-0.78200	2.11616
C	-3.55060	-1.94578	-0.64024
H	-3.06694	-2.91809	-0.82606
H	-4.38766	-2.07663	0.06515
H	-3.92762	-1.53699	-1.59154
C	2.00030	-2.13336	1.01845
H	2.91780	-2.74135	0.94626
H	1.92853	-1.67941	2.01892
H	1.12232	-2.77732	0.84981
C	3.68131	0.03498	0.03310
H	4.48521	-0.71963	-0.01017
H	3.84854	0.79743	-0.74473
H	3.67041	0.52609	1.01769
C	2.30865	-1.69037	-1.84733
H	2.43847	-0.95983	-2.66215
H	3.21201	-2.31860	-1.77034
H	1.44148	-2.32893	-2.07864
Cl	-0.63372	2.57537	-1.11164
C	-0.88673	-0.56857	-1.04636
H	-1.27360	-0.13916	-1.99183
H	-0.54033	-1.60065	-1.25050

^{4}11

SCF (BP86) Energy =-468.104680886
Enthalpy 0K = -467.855326
Enthalpy 298K = -467.833422
Free Energy 298K =-467.908743

Co	0.34531	-0.34024	0.01087
Cl	0.35134	-1.72156	-1.85471
P	-2.81655	0.54747	-0.02195
P	2.47150	0.68634	-0.02330
C	-3.17007	-0.39105	1.51507
H	-4.20124	-0.77787	1.48500
H	-2.44488	-1.21503	1.60526
H	-3.05267	0.28367	2.37870
C	-3.17646	-0.53874	-1.45612
H	-4.20630	-0.92296	-1.38239
H	-3.06484	0.04778	-2.38253
H	-2.44930	-1.36561	-1.46824
C	-4.06156	1.91424	-0.08728
H	-3.91501	2.48880	-1.01598
H	-5.08322	1.49970	-0.06596
H	-3.91331	2.57788	0.77968
C	2.85802	1.70761	-1.53355
H	3.87950	2.12089	-1.48195
H	2.76265	1.06926	-2.42669
H	2.13203	2.53325	-1.61016
C	3.89674	-0.51121	0.04930

H 4.86230 0.02184 0.02916
H 3.81687 -1.10260 0.97546
H 3.83082 -1.19483 -0.81212
C 2.83589 1.85735 1.38059
H 2.72348 1.31503 2.33319
H 3.85956 2.26140 1.30328
H 2.11151 2.68756 1.35871
Cl 0.33747 -1.57098 1.97510
C -1.10949 1.10443 -0.05168
H -0.97087 1.77551 0.81920
H -0.97293 1.69303 -0.98097

B3P86 Results

^{3}1.CH_2Cl_2
SCF (B3P86) Energy = -612.082034426
Enthalpy 0K = -611.708974
Enthalpy 298K = -611.675671
Free Energy 298K = -611.784366

Co 0.91817 -0.05383 -0.28215
Cl -0.91403 -0.24982 -1.71200
P 0.88462 1.85977 1.02612
P 1.13890 -1.79127 1.23427
P 2.95117 0.02883 -1.38597
C -0.39464 1.90692 2.37022
H -0.40313 2.87300 2.88475
H -1.37865 1.72273 1.93034
H -0.18856 1.11563 3.09641
C 0.46963 3.42014 0.11078
H 0.40636 4.27870 0.78658
H 1.23523 3.61177 -0.64572
H -0.48875 3.28688 -0.39843
C 2.39325 2.40088 1.96244
H 3.21125 2.57559 1.25801
H 2.20472 3.31957 2.52692
H 2.69705 1.60966 2.65270
C 2.26893 -1.63218 2.69816
H 2.26309 -2.54094 3.30833
H 3.28702 -1.43671 2.35148
H 1.94619 -0.78716 3.31282
C 1.69423 -3.42102 0.54129
H 2.70680 -3.32018 0.14067
H 1.68671 -4.20635 1.30367
H 1.02657 -3.70483 -0.27692
C -0.43860 -2.30035 2.06897
H -1.17324 -2.56598 1.30396
H -0.28425 -3.15383 2.73647
H -0.83278 -1.45832 2.64416
C 3.30191 1.58653 -2.33247
H 4.23203 1.50946 -2.90430
H 2.47125 1.78077 -3.01650
H 3.37828 2.42609 -1.63583
C 3.14963 -1.23464 -2.73067
H 4.10072 -1.11521 -3.25893
H 3.10079 -2.23697 -2.29683
H 2.32417 -1.12785 -3.43970
C 4.54826 -0.18797 -0.46587
H 4.55375 -1.16788 0.01952
H 5.40997 -0.11617 -1.13705
H 4.62886 0.57943 0.30837
C -5.14504 0.00929 -0.95126
H -4.07676 -0.17589 -0.82056
H -5.41660 0.23734 -1.98346
Cl -6.03044 -1.46788 -0.45995
Cl -5.59226 1.41745 0.06144

