Electronic Supplementary Information

Understanding the Reaction Mechanism of Gold-Catalyzed Reactions of 2,1-Benzisoxazoles with Propiolates and Ynamides

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CONTENT

Complete reference of Gaussian 09

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

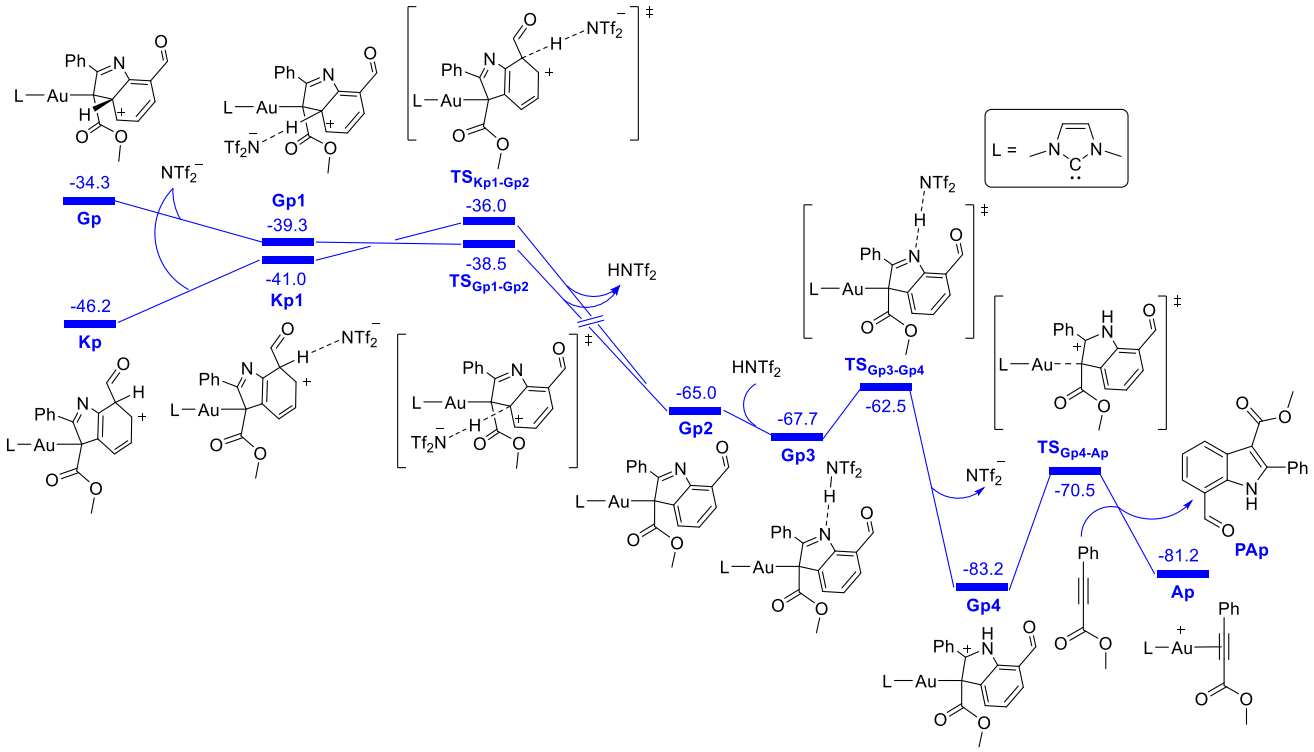

Figure S1. Energy profiles calculated for the 1,3-proton migrations from **Gp** and **Kp**. The relative free energies are given in kcal/mol.

One point is worth commenting on here. As mentioned, in the gold-catalyzed annulation of anthranil with the propiolate PhC≡CCO$_2$Me, we failed to locate an isomerization process between **Fp** and **Mp**. Instead, we were able to calculate the isomerization process between **Fp1** and **Np** (Figure S3). We see that the isomerization process gives slightly higher barrier than the direct C–C bond coupling process (Paths A and B shown in Figure 2).

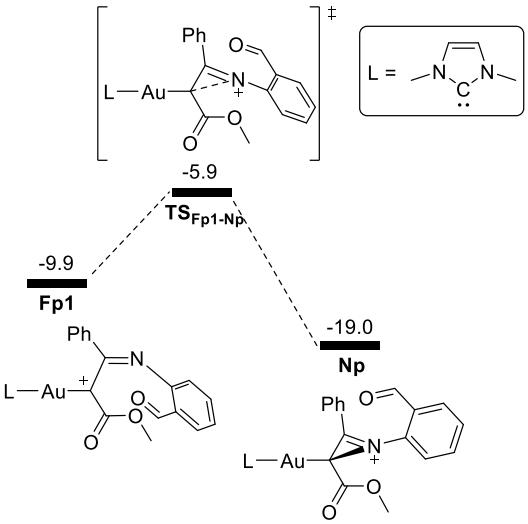

Figure S2. Energy profile for the isomerization process in gold-catalyzed annulation of anthranil with the propiolate PhC≡CCO_2Me. The relative free energies are given in kcal/mol.

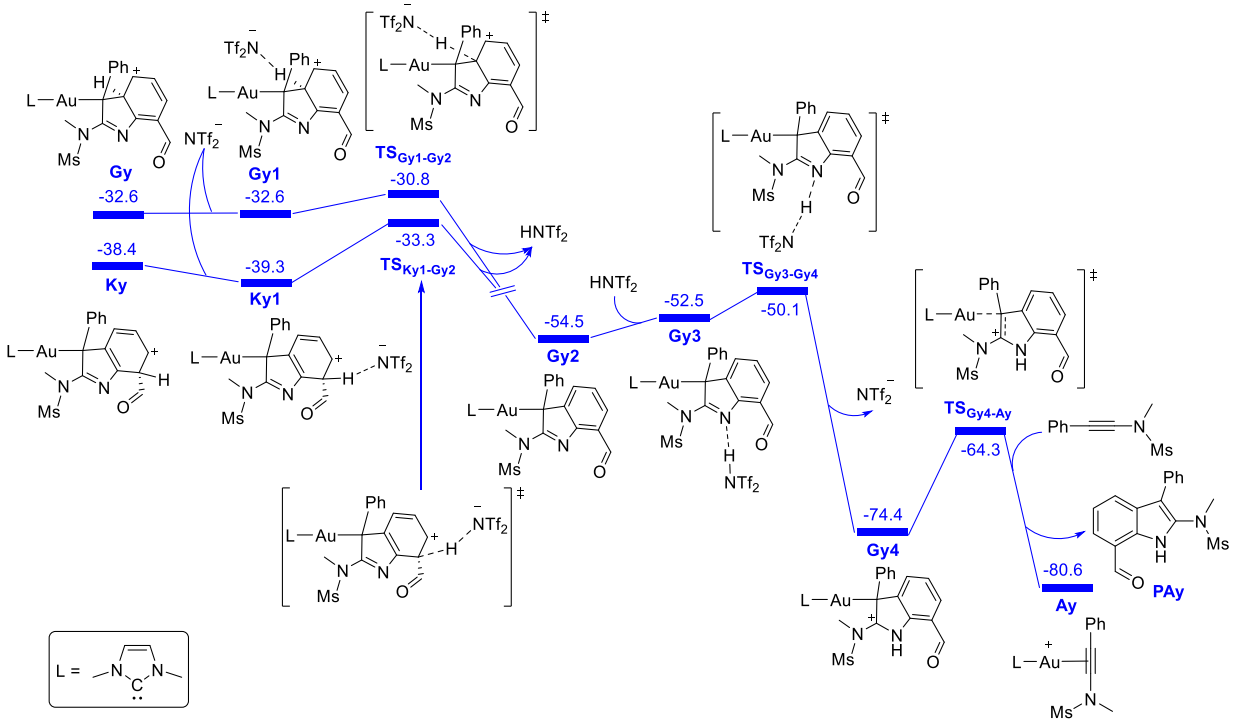

Figure S3. Energy profiles calculated for the 1,3-proton migrations from **Gy** and **Ky**. The relative free energies are given in kcal/mol.

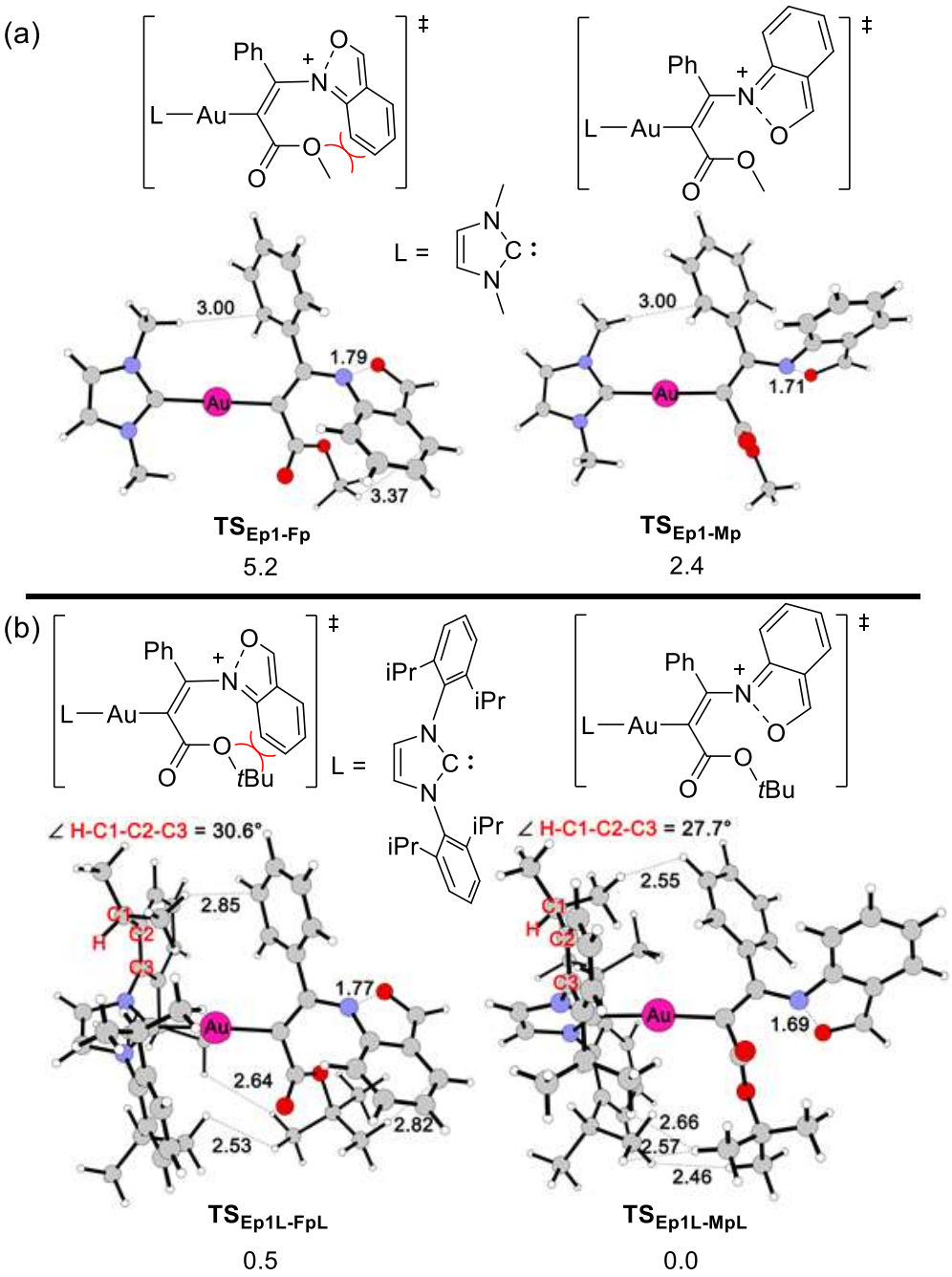

Figure S4. (a) The optimized geometries for the N–O bond cleavage transition states **TS$_{Ep1-Fp}$** and **TS$_{Ep1-Mp}$.** (b) The optimized geometries for the of N–O bond cleavage transition states **TS$_{Ep1L-FpL}$** and **TS$_{Ep1L-MpL}$** by employing the experimentally used ligand IPr and the real substrate PhC≡CCO$_2$*t*Bu. The relative free energies are given in kcal/mol. The distances are given in angstroms (Å).

Table S1. B3LYP-D3 electronic energies in gas phase, M06 electronic energies in dichloroethane, thermal correction to enthalpies, thermal correction to Gibbs free energies and B3LYP-D3 calculated imaginary frequencies.

Geometry	$E_{B3LYP-D3}$[1]	$E_{M06(dichloroethane)}$[2]	Correction of H[3]	Correction of G[4]	IF[5]
Ap	-976.442519	-976.409896	0.307692	0.226554	-
anthranil	-399.664692	-399.494410	0.112155	0.075194	-
TS_{Ap-Ep1}	-1376.129654	-1375.905286	0.421017	0.324197	-114.6
TS_{Ap-Ep2}	-1376.119982	-1375.895991	0.420819	0.324902	-172.6
Ep1	-1376.163974	-1375.937861	0.423464	0.330385	-
Ep2	-1376.162366	-1375.937664	0.423464	0.330797	-
TS_{Ep1-Fp}	-1376.151694	-1375.922525	0.420690	0.328209	-353.5
Fp	-1376.159433	-1375.941719	0.421358	0.324619	-
TS_{Fp-Gp}	-1376.160228	-1375.943823	0.420668	0.327414	-36.8
Gp	-1376.196238	-1375.986110	0.422385	0.328914	-
NTf_2^-	-1827.204122	-1827.212931	0.068847	0.009663	-
Gp1	-3203.559623	-3203.233546	0.491770	0.365108	-
$TS_{Gp1-Gp2}$	-3203.559506	-3203.231074	0.488866	0.363914	-282.3
$HNTf_2$	-1827.699832	-1827.639562	0.081470	0.020817	-
Gp2	-1375.848894	-1375.608741	0.410951	0.318097	-
Gp3	-3203.610405	-3203.281211	0.493142	0.367471	-
$TS_{Gp3-Gp4}$	-3203.599111	-3203.272193	0.489972	0.366756	-739.3
Gp4	-1376.268504	-1376.067014	0.424808	0.331801	-
TS_{Gp4-Ap}	-1376.254140	-1376.047169	0.423795	0.332332	-117.0
$PhC{\equiv}CCO_2Me$	-536.272273	-536.056779	0.165738	0.114830	-
PAp	-936.096068	-935.708470	0.282678	0.217933	-
Fp1	-1376.167323	-1375.943630	0.421597	0.325245	-
TS_{Fp1-Ip}	-1376.165148	-1375.943047	0.420593	0.329583	-62.1
TS_{Fp1-Np}	-1376.169303	-1375.939841	0.420699	0.327937	-30.0
Ip	-1376.193484	-1375.979608	0.422283	0.331289	-
TS_{Ip-Jp}	-1376.186107	-1375.975003	0.420179	0.329723	-114.0
Jp	-1376.193058	-1375.983431	0.422151	0.329423	-
TS_{Jp-Kp}	-1376.190508	-1375.981982	0.420516	0.329341	-113.3
Kp	-1376.212926	-1376.004752	0.422710	0.328513	-
Kp1	-3203.534792	-3203.233421	0.493166	0.362269	-

$TS_{Kp1-Gp2}$	-3203.533980	-3203.224906	0.489250	0.361675	-203.3
TS_{Fp-Lp}	-1376.161136	-1375.938101	0.420462	0.328024	-19.3
Lp	-1376.203623	-1375.983572	0.423331	0.333343	-
TS_{Lp-Ap}	-1376.175656	-1375.961998	0.421248	0.331796	-71.0
PQ'p	-936.038276	-935.650385	0.281512	0.218309	-
TS_{Ep1-Mp}	-1376.150583	-1375.925418	0.421011	0.326642	-412.2
Mp	-1376.165273	-1375.945061	0.421726	0.325527	-
TS_{Mp-Np}	-1376.172627	-1375.946191	0.420999	0.327832	-13.0
Np	-1376.179515	-1375.958352	0.422316	0.325476	-
TS_{Np-Op}	-1376.167420	-1375.949706	0.420989	0.328134	-244.1
Op	-1376.173966	-1375.961167	0.422677	0.330507	-
TS_{Op-Pp}	-1376.161285	-1375.945076	0.421467	0.331022	-356.9
Pp	-1376.171171	-1375.952380	0.422561	0.329491	-
TS_{Pp-Qp}	-1376.171138	-1375.952372	0.421595	0.331484	-14.9
Qp	-1376.204589	-1375.973619	0.423748	0.333612	-
TS_{Qp-Ap}	-1376.180561	-1375.970052	0.422057	0.333858	-19.1
PQp	-936.034325	-935.645623	0.281329	0.217471	-
$TS_{Ep1L-FpL}$	-2349.437489	-2348.612214	0.978569	0.829532	-384.4
$TS_{Ep1L-MpL}$	-2349.436150	-2348.614853	0.979241	0.831437	-426.3

[1]The electronic energy calculated by B3LYP-D3 in gas phase. [2]The electronic energies calculated by M06 in dichloroethane. [3]The thermal correction to enthalpy calculated by B3LYP-D3 in gas phase. [4]The thermal correction to Gibbs free energy calculated by B3LYP-D3 in gas phase. [5]The B3LYP-D3 calculated imaginary frequencies for the transition states in gas phase.