^{1}TS(1-2$^+$)
SCF (B3P86) Energy = -612.013198537
Enthalpy 0K = -611.637780
Enthalpy 298K = -611.607172
Free Energy 298K = -611.698064

Co -0.03250 -0.38298 -0.42007
Cl 0.15554 0.26184 -2.62337
P -0.13426 -1.55184 1.44764
P -2.27632 -0.14174 -0.82921
P 2.26113 -0.57443 -0.59284
C -1.72735 -2.06821 2.23745
H -1.50300 -2.69452 3.10613
H -2.29123 -1.19404 2.56540
H -2.32821 -2.64690 1.53286
C 0.71669 -0.92017 2.96949
H 0.72940 -1.69663 3.74018
H 1.73872 -0.60757 2.75908
H 0.15717 -0.05789 3.34181
C 0.59867 -3.24189 1.21518
H 1.63541 -3.19198 0.88052
H 0.55297 -3.80666 2.15127
H 0.01692 -3.76574 0.45160
C -3.67715 -0.28093 0.38339
H -4.59501 0.04853 -0.11263
H -3.81120 -1.31131 0.71230
H -3.49587 0.35539 1.25176
C -2.84916 -1.34979 -2.10952
H -2.76718 -2.36429 -1.70980
H -3.89054 -1.15297 -2.38136
H -2.21052 -1.26171 -2.98958
C -2.73670 1.48847 -1.58060
H -2.07131 1.70871 -2.41481
H -3.77393 1.45228 -1.92685
H -2.64273 2.27160 -0.82374
C 3.10577 0.91814 -1.28843
H 4.17377 0.71409 -1.40957
H 2.65823 1.17052 -2.24920
H 2.97502 1.76170 -0.60490
C 2.73811 -1.90397 -1.78657
H 3.81991 -1.89617 -1.94979
H 2.44011 -2.87958 -1.39393
H 2.21737 -1.72708 -2.72891
C 3.44644 -0.91658 0.79982
H 3.19619 -1.82612 1.34845
H 4.45355 -1.02438 0.38612
H 3.44874 -0.07190 1.49466
C 0.20358 1.90635 0.65721
H 1.02335 1.34312 1.07757
H -0.00085 2.00961 -0.40130
Cl -1.16576 2.08314 1.72371
Cl 1.26614 3.82643 0.79791

^{3}TS(1-2$^+$)

SCF (B3P86) Energy = -612.033158753
Enthalpy 0K = -611.660068
Enthalpy 298K = -611.628189
Free Energy 298K = -611.724631

Co	-0.14527	-0.00915	-0.25084
Cl	0.08500	-0.13220	-2.57595
P	0.31168	0.26488	2.03746
P	-1.50598	2.03045	-0.46822
P	-1.57398	-1.98328	-0.14205
C	1.06196	1.86220	2.60931
H	1.13910	1.87668	3.70050
H	2.05977	1.99472	2.18173
H	0.43705	2.69852	2.28581
C	1.36402	-0.98131	2.91524
H	1.37666	-0.77855	3.99024
H	0.95626	-1.98030	2.73998
H	2.38780	-0.95684	2.53409
C	-1.20559	0.21787	3.09927
H	-1.64780	-0.77851	3.06295
H	-0.94489	0.45408	4.13532
H	-1.94026	0.94011	2.74002
C	-2.47762	2.90251	0.85023
H	-2.91293	3.82578	0.45550
H	-3.28446	2.25373	1.20231
H	-1.83450	3.15279	1.69810
C	-2.75574	1.95737	-1.82856
H	-3.58590	1.31312	-1.52877
H	-3.13816	2.95753	-2.05351
H	-2.28034	1.53058	-2.71370
C	-0.39422	3.38640	-1.06199
H	0.14356	3.03400	-1.94576
H	-0.96859	4.28252	-1.31591
H	0.33493	3.63412	-0.28591
C	-0.73302	-3.45250	-0.88746
H	-1.44653	-4.26698	-1.04572
H	-0.28986	-3.15726	-1.84112
H	0.06358	-3.79284	-0.22093
C	-3.04082	-1.78941	-1.25181
H	-3.56487	-2.74261	-1.37193
H	-3.72624	-1.05421	-0.82197
H	-2.70073	-1.42856	-2.22489
C	-2.36414	-2.74877	1.35027
H	-3.06124	-2.04114	1.80636
H	-2.91229	-3.65198	1.06521
H	-1.59876	-3.01592	2.08391
C	2.44068	0.06478	-0.29341
H	2.08136	0.59990	-1.16341
H	2.64182	0.49246	0.67580
Cl	2.48250	-1.65606	-0.39697
Cl	4.62603	0.70924	-0.87801