Table S2. B3LYP-D3 electronic energies in gas phase, M06 electronic energies in trifluoromethylbenzene, thermal correction to enthalpies, thermal correction to Gibbs free energies and B3LYP-D3 calculated imaginary frequencies.

Geometry	$E_{B3LYP-D3}$[1]	$E_{B3LYP-D3(trifluoromethylbenzene)}$[2]	Correction of H[3]	Correction of G[4]	IF[5]
Ay	-1431.137816	-1431.062971	0.350729	0.264301	-
anthranil	-399.664692	-399.492110	0.112155	0.075194	-
TS_{Ay-Ey1}	-1830.823251	-1830.555509	0.464193	0.364594	-229.0
TS_{Ay-Ey2}	-1830.805767	-1830.538697	0.463937	0.362541	-168.5
Ey1	-1830.850506	-1830.582200	0.466507	0.369244	-
Ey2	-1830.847020	-1830.577895	0.466516	0.369702	-
$TS_{Ey1-Fy1}$	-1830.844993	-1830.571279	0.464225	0.366903	-404.2
$TS_{Ey1-My1}$	-1830.840769	-1830.568904	0.464386	0.367859	-436.6
Fy1	-1830.883942	-1830.619450	0.465855	0.366562	-
My1	-1830.884555	-1830.617012	0.465808	0.365732	-
TS_{Fy1-Gy}	-1830.859381	-1830.601665	0.463881	0.367339	-337.4
Gy	-1830.886989	-1830.635779	0.465581	0.368170	-
NTf_2^-	-1827.204122	-1827.214416	0.068847	0.009663	-
Gy1	-3658.243208	-3657.877893	0.535569	0.405563	-
$TS_{Gy1-Gy2}$	-3658.242540	-3657.872826	0.532045	0.403479	-543.3
$HNTf_2$	-1827.699832	-1827.642151	0.081470	0.020817	-
Gy2	-1830.529669	-1830.243463	0.454107	0.357549	-
Gy3	-3658.266089	-3657.909305	0.536862	0.405308	-
$TS_{Gy3-Gy4}$	-3658.274019	-3657.905985	0.533162	0.405845	-630.4
Gy4	-1830.942381	-1830.701042	0.467557	0.366924	-
TS_{Gy4-Ay}	-1830.934794	-1830.688524	0.466491	0.370539	-72.3
PhC≡CNMeMs	-990.945485	-990.701103	0.208962	0.150363	-
PAy	-1390.777448	-1390.350938	0.325909	0.254820	-
Fy2	-1830.881354	-1830.616154	0.465776	0.367053	-
TS_{Fy2-Iy}	-1830.862224	-1830.603002	0.463935	0.368390	-292.9
Iy	-1830.880473	-1830.626625	0.465494	0.370424	-
TS_{Iy-Jy}	-1830.872154	-1830.616339	0.463559	0.368787	-107.2
Jy	-1830.865778	-1830.622927	0.465555	0.366603	-
TS_{Jy-Ky}	-1830.870780	-1830.618415	0.463883	0.367982	-66.4

Ky	-1830.895003	-1830.643525	0.466106	0.366700	-
Ky1	-3658.233300	-3657.883485	0.536862	0.400450	-
$TS_{Ky1-Gy2}$	-3658.228417	-3657.871145	0.531710	0.397712	-824.4
TS_{Fy1-Ly}	-1830.852058	-1830.593215	0.464213	0.367492	-89.8
Ly	-1830.873919	-1830.618517	0.466310	0.369428	-
TS_{Ly-Ly1}	-1830.865055	-1830.601306	0.464626	0.372212	-62.0
Ly1	-1830.900325	-1830.631268	0.467190	0.373007	-
TS_{Ly1-Ay}	-1830.880354	-1830.624471	0.465340	0.371372	-36.3
PQ'y	-1390.724051	-1390.298196	0.324865	0.256118	-
TS_{My1-Oy}	-1830.857471	-1830.598972	0.464041	0.366862	-262.6
Oy	-1830.859216	-1830.605842	0.465624	0.369518	-
TS_{Oy-Qy}	-1830.839454	-1830.581144	0.464710	0.371737	-373.8
Qy	-1830.895596	-1830.630745	0.466903	0.371928	-
TS_{Qy-Ay}	-1830.865245	-1830.611328	0.465151	0.372343	-51.9
PQy	-1390.719283	-1390.291061	0.324915	0.256383	-
$TS_{My1-Fy3}$	-1830.878837	-1830.609140	0.464345	0.366123	-76.9
Fy3	-1830.890677	-1830.621956	0.465811	0.368024	-

[1]The electronic energy calculated by B3LYP-D3 in gas phase. [2]The electronic energies calculated by M06 in trifluoromethylbenzene. [3]The thermal correction to enthalpy calculated by B3LYP-D3 in gas phase. [4]The thermal correction to Gibbs free energy calculated by B3LYP-D3 in gas phase. [5]The B3LYP-D3 calculated imaginary frequencies for the transition states in gas phase.

Table S3. Comparison of the relative free energies calculated for the gold-catalyzed reaction of anthranil with the propiolate (PhC≡CCO$_2$Me) using M06 and B3LYP-D3 methods.

Geometry	M06	B3D3
Ap	0.0	0.0
TS$_{Ap-Ep1}$	13.5	12.4
TS$_{Ap-Ep2}$	19.7	19.7
Ep1	-3.1	-4.6
Ep2	-2.7	-3.5
TS$_{Ep1-Fp}$	5.2	0.9
Fp	-9.1	-11.9
TS$_{Fp-Gp}$	-8.7	-11.0
Gp	-34.3	-31.1
Gp1	-39.3	-41.4
TS$_{Gp1-Gp2}$	-38.5	-41.3
Gp2	-65.0	-61.4
Gp3	-67.7	-68.9
TS$_{Gp3-Gp4}$	-62.5	-63.6
Gp4	-83.2	-81.0
TS$_{Gp4-Ap}$	-70.5	-68.0
Fp1	-9.9	-12.5
TS$_{Fp1-Ip}$	-6.8	-8.8
TS$_{Fp1-Np}$	-5.9	-8.6
Ip	-28.7	-25.7
TS$_{Ip-Jp}$	-26.8	-24.8
Jp	-32.3	-28.8
TS$_{Jp-Kp}$	-31.4	-28.4
Kp	-46.2	-42.7
Kp1	-41.0	-39.4
TS$_{Kp1-Gp2}$	-36.0	-35.7
TS$_{Fp-Lp}$	-4.7	-7.2
Lp	-29.9	-28.7
TS$_{Lp-Ap}$	-17.3	-13.7

TS_{Ep1-Mp}	2.4	-1.9
Mp	-10.7	-13.8
TS_{Mp-Np}	-9.9	-12.1
Np	-19.0	-17.4
TS_{Np-Op}	-11.9	-10.1
Op	-17.6	-12.8
TS_{Op-Pp}	-7.2	-4.8
Pp	-12.8	-11.8
TS_{Pp-Qp}	-11.5	-10.6
Qp	-23.5	-24.7
TS_{Qp-Ap}	-21.1	-15.1
$TS_{Ep1L-FpL}$	0.0	0.0
$TS_{Ep1L-MpL}$	-0.5	-0.3

Table S4. Comparison of the relative free energies calculated for the gold-catalyzed reaction of anthranil with the ynamide (PhC≡CNMeMs) using M06 and B3LYP-D3 methods.

Geometry	M06	B3D3
Ay	0.0	0.0
TS_{Ay-Ey1}	15.5	14.6
TS_{Ay-Ey2}	24.7	23.2
Ey1	1.7	0.4
Ey2	4.6	2.0
$TS_{Ey1-Fy1}$	7.0	3.1
$TS_{Ey1-My1}$	9.1	5.2
Fy1	-23.4	-25.8
My1	-22.4	-24.4
TS_{Fy1-Gy}	-11.8	-10.8
Gy	-32.6	-28.7
Gy1	-32.6	-33.8
$TS_{Gy1-Gy2}$	-30.8	-33.1
Gy2	-54.5	-50.0
Gy3	-52.5	-50.5
$TS_{Gy3-Gy4}$	-50.1	-51.3
Gy4	-74.4	-70.5
TS_{Gy4-Ay}	-64.3	-62.5
Fy2	-21.0	-22.7
TS_{Fy2-Iy}	-11.9	-10.4
Iy	-25.5	-21.2
TS_{Iy-Jy}	-20.1	-16.6
Jy	-25.6	-20.8
TS_{Jy-Ky}	-21.9	-17.4
Ky	-38.4	-34.9
Ky1	-39.3	-37.6
$TS_{Ky1-Gy2}$	-33.3	-31.9
TS_{Fy2-Ly}	-6.4	-7.1
Ly	-21.0	-19.1

TS_{Ly-Ly1}	-8.5	-7.8
Ly1	-26.8	-28.0
TS_{Ly1-Ay}	-23.5	-17.4
TS_{My1-Oy}	-10.4	-6.9
Oy	-13.0	-7.6
TS_{Oy-Qy}	3.9	7.4
Qy	-27.1	-27.3
TS_{Qy-Ay}	-14.7	-9.5
$TS_{My1-Fy3}$	-17.2	-18.9
Fy3	-24.1	-26.1

B3LYP-D3 geometries for all the optimized compounds and transition states

Ap $E_{M06(dichloroethane)}$ = -976.409896

C	-3.98080500	4.55235000	5.95531800
C	-3.69770500	4.43198200	7.16639000
C	-3.10327200	5.16160800	8.31689100
O	-3.20862600	6.35402900	8.46347200
O	-2.46640800	4.31605000	9.13603700
C	-1.83307000	4.93587800	10.28307500
C	-4.89540200	0.45578200	7.70977100
C	-4.81637900	-1.74627500	8.17368900
C	-6.12380800	-1.37650300	8.16133600
H	-4.35260800	-2.70242700	8.36088300
H	-7.02299100	-1.94981200	8.32581000
C	-2.61361400	-0.59252500	7.85667300
C	-7.38895300	0.74945500	7.72739300
N	-6.15411700	-0.02216400	7.88117800
N	-4.07685600	-0.61073200	7.89447100
Au	-4.35412500	2.37492600	7.29539800
H	-7.18621400	1.79950700	7.93911200
H	-7.77260300	0.64778500	6.70858000
H	-8.13000300	0.37800500	8.43780000
H	-2.21488800	-0.76473200	8.85978300
H	-2.25842500	-1.37334300	7.18000100
H	-2.27745100	0.37926600	7.49576900
H	-1.37064100	4.11653700	10.83135200
H	-1.08247300	5.65741300	9.95220200
H	-2.58281000	5.44368200	10.89441000
C	-4.32765400	4.67254900	4.59593500
C	-3.48698600	4.13094700	3.59539200
C	-5.50507300	5.37043600	4.23757300
C	-3.82567700	4.28940600	2.25828700
H	-2.58597600	3.59940200	3.88440100
C	-5.82683400	5.52330300	2.89489900
H	-6.13755500	5.78660500	5.01503600
C	-4.99137100	4.98358500	1.90924000
H	-3.18469800	3.87851800	1.48481500
H	-6.72482900	6.06312700	2.61196000
H	-5.24868300	5.10680600	0.86133000

anthranil $E_{M06(dichloroethane)}$ = -399.494410

C	-3.43000300	0.39383400	0.00005400
C	-1.98788800	0.43195800	-0.00002700
C	-1.29555800	1.67785300	0.00004400
C	-2.04488900	2.82410600	0.00017800
C	-3.48304600	2.78528300	0.00025300
C	-4.18240400	1.60824200	0.00019800
C	-1.64756700	-0.90010100	-0.00020500
H	-0.21021600	1.71071200	-0.00002800
H	-1.55212700	3.79204400	0.00022200
H	-4.02357300	3.72794100	0.00036700
H	-5.26673600	1.57716100	0.00027200
H	-0.71026300	-1.43808900	-0.00034100
N	-3.89916100	-0.84981100	0.00003500
O	-2.75633300	-1.64997700	-0.00013500

TS_{Ap-Ep1} $E_{M06(dichloroethane)}$ = -1375.905286

C	-3.45753800	3.71435800	5.65624100
C	-3.01862200	3.19499400	6.73454400
C	-1.80204500	3.53753600	7.51969900
O	-1.61285300	4.61055900	8.04725400
O	-0.97540000	2.48609500	7.59587000
C	0.25298000	2.72345700	8.32173900
C	-2.36192300	6.52804700	5.24486600
C	-2.45860700	7.21456000	3.98656600
C	-2.89597900	8.56749200	3.92686500
C	-3.23610100	9.17273300	5.10935600
C	-3.14822600	8.47677900	6.36148800
C	-2.71981600	7.17461300	6.45841600
C	-2.06283100	6.25880200	3.07332500
H	-2.95409500	9.09291100	2.97927200
H	-3.57508400	10.20392600	5.11070600
H	-3.42641800	9.01025500	7.26589800
H	-2.63424800	6.64387100	7.39925400
H	-1.93847900	6.25608000	1.99924000
N	-1.93309900	5.26626400	5.07959000
O	-1.75800600	5.12249700	3.69846200
C	-5.29890000	0.04207300	8.16809900
C	-5.84154600	-1.85951200	9.25336200
C	-6.97621000	-1.37482700	8.68615300
H	-5.67062400	-2.73712200	9.85735400
H	-7.98702600	-1.75224600	8.68929600
C	-3.44478100	-1.12772100	9.39147000
C	-7.56520500	0.59277800	7.24377000
N	-6.62598100	-0.20783400	8.02785200
N	-4.82342100	-0.98096000	8.92361000
Au	-4.22579000	1.61474700	7.41963200
H	-7.13249900	1.57759400	7.06717600
H	-7.76620500	0.10608000	6.28521500
H	-8.49762400	0.70361100	7.80205600
H	-3.37366400	-0.84257800	10.44481100
H	-3.13252300	-2.16749400	9.27020000
H	-2.79471000	-0.48544700	8.79679500
H	0.80253600	1.78427500	8.27094300
H	0.81922100	3.53032200	7.85053800
H	0.03209800	2.99306400	9.35777600
C	-4.34137500	3.93017900	4.56546600
C	-4.24530100	3.13240800	3.40541900
C	-5.30436700	4.96064600	4.63555000
C	-5.12401100	3.34399100	2.34831500
H	-3.48651200	2.35834800	3.35638200
C	-6.17449300	5.16501300	3.57020300
H	-5.35160900	5.58413200	5.52262200
C	-6.08733300	4.35638600	2.43087700
H	-5.05942000	2.72482500	1.45885500
H	-6.91998300	5.95240700	3.62392100
H	-6.77050900	4.51835500	1.60204000

TS_{Ap-Ep2} $E_{M06(dichloroethane)}$ = -1375.895991

C	-2.92403500	4.92651100	5.27705300
C	-3.33386100	4.73687300	6.45697800
C	-4.25559500	4.81463900	7.59278600
O	-5.46393200	4.82440700	7.43892900
O	-3.63080700	4.91386200	8.76281900
C	-4.49519200	4.96945800	9.92392500
C	-0.62939800	3.54236500	8.10578700
C	0.41517400	2.67484700	7.62522500
C	1.71989900	2.72528600	8.19501900
C	1.93990300	3.63219200	9.19798000
C	0.89717100	4.50304500	9.66576100
C	-0.37304000	4.47797800	9.14852800
C	-0.20190500	1.96178700	6.62154800
H	2.50576500	2.06561100	7.84163600
H	2.92041500	3.70324700	9.65804300
H	1.13256000	5.20461400	10.46094600
H	-1.16079500	5.13481500	9.49715400
H	0.12130500	1.18430100	5.94409500
N	-1.76801800	3.33482300	7.44157800
O	-1.47416300	2.34887700	6.50209600