^{3}TS(1-3)

SCF (B3P86) Energy = -612.047924180
Enthalpy 0K = -611.675898
Enthalpy 298K = -611.643688
Free Energy 298K = -611.742362

Co	0.45005	-0.05602	-0.30330
Cl	2.04344	-0.66156	-2.05973
P	1.49562	-0.73521	1.68059
P	1.27272	2.08299	-0.41956
P	-0.68232	-1.99517	-0.78038
C	1.87636	0.53733	2.97593
H	2.35935	0.07592	3.84277
H	2.54029	1.30431	2.56990
H	0.94552	1.01388	3.29572
C	3.15239	-1.51677	1.42972
H	3.59602	-1.82181	2.38227
H	3.04013	-2.38594	0.77739
H	3.80914	-0.80325	0.92644
C	0.64797	-1.99252	2.74914
H	0.49325	-2.91962	2.19210
H	1.24585	-2.21150	3.63922
H	-0.32627	-1.60353	3.05787
C	0.70279	3.36888	0.78116
H	1.11676	4.34708	0.51860
H	-0.38795	3.41354	0.75808
H	1.02188	3.10365	1.79150
C	0.85449	2.86448	-2.04011
H	-0.23206	2.92617	-2.13387
H	1.28923	3.86606	-2.11299
H	1.24526	2.23183	-2.84027
C	3.10881	2.28381	-0.36751
H	3.54449	1.61839	-1.11535
H	3.38793	3.32059	-0.57789
H	3.49118	2.00431	0.61756
C	0.31621	-3.54714	-0.87640
H	-0.29452	-4.37390	-1.25132
H	1.15862	-3.36836	-1.54742
H	0.70256	-3.80966	0.11167
C	-1.43174	-1.92409	-2.46722
H	-1.92554	-2.86907	-2.71332
H	-2.15924	-1.10983	-2.49708
H	-0.63865	-1.72080	-3.19027
C	-2.12224	-2.51165	0.25692
H	-2.83402	-1.68513	0.30968
H	-2.60952	-3.39020	-0.17641
H	-1.78618	-2.75059	1.26837
C	-3.74503	1.90112	0.31573
H	-3.44961	2.58662	1.10685
H	-4.05070	2.31265	-0.64390
Cl	-4.86449	0.67980	0.89271
Cl	-1.76101	0.99003	-0.24067

OPBE Results

^{3}1.CH_2Cl_2

SCF (OPBE) Energy = -609.630293193
Enthalpy 0K = -609.261143
Enthalpy 298K = -609.227964
Free Energy 298K = -609.334194

Co	-0.99396	-0.01871	-0.34155
Cl	0.41246	-0.12490	-2.20824
P	-0.48888	-1.54536	1.28577
P	-0.97485	2.01711	0.70039
P	-3.18064	-0.41234	-0.88826