C	-6.48014200	6.41994000	3.59252000
C	-7.91598900	7.45220500	2.19871900
C	-8.64917500	6.84369400	3.16725900
H	-8.21651100	8.05029900	1.35247100
H	-9.71559300	6.79958700	3.32537500
C	-5.47123300	7.70113900	1.68442100
C	-8.15581300	5.40054500	5.16540500
N	-7.75323400	6.21701300	4.01571600
N	-6.58671500	7.17963200	2.47377700
Au	-4.79570000	5.71149000	4.48350000
H	-7.31346900	5.28336100	5.84765100
H	-8.97482000	5.90266000	5.68502400
H	-8.48738800	4.41650200	4.82271600
H	-5.67327500	7.53998800	0.62294300
H	-5.34276700	8.76982900	1.87675600
H	-4.56009000	7.17132400	1.96289900
H	-5.13477200	5.85367600	9.87439300
H	-5.11316000	4.07003000	9.97237400
H	-3.81979600	5.02289300	10.77641000
C	-1.74425900	4.79154300	4.44264200
C	-0.47734800	5.04378100	5.00198400
C	-1.84512000	4.40336900	3.09532600
C	0.66753700	4.88616600	4.22630100
H	-0.40324800	5.36148500	6.03563000
C	-0.69287400	4.23503300	2.33080200
H	-2.82367600	4.21163900	2.66500000
C	0.56370800	4.47699300	2.89298600
H	1.64203800	5.08256400	4.66346500
H	-0.77498100	3.91821500	1.29544900
H	1.45975000	4.35326400	2.29188800

Ep1 $E_{M06(dichloroethane)}$ = -1375.937861

C	-3.37505900	4.23733700	5.27977700
C	-2.95322500	3.52078000	6.34563800
C	-1.70667600	3.92525500	7.05722200
O	-1.47305700	5.03168500	7.51336300
O	-0.86231400	2.88402300	7.17691400
C	0.36855700	3.16145400	7.87479000
C	-2.63971900	6.69312800	5.36908300
C	-1.98193800	7.52448800	4.40458000
C	-1.81225100	8.91721700	4.65075900
C	-2.31969000	9.41286200	5.82272800
C	-2.98930400	8.56590700	6.76765400
C	-3.16021800	7.21540700	6.57244500
C	-1.67398300	6.67157500	3.36509800
H	-1.30393100	9.54877400	3.93047900
H	-2.21695500	10.46802700	6.05334600
H	-3.36796700	9.01441600	7.68103500
H	-3.62738900	6.56523600	7.29924000
H	-1.18198300	6.80466000	2.41106600
N	-2.66774400	5.43491300	4.89604000
O	-2.07999300	5.43176900	3.62535800
C	-5.04343200	0.32096200	7.88113300
C	-5.67745500	-1.48888800	9.07680200
C	-6.70905800	-1.15958800	8.25708200
H	-5.57042900	-2.28676400	9.79530800
H	-7.68034900	-1.61077500	8.12582700
C	-3.37824100	-0.58887300	9.52015500
C	-7.15160200	0.64636900	6.56608000
N	-6.30230800	-0.05387000	7.52947600
N	-4.66756400	-0.57333400	8.83208000
Au	-3.97826100	1.91085300	7.11791500
H	-6.52612300	1.17036900	5.84232200
H	-7.77379300	-0.08370600	6.04350400
H	-7.79087100	1.36941400	7.08066400
H	-3.52447200	-0.40308700	10.58780900
H	-2.89705800	-1.56048800	9.37986800
H	-2.74485000	0.19210500	9.09935100
H	0.92710100	2.22597800	7.85968400
H	0.92758000	3.95294200	7.36845900
H	0.15980600	3.47403700	8.90155500
C	-4.54169900	3.95346500	4.40586900
C	-4.76825600	2.65668400	3.91651500
C	-5.43477600	4.97861100	4.05316800
C	-5.88545200	2.38506000	3.12580400
H	-4.05375800	1.87203200	4.14439300
C	-6.55077300	4.70486700	3.26396400
H	-5.27157800	5.99002200	4.41755300
C	-6.78206100	3.40627400	2.80185100
H	-6.04299000	1.37957200	2.74559700
H	-7.24218100	5.50386800	3.01236400
H	-7.64840500	3.19588400	2.18153100

Ep2 $E_{M06(dichloroethane)}$ = -1375.937664

C	-2.92985600	4.71945400	5.65742300
C	-3.04041600	4.01550300	6.81908700
C	-4.20984700	3.81840900	7.71952000
O	-4.11982600	3.23941200	8.78883000
O	-5.34945500	4.36471600	7.26877900
C	-6.47626200	4.24703300	8.16196300
C	-1.15644000	3.36776300	8.43470200
C	-0.11839400	2.38534600	8.34144300
C	0.84545500	2.25710400	9.38146700
C	0.73381600	3.10727900	10.45052000
C	-0.31293300	4.08505400	10.52427500
C	-1.26378300	4.23688900	9.54199300
C	-0.34012500	1.76560200	7.12841400
H	1.63091300	1.51184900	9.31974300
H	1.44453100	3.04540500	11.26786600
H	-0.35684300	4.72574300	11.39981100
H	-2.07114800	4.95417700	9.61039600
H	0.16314000	0.97643100	6.58722800
N	-1.90145100	3.30073200	7.32331100
O	-1.40604300	2.27801700	6.52053200
C	-5.99255900	6.60350300	3.64600500
C	-8.03587700	7.18492500	2.87137100
C	-7.12611500	7.99808800	2.27509300
H	-9.10894300	7.12962000	2.77222400
H	-7.25144800	8.79645900	1.56009300
C	-7.94398100	5.28749700	4.50965400
C	-4.63605200	8.29234700	2.38416900
N	-5.88270400	7.62586700	2.75742200
N	-7.32504700	6.33957000	3.70669900
Au	-4.48005900	5.65672300	4.68415000
H	-3.79621100	7.66620900	2.68557100
H	-4.61214200	8.43446000	1.30101900
H	-4.56336600	9.26286900	2.88315700
H	-8.72185400	5.72021900	5.14491000
H	-8.38673200	4.53026400	3.85643700
H	-7.17879700	4.82404500	5.13265100
H	-6.73849300	3.19618700	8.30781200
H	-6.24424000	4.69708300	9.13016900
H	-7.28760800	4.78529600	7.67229000
C	-1.59337100	4.84142400	5.02278200
C	-0.49835800	5.37082000	5.73094200
C	-1.40466700	4.45211900	3.68513400
C	0.74917800	5.49764200	5.12027000
H	-0.63620700	5.71281500	6.75321400
C	-0.14843300	4.54896600	3.08843700
H	-2.24893300	4.06191900	3.12365600

C	0.93234400	5.07556000	3.80125700
H	1.57791800	5.92919600	5.67492800
H	-0.01626900	4.22585500	2.05966200
H	1.90540700	5.16910200	3.32798400

TS_{Ep1-Fp} $E_{M06(dichloroethane)}$ = -1375.922525

C	-4.09567500	5.81532600	-5.98815300
C	-4.46033200	5.00891100	-7.05763800
C	-4.10221400	5.39497600	-8.45295000
O	-3.51051800	4.65964500	-9.21833200
O	-4.53775500	6.63009000	-8.77205200
C	-4.26522400	7.04747400	-10.12814700
C	-2.16363000	6.99849900	-7.03626600
C	-2.03024100	8.34939300	-7.46126000
C	-0.97580700	8.75274200	-8.30804000
C	-0.07462300	7.79670400	-8.72999800
C	-0.21185400	6.45145300	-8.30545400
C	-1.23302900	6.03359000	-7.46728200
C	-3.07089200	9.09258400	-6.86606600
H	-0.89206600	9.78904200	-8.62042800
H	0.74137200	8.06742600	-9.39122300
H	0.50570300	5.71491600	-8.65459500
H	-1.33428100	5.00060800	-7.15702400
H	-3.19775100	10.17652900	-6.93036600
N	-3.16026900	6.80382200	-6.12785100
O	-3.89009500	8.44085900	-6.15446400
C	-6.06641300	1.26355000	-6.61955000
C	-6.76624000	-0.84442600	-7.02220000
C	-6.97474400	-0.58911100	-5.70366500
H	-6.96524500	-1.72533500	-7.61279100
H	-7.38413600	-1.20679600	-4.91930100
C	-5.86398100	0.44001000	-8.98048900
C	-6.55964300	1.34327100	-4.15857800
N	-6.54240100	0.70523300	-5.47518800
N	-6.20797100	0.29871500	-7.56559600
Au	-5.28911900	3.15706200	-6.85240100
H	-6.34974200	2.40745600	-4.26835500
H	-5.80063800	0.89073400	-3.51432100
H	-7.54660400	1.21455800	-3.70715200
H	-5.28962900	-0.43199500	-9.30242600
H	-5.25972500	1.33787400	-9.11185200
H	-6.77435300	0.52222800	-9.58078500
H	-4.76292200	8.01015400	-10.24119200
H	-4.66218600	6.31861700	-10.83847500
H	-3.18626200	7.14559300	-10.27762600
C	-4.61759300	5.64578800	-4.60805400
C	-3.76467500	5.76847600	-3.50083300
C	-5.97995600	5.37791000	-4.39539700
C	-4.25659000	5.59105800	-2.20868900
H	-2.71372800	5.99317300	-3.65717900
C	-6.47174900	5.20732200	-3.10124100
H	-6.65448000	5.32720800	-5.24508900
C	-5.60974600	5.30580700	-2.00575000
H	-3.58466000	5.67589100	-1.35968800
H	-7.53038500	5.01747900	-2.94784200
H	-5.99283100	5.17587500	-0.99769600

Fp $E_{M06(dichloroethane)}$ = -1375.941719

C	-4.09090800	5.40109200	-5.90370900
C	-4.33662700	4.53800200	-7.04635300
C	-4.23268800	5.10220800	-8.41453500
O	-4.92032900	6.06613100	-8.69675300
O	-3.48317100	4.39730800	-9.26029600
C	-3.39966900	4.92958100	-10.60520400
C	-2.24859900	6.50085800	-6.88221800
C	-2.03739100	7.77798200	-7.47420300
C	-0.99935700	7.95627700	-8.38607900
C	-0.15114000	6.89383700	-8.72101200
C	-0.35141600	5.64131300	-8.13761600
C	-1.39026900	5.43768700	-7.22865600
C	-2.99668800	8.85276100	-7.16826300
H	-0.86783100	8.92768600	-8.85600900
H	0.65330400	7.04349900	-9.43380700
H	0.30570200	4.81353100	-8.38668200
H	-1.51345600	4.48267300	-6.72684500
H	-2.74285100	9.85618000	-7.56550300
N	-3.20188200	6.36427100	-5.89820300
O	-4.00842900	8.67548600	-6.51487900
C	-5.65310900	0.74347100	-6.39909600
C	-6.29482400	-1.41195600	-6.54491100
C	-6.33681000	-1.05817500	-5.23059500
H	-6.53110800	-2.34418100	-7.03430100
H	-6.60932300	-1.62729600	-4.35530200
C	-5.72156200	-0.25841200	-8.69752500
C	-5.80482700	1.02580900	-3.91559300
N	-5.94434100	0.26337100	-5.16064500
N	-5.87263000	-0.29724100	-7.24288000
Au	-5.02206200	2.66266000	-6.79979000
H	-6.19705400	2.03519100	-4.05113800
H	-4.75233600	1.08252400	-3.62695900
H	-6.37177000	0.52178400	-3.13132300
H	-5.06837600	-1.07347500	-9.01864300
H	-5.27636000	0.69544600	-8.98036500
H	-6.69931500	-0.36001000	-9.17589100
H	-2.74737100	4.24406600	-11.14397400
H	-2.97012400	5.93424000	-10.58002500
H	-4.39236100	4.96592500	-11.05939800
C	-4.85913100	5.17406800	-4.64994100
C	-4.20706200	5.22588500	-3.40953000
C	-6.24138200	4.92508400	-4.69440300
C	-4.91955500	4.99486600	-2.23349800
H	-3.14421400	5.44441400	-3.37606900
C	-6.95466600	4.71069200	-3.51469300
H	-6.76194300	4.93419400	-5.64810900
C	-6.29217100	4.73392800	-2.28374400
H	-4.40617300	5.02796000	-1.27711500
H	-8.02696500	4.54272400	-3.55589200
H	-6.84684800	4.56638000	-1.36498400

TS_{Fp-Gp} $E_{M06(dichloroethane)}$ = -1375.943823

C	-3.97097000	5.43493400	-5.93243000
C	-4.25989500	4.60220400	-7.14426800
C	-4.73312100	5.33605700	-8.34267000
O	-5.81482900	5.88250900	-8.20737900
O	-4.01743300	5.27044000	-9.45482400
C	-4.58703600	5.95612500	-10.60038200
C	-2.12313700	6.00918300	-7.03056700
C	-1.61608800	7.08457200	-7.80954400
C	-0.89224700	6.78728000	-8.96049100
C	-0.64776000	5.46148500	-9.36948300
C	-1.10285800	4.40912900	-8.59313300
C	-1.82549700	4.67192700	-7.41417100
C	-1.93293500	8.50514800	-7.49739700
H	-0.52892300	7.60865100	-9.57449500
H	-0.08064400	5.27375300	-10.27563100
H	-0.88395400	3.38212500	-8.86847000
H	-1.96879100	3.87824200	-6.68884400
H	-1.33415600	9.23853200	-8.08024300
N	-2.93440600	6.21437400	-5.93122500
O	-2.77136200	8.86630000	-6.70115300

C	-5.47690500	0.75973600	-6.48258600
C	-6.16980300	-1.38277900	-6.57731900
C	-6.22314700	-0.99127200	-5.27557300
H	-6.41795800	-2.32320900	-7.04451500
H	-6.52427100	-1.52751100	-4.38903300
C	-5.52692900	-0.30690200	-8.75121000
C	-5.67986100	1.12862900	-4.01654900
N	-5.79793900	0.32308800	-5.23648500
N	-5.71147100	-0.29646300	-7.30056400
Au	-4.82516100	2.66574300	-6.91003100
H	-6.14877000	2.10351800	-4.16515400
H	-4.62677500	1.26930200	-3.76155200
H	-6.18414700	0.60593200	-3.20251800
H	-4.80078200	-1.07645200	-9.02568700
H	-5.15829200	0.66934600	-9.06609500
H	-6.48146100	-0.51034400	-9.24337900
H	-3.87072900	5.80109400	-11.40573100
H	-4.70168800	7.01949800	-10.37798700
H	-5.55940000	5.52618500	-10.85061400
C	-4.84070700	5.29698500	-4.75065600
C	-4.29039700	5.43067800	-3.46442100
C	-6.21441700	5.02909200	-4.89897900
C	-5.09815900	5.26468300	-2.34248100
H	-3.23503900	5.66147800	-3.36113400
C	-7.01885600	4.87371600	-3.77050500
H	-6.65046500	4.98993400	-5.89251100
C	-6.46015300	4.98019900	-2.49323900
H	-4.66933900	5.36381800	-1.34980100
H	-8.08249800	4.68845500	-3.88813100
H	-7.08789900	4.85904900	-1.61504500

Gp $E_{M06(dichloroethane)}$ = -1375.986110

C	-0.63312800	2.53027100	-7.42963800
C	-1.02022200	2.94144800	-8.78683000
C	-2.18558300	2.22909600	-9.44688600
O	-2.11858800	1.22345200	-10.12715300
O	-3.33911900	2.85311100	-9.16426500
C	-4.53500900	2.26765100	-9.73292200
C	-0.80777700	4.69258400	-7.21133200
C	-0.97548200	5.98909200	-6.64390800
C	-1.76142900	6.87786100	-7.35168100
C	-2.37526800	6.56542300	-8.61346600
C	-2.12837800	5.38409400	-9.23924800
C	-1.10351400	4.47291000	-8.65739100
C	-0.46423900	6.33904300	-5.28766200
H	-1.95170400	7.84419300	-6.89013100
H	-3.04681800	7.29279100	-9.05819100
H	-2.55905400	5.14700300	-10.20564900
H	-0.18283000	4.87879300	-9.14257300
H	0.08731600	5.53365100	-4.76796600
N	-0.43446800	3.59052900	-6.58507700
O	-0.62946300	7.43398900	-4.79034100
C	2.31477400	1.78976300	-11.12112100
C	3.44270800	0.78751600	-12.79527800
C	4.34395800	1.48004200	-12.05170300
H	3.57154000	0.17433000	-13.67378800
H	5.41272100	1.58844000	-12.15348600
C	0.96060000	0.41447100	-12.73374100
C	4.25084700	2.93749900	-10.01047000
N	3.63505600	2.08736800	-11.02848600
N	2.20372900	0.98608200	-12.20997800
Au	0.76754100	2.37751400	-9.92064500
H	3.50918300	3.16544000	-9.24494100
H	4.60510600	3.86707500	-10.46435600
H	5.09064400	2.40906100	-9.55268700
H	0.69275300	0.90677400	-13.67254000
H	0.15885600	0.55836200	-12.00819800
H	1.10121000	-0.65496600	-12.90787800
H	-5.35132900	2.91288300	-9.41067000
H	-4.66778100	1.25143800	-9.35542100
H	-4.46056800	2.24288300	-10.82287400
C	-0.47295300	1.18768200	-6.88376300
C	-0.24236700	1.05207200	-5.49498400
C	-0.56119600	0.02192400	-7.67813800
C	-0.11468600	-0.20755200	-4.92168200
H	-0.17553900	1.94402300	-4.88420600
C	-0.43348900	-1.23265500	-7.09497900
H	-0.72727400	0.09795300	-8.74511100
C	-0.21009600	-1.35256100	-5.71831000
H	0.05863800	-0.29853900	-3.85387100
H	-0.50301900	-2.12179200	-7.71416600
H	-0.10743500	-2.33635500	-5.26938600