C	1.06242	-1.22803	2.27342
H	1.30338	-2.07812	2.92464
H	1.89508	-1.05552	1.58130
H	0.93009	-0.33132	2.88886
C	-0.09243	-3.24337	0.61956
H	0.21126	-3.92917	1.42092
H	-0.96973	-3.65172	0.10629
H	0.72129	-3.15203	-0.10956
C	-1.67713	-1.98483	2.65432
H	-2.59898	-2.38407	2.21723
H	-1.24634	-2.73425	3.33076
H	-1.92553	-1.08307	3.22480
C	-1.70449	2.29155	2.39420
H	-1.60115	3.33796	2.70910
H	-2.76598	2.02072	2.38067
H	-1.19165	1.64738	3.11698
C	-1.75427	3.42854	-0.23897
H	-2.83490	3.26513	-0.31605
H	-1.57079	4.39051	0.25662
H	-1.33290	3.45572	-1.25100
C	0.73894	2.71352	0.94957
H	1.24561	2.75193	-0.02196
H	0.70453	3.72164	1.38235
H	1.31140	2.05469	1.61143
C	-3.60017	-2.16428	-1.37502
H	-4.62313	-2.23874	-1.76578
H	-2.89293	-2.49618	-2.14454
H	-3.50019	-2.82118	-0.50388
C	-3.73699	0.48423	-2.42771
H	-4.76293	0.20965	-2.70463
H	-3.68355	1.56575	-2.26290
H	-3.05647	0.22624	-3.24758
C	-4.59821	-0.02948	0.26161
H	-4.59611	1.04172	0.49189
H	-5.56213	-0.29806	-0.18955
H	-4.46920	-0.58542	1.19669
C	5.03819	0.04593	-1.05658
H	3.94160	0.02434	-1.10183
H	5.50600	0.16613	-2.04224
Cl	5.51898	1.43985	-0.04913
Cl	5.58983	-1.50963	-0.37510

^{1}TS(1-2^{+})

SCF (OPBE) Energy = -609.561891465
Enthalpy 0K = -609.191170
Enthalpy 298K = -609.160191
Free Energy 298K = -609.252136

Co	-0.07055	-0.41529	-0.35475
Cl	0.14842	-0.04452	-2.60015
P	-0.24717	-1.33130	1.61357
P	-2.28372	-0.11597	-0.83253
P	2.17450	-0.85560	-0.54311
C	-1.85631	-1.56759	2.52444
H	-1.64072	-2.06812	3.47667
H	-2.32914	-0.60406	2.73011
H	-2.53436	-2.20012	1.94434
C	0.71201	-0.64463	3.06154
H	0.74687	-1.38645	3.86912
H	1.72797	-0.35901	2.78840
H	0.18473	0.24599	3.42062
C	0.24987	-3.13126	1.57325
H	1.28755	-3.26523	1.26114
H	0.11490	-3.58011	2.56543
H	-0.39814	-3.64730	0.85473
C	-3.72347	0.02292	0.34898
H	-4.60953	0.30884	-0.23106
H	-3.92785	-0.92893	0.84307
H	-3.53041	0.79247	1.10187
C	-2.88996	-1.52775	-1.88102
H	-2.83461	-2.45477	-1.29820
H	-3.92915	-1.35467	-2.18771
H	-2.25075	-1.62124	-2.76329
C	-2.69386	1.37946	-1.86519
H	-1.99885	1.46367	-2.70254
H	-3.72205	1.28921	-2.23692
H	-2.61905	2.27357	-1.23659
C	3.18861	0.40811	-1.45705
H	4.20567	0.02076	-1.59528
H	2.73180	0.61985	-2.42571
H	3.23010	1.33066	-0.86942
C	2.45994	-2.38977	-1.55581
H	3.53540	-2.53680	-1.71523
H	2.04770	-3.26405	-1.04165
H	1.95397	-2.27175	-2.51817
C	3.37929	-1.14302	0.85566
H	3.05793	-1.93476	1.53700
H	4.34803	-1.42578	0.42511
H	3.51266	-0.21313	1.42012
C	0.35474	2.06512	0.48181
H	1.10290	1.44521	0.96575
H	0.13584	2.04970	-0.58435
Cl	-0.96639	2.53653	1.50761
Cl	1.67481	3.87286	0.36856

^{3}TS(1-2^{+})

SCF (OPBE) Energy = -609.569456116
Enthalpy 0K = -609.200875
Enthalpy 298K = -609.168592
Free Energy 298K = -609.266343