NTf_2^- $E_{M06(dichloroethane)}$ = -1827.212931

N	4.95988200	11.70760600	7.69350500
S	4.66794100	12.37260400	9.14103300
S	6.45036100	11.37726100	7.15288900
C	4.50539000	10.86788600	10.23899100
C	6.91417500	12.96524200	6.28137600
F	5.61005400	10.11247400	10.19691400
F	3.46010300	10.11329300	9.86521300
F	4.30539200	11.25536100	11.51338700
F	6.86037600	14.01267900	7.11359200
F	6.09079200	13.20087600	5.24803600
F	8.16911800	12.86942600	5.80148100
O	3.31289900	12.93602100	9.12027700
O	5.75470000	13.15219800	9.74876000
O	7.50147500	11.19434200	8.16276600
O	6.33472000	10.40331500	6.06097100

Gp1 $E_{M06(dichloroethane)}$ = -3203.233546

C	-0.53944200	2.56654200	-7.28686200
C	-1.10175500	2.92481400	-8.59643300
C	-2.20688900	2.16575500	-9.24466400
O	-2.68364400	1.10899300	-8.88260600
O	-2.64242700	2.81620800	-10.35838800
C	-3.70066700	2.16111500	-11.07410700
C	-0.65033400	4.73654800	-7.18861600
C	-0.63909400	6.07010900	-6.71306500
C	-1.39991000	6.99955100	-7.40964500
C	-2.17546400	6.66321100	-8.54946700
C	-2.13526800	5.39910400	-9.08005400
C	-1.17397800	4.44386800	-8.52628700
C	0.11063200	6.45748800	-5.49455700
H	-1.40247100	8.01936700	-7.03374500
H	-2.77150900	7.42981400	-9.03171300
H	-2.64751900	5.15359900	-10.00068700
H	-0.28673300	4.90341400	-9.16368300
H	0.70436800	5.64523100	-5.03536500
N	-0.22741000	3.64438800	-6.53828500
O	0.09766700	7.58374400	-5.03174200
C	2.21671400	1.89119800	-11.06489800
C	3.40715700	1.35249200	-12.90209000
C	4.28790400	1.64793400	-11.91090800
H	3.56572500	1.05689600	-13.92722900
H	5.36627500	1.66527800	-11.90159400
C	0.88859300	1.28804700	-13.08304500
C	4.13615100	2.35006800	-9.50984100
N	3.54048500	1.96707200	-10.79081500
N	2.14134500	1.50009400	-12.36279100

Au	0.64314400	2.36962900	-9.86347600
H	3.34312500	2.55369800	-8.79299900
H	4.71566200	3.26415600	-9.64550700
H	4.77043800	1.53465600	-9.15113400
H	0.29403800	2.20114500	-13.06262400
H	0.32350900	0.47842500	-12.61497800
H	1.11869300	1.02270300	-14.11648500
H	-3.92494200	2.81216500	-11.91975000
H	-4.58138900	2.03585800	-10.43812000
H	-3.37416300	1.17644200	-11.42150500
C	-0.24137400	1.23769100	-6.72640800
C	0.15018500	1.16256000	-5.37427300
C	-0.31758200	0.04623000	-7.47228000
C	0.44549800	-0.06374500	-4.78675700
H	0.21702800	2.07968800	-4.80139300
C	-0.01578200	-1.17726400	-6.88162900
H	-0.61937700	0.07367400	-8.51016500
C	0.36486900	-1.23889500	-5.53832800
H	0.74146500	-0.10221900	-3.74217200
H	-0.07979200	-2.08644500	-7.47281200
H	0.59819100	-2.19683900	-5.08110500
N	0.90029500	5.82436700	-9.99713100
S	0.57198400	6.54666400	-11.42847100
S	2.39663600	5.55312300	-9.41402200
C	0.43591700	5.08682000	-12.58584500
C	2.86147100	7.18091700	-8.61423400
F	1.57426600	4.38143400	-12.61595800
F	-0.55950200	4.26900600	-12.18356400
F	0.15890900	5.51273700	-13.82032500
F	2.89529000	8.16073000	-9.51275500
F	1.96606900	7.48082800	-7.66641600
F	4.06698200	7.04488300	-8.05212200
O	-0.80033600	7.04943100	-11.35451600
O	1.65229000	7.36804600	-11.96726700
O	3.43133300	5.26853800	-10.41383600
O	2.21980500	4.63805500	-8.27502400

$TS_{Gp1\text{-}Gp2}$ $E_{M06(dichloroethane)}$ = -3203.231074

C	-0.58720800	2.55457200	-7.23542500
C	-1.16506100	2.90816900	-8.54959100
C	-2.29895000	2.15103000	-9.15153300
O	-2.78479300	1.11284000	-8.75027600
O	-2.75215700	2.77753900	-10.27346200
C	-3.84646600	2.12564800	-10.93563000
C	-0.73219100	4.72215000	-7.14116500
C	-0.74027400	6.05030300	-6.66024300
C	-1.50201900	6.98108400	-7.36175000
C	-2.25632700	6.64032900	-8.50608700
C	-2.20052900	5.36872400	-9.03470900
C	-1.26154500	4.42168100	-8.46515000
C	-0.00598700	6.43814200	-5.43356200
H	-1.51589800	7.99911700	-6.98178800
H	-2.85271000	7.39916400	-9.00001300
H	-2.70639100	5.11952700	-9.95771300
H	-0.33528600	4.94008400	-9.13425100
H	0.58080200	5.62567300	-4.96567000
N	-0.28640100	3.62833100	-6.49170500
O	-0.02252300	7.56513800	-4.97141000
C	2.11041200	1.83742100	-11.04943800
C	3.36209200	1.33338700	-12.85832100
C	4.20923300	1.57384500	-11.82522500
H	3.55260500	1.06765100	-13.88636500
H	5.28652000	1.55767400	-11.77222700
C	0.87732600	1.39118900	-13.18465300
C	3.98259900	2.20599100	-9.41255800
N	3.42600100	1.87263400	-10.72443800
N	2.07838000	1.48950100	-12.36276700
Au	0.53272700	2.33032900	-9.84990900
H	3.16956600	2.40137400	-8.71627300
H	4.58188200	3.11349400	-9.50058900
H	4.59151900	1.37058300	-9.05609700
H	0.77694200	2.28326100	-13.80704400
H	0.00808200	1.31125900	-12.53227700
H	0.94278700	0.50168900	-13.81627700
H	-4.08582700	2.75750500	-11.79177700
H	-4.70832700	2.03680500	-10.26837300
H	-3.55244600	1.12474400	-11.26537600
C	-0.26064900	1.22513400	-6.68788300
C	0.18917800	1.15041400	-5.35426700
C	-0.36394700	0.03350600	-7.42957800
C	0.51745900	-0.07441700	-4.78139800
H	0.27517400	2.06776100	-4.78415500
C	-0.03073500	-1.18935900	-6.85348100
H	-0.71347100	0.05835800	-8.45249600
C	0.40989300	-1.25014600	-5.52897100
H	0.85908800	-0.11154800	-3.75069100
H	-0.11839300	-2.09850700	-7.44181600
H	0.66739100	-2.20713800	-5.08278000
N	0.78417400	5.70349300	-9.91977300
S	0.45426900	6.44045500	-11.35459800
S	2.29786100	5.45195500	-9.33743700
C	0.38659200	5.01004000	-12.55525400
C	2.76005400	7.09095600	-8.55415400
F	1.55337300	4.35442500	-12.59009200
F	-0.58283100	4.15016400	-12.19668700
F	0.11499900	5.46999000	-13.77917800
F	2.85975800	8.05048800	-9.46715100
F	1.83116600	7.42743300	-7.65389200
F	3.93559400	6.93244300	-7.93794300
O	-0.93220300	6.89998900	-11.29261300
O	1.52478600	7.30500700	-11.83936000
O	3.31547200	5.16864300	-10.35275900
O	2.13311500	4.54578100	-8.19341400