Co	-0.22219	0.00893	-0.20855
Cl	0.02910	-0.06899	-2.51050
P	0.22029	0.00533	2.04151
P	-1.17464	2.22217	-0.36798
P	-1.91661	-1.71430	-0.28785
C	1.28918	1.36321	2.74704
H	1.38940	1.22918	3.83125
H	2.28800	1.35746	2.29780
H	0.83002	2.33700	2.54986
C	1.02140	-1.50120	2.79121
H	1.06564	-1.39960	3.88268
H	0.43608	-2.39104	2.53484
H	2.03643	-1.62952	2.40296
C	-1.24707	0.16006	3.17768
H	-1.87614	-0.72824	3.09473
H	-0.89561	0.25014	4.21304
H	-1.84334	1.03922	2.92390
C	-1.95471	3.22468	0.99437
H	-2.25253	4.20905	0.61163

H	-2.84506	2.70353	1.36534
H	-1.25405	3.36587	1.82334
C	-2.46930	2.43197	-1.68268
H	-3.39860	1.95617	-1.35193
H	-2.65525	3.49820	-1.86321
H	-2.12844	1.94971	-2.60275
C	0.15444	3.38060	-0.95566
H	0.58682	2.97974	-1.87833
H	-0.25545	4.38080	-1.14440
H	0.94385	3.44885	-0.19825
C	-1.17089	-3.29104	-0.93165
H	-1.95202	-4.03878	-1.11747
H	-0.63470	-3.07484	-1.86080
H	-0.45893	-3.68270	-0.19650
C	-3.24709	-1.38610	-1.54059
H	-3.82490	-2.29958	-1.72903
H	-3.91786	-0.60884	-1.15853
H	-2.78471	-1.03677	-2.46768
C	-2.95283	-2.37702	1.11098
H	-3.57135	-1.57388	1.52706
H	-3.60811	-3.17651	0.74298
H	-2.31103	-2.78369	1.90009
C	2.47669	-0.31706	-0.29957
H	2.18879	0.34398	-1.11253
H	2.69817	-0.03716	0.72160
Cl	2.60930	-1.98375	-0.66038
Cl	4.75393	0.60242	-0.67398

^{3}TS(1-3)

SCF (OPBE) Energy = -609.582395032
Enthalpy 0K = -609.214746
Enthalpy 298K = -609.181400
Free Energy 298K = -609.281205

Co	-0.48873	0.03358	-0.28273
Cl	-2.04645	0.31091	-2.08128
P	-1.72199	0.30966	1.65328
P	-0.72663	-2.22149	-0.59591
P	0.14627	2.20212	-0.66727
C	-1.83192	-1.10195	2.86618
H	-2.41682	-0.80700	3.74658
H	-2.30915	-1.96937	2.40063
H	-0.82074	-1.38110	3.18419
C	-3.52202	0.70337	1.40842
H	-4.03473	0.81997	2.37138
H	-3.61121	1.62679	0.82695
H	-3.98841	-0.10510	0.83574
C	-1.22251	1.64726	2.85232
H	-1.30311	2.63098	2.38015
H	-1.86631	1.62737	3.74077
H	-0.18251	1.48413	3.15797
C	0.07789	-3.45575	0.53769
H	-0.04860	-4.46717	0.13157
H	1.14309	-3.22252	0.62023
H	-0.37471	-3.40957	1.53244
C	0.02564	-2.69533	-2.22630
H	1.09343	-2.45329	-2.20729
H	-0.10701	-3.76859	-2.41275
H	-0.45995	-2.11760	-3.01888
C	-2.43457	-2.93292	-0.75069
H	-2.99052	-2.34897	-1.48955
H	-2.37673	-3.98177	-1.06745
H	-2.95412	-2.87748	0.21146
C	-1.16093	3.50963	-0.84057
H	-0.71115	4.44564	-1.19460
H	-1.91149	3.16123	-1.55564
H	-1.64403	3.68764	0.12585
C	1.00364	2.30698	-2.31144
H	1.29336	3.34318	-2.52719
H	1.89595	1.67261	-2.28618
H	0.32384	1.94148	-3.08731
C	1.37817	3.06201	0.42726
H	2.27686	2.44397	0.50646
H	1.63767	4.03723	-0.00332
H	0.96006	3.21139	1.42696
C	3.91797	-0.75792	1.30613
H	3.76230	-0.03992	2.11457
H	3.82046	-1.82776	1.50435
Cl	5.30911	-0.38117	0.33199
Cl	1.81071	-0.41972	0.11399