$HNTf_2$ $E_{M06(dichloroethane)}$ = -1827.639562

N	4.98099800	11.71377200	7.70912500
S	4.58944900	12.40443300	9.21609600
S	6.51388000	11.34087800	7.06640300
C	4.52055100	10.87084600	10.29360500
C	6.96839300	12.98143100	6.27935200
F	5.70381800	10.27250500	10.29993800
F	3.59603600	10.04714800	9.79971800
F	4.18580200	11.24731500	11.52393600
F	7.02973800	13.92524800	7.20868100
F	6.03672600	13.28982100	5.37713200
F	8.14915200	12.83948700	5.68510000
O	3.22402500	12.88273700	9.06689300
O	5.70039200	13.21564200	9.67279200
O	7.44154200	11.09901000	8.15345100
O	6.25004400	10.40747400	5.98263700
H	4.18835600	11.49310000	7.10884100

Gp2 $E_{M06(dichloroethane)}$ = -1375.608741

C	-0.61732000	2.58857900	-7.16464700
C	-1.29612400	2.75187500	-8.49460100
C	-2.41518500	1.84999400	-8.89279600
O	-2.77211800	0.83344400	-8.33030400
O	-3.02645800	2.29476700	-10.02915500
C	-4.13701500	1.50103400	-10.46614400
C	-0.89947600	4.74450300	-7.37900000

C	-0.86808000	6.12959100	-7.12791200
C	-1.48418700	6.98090300	-8.05807500
C	-2.10814800	6.46814100	-9.19675400
C	-2.12269200	5.08949300	-9.45588800
C	-1.50837500	4.22778700	-8.54918200
C	-0.21369800	6.67715000	-5.92431300
H	-1.46405200	8.04844100	-7.86031500
H	-2.58770400	7.14633800	-9.89795000
H	-2.60512400	4.69538400	-10.34351300
H	0.23265100	5.91786700	-5.25232200
N	-0.36771400	3.74192900	-6.58029400
O	-0.14811400	7.86837200	-5.66053500
C	1.97043400	1.97217900	-11.03324200
C	3.50701100	1.98355000	-12.69084900
C	3.93339100	1.10837700	-11.74425300
H	3.94346500	2.27793100	-13.63268400
H	4.81434500	0.48704000	-11.69905200
C	1.53294300	3.51722100	-12.95215400
C	3.08725000	0.30675300	-9.52017200
N	2.98129800	1.11185300	-10.73783900
N	2.30294100	2.50038400	-12.24039700
Au	0.34206300	2.37526700	-9.85891400
H	2.17753700	0.41756600	-8.92957800
H	3.94170900	0.64389700	-8.92673000
H	3.21795100	-0.74520800	-9.78801700
H	2.03397700	4.48705200	-12.88150500
H	0.54420700	3.58979500	-12.49873800
H	1.43275900	3.23050400	-14.00228800
H	-4.51899100	1.99822900	-11.35925800
H	-4.91038800	1.45402400	-9.69385300
H	-3.81574500	0.48179900	-10.70190700
C	-0.12155500	1.34053200	-6.54584300
C	0.39953700	1.39497100	-5.23958200
C	-0.09737500	0.10700400	-7.22182200
C	0.93245800	0.25952500	-4.63467200
H	0.38274100	2.34550400	-4.71813600
C	0.44155500	-1.02739900	-6.61558300
H	-0.51891200	0.02891900	-8.21579300
C	0.96076600	-0.95805200	-5.32061300
H	1.32746900	0.32482300	-3.62410300
H	0.44445400	-1.97147200	-7.15489600
H	1.37607100	-1.84460600	-4.84820800

Gp3 $E_{M06(dichloroethane)}$ = -3203.281211

C	-1.26200500	2.31691300	-6.42695600
C	-1.66535600	2.42577000	-7.84483600
C	-2.46490000	1.37509700	-8.53065700
O	-2.70218700	0.25757400	-8.11796200
O	-2.90816400	1.80871000	-9.74311400
C	-3.68909100	0.85567600	-10.47785600
C	-1.62445900	4.46835200	-6.75767700
C	-1.73908900	5.86204200	-6.56961300
C	-2.20815600	6.62726200	-7.64814400
C	-2.55384300	6.03759700	-8.86782000
C	-2.43310100	4.65746600	-9.05290900
C	-1.96359400	3.87185600	-7.99635900
C	-1.43783000	6.53754900	-5.30043100
H	-2.31263900	7.70258100	-7.52011800
H	-2.92282400	6.65735100	-9.68018800
H	-2.69649700	4.19551600	-9.99692400
H	0.00212600	3.83618100	-4.86037500
H	-1.59689700	7.63970900	-5.32879200
N	-1.18696900	3.51684500	-5.85008500
O	-1.05947800	6.00185200	-4.27290300
C	2.28188500	2.39687500	-9.37944300
C	4.44151500	1.83354400	-9.69664100
C	4.31607000	3.15787900	-9.97711100
H	5.30013100	1.18138400	-9.72554600
H	5.04406800	3.88542500	-10.29973500
C	2.87184100	0.04150200	-8.85044400
C	2.42784700	4.83302100	-9.88281600
N	2.98428600	3.48216200	-9.78535800
N	3.18237600	1.38319700	-9.34012800
Au	0.36002800	2.35698500	-8.72442400
H	2.35512200	5.26970600	-8.88513500
H	1.43075900	4.77738200	-10.32268200
H	3.07686100	5.43603700	-10.52096100
H	3.71128900	-0.62003700	-9.07220100
H	1.97294100	-0.32819900	-9.34689700
H	2.69693400	0.07734200	-7.77314100
H	-3.97426600	1.36183200	-11.40119500
H	-4.57685100	0.56115200	-9.91097500
H	-3.09904400	-0.03929400	-10.69722000
C	-0.88413100	1.12417800	-5.65272700
C	-0.91154500	1.19971400	-4.24907800
C	-0.42966800	-0.06209900	-6.25591400
C	-0.45878600	0.13675700	-3.47071500
H	-1.28462200	2.09564700	-3.76931500
C	0.01394200	-1.12551800	-5.47575300
H	-0.41699100	-0.14379100	-7.33555000
C	0.01037000	-1.02829400	-4.08041200
H	-0.47183200	0.22834200	-2.38867300
H	0.36653600	-2.03386600	-5.95763400
H	0.36574200	-1.85783400	-3.47475800
N	1.00665500	3.93522900	-4.39327800
S	2.25966600	4.20632400	-5.44083700
S	1.14132000	3.97086500	-2.71113100
C	3.00378200	2.50141400	-5.67294300
C	1.25794900	5.82621400	-2.28054200
F	3.64985300	2.11331000	-4.58414000
F	2.05230500	1.60902000	-5.97052400
F	3.86597800	2.56861700	-6.70339700
F	1.49809100	6.56059200	-3.36124500
F	0.12639100	6.20589900	-1.70560300
F	2.26520400	5.96587700	-1.41734500
O	1.65729900	4.54578600	-6.73008300
O	3.31897400	5.00738200	-4.84593100
O	2.41577900	3.38307500	-2.32147200
O	-0.13412300	3.49508400	-2.19617800

$TS_{Gp3\text{-}Gp4}$ $E_{M06(dichloroethane)}$ = -3203.272193

C	-1.28877500	2.30995900	-6.42236300
C	-1.67418700	2.42074500	-7.83836700
C	-2.47700900	1.37104600	-8.52568000
O	-2.72006100	0.25630000	-8.11031600
O	-2.91224800	1.80457600	-9.73995400
C	-3.69004200	0.85215200	-10.47964200
C	-1.61941700	4.47378000	-6.76804600
C	-1.71670100	5.87218800	-6.60509100
C	-2.13618100	6.62810200	-7.70854100
C	-2.46346200	6.02894700	-8.92920300
C	-2.37159600	4.64561900	-9.08664800
C	-1.94327900	3.86864200	-8.00488500
C	-1.48143300	6.56991300	-5.33073200
H	-2.22338400	7.70668600	-7.59725100
H	-2.79708900	6.64432300	-9.75991400
H	-2.62194900	4.17092500	-10.02761900
H	-0.16899800	3.82477100	-4.88583300
H	-1.58837500	7.67633800	-5.39598300
N	-1.20930500	3.51443700	-5.84440800

O	-1.22201000	6.03997500	-4.26696500
C	2.26955900	2.37468400	-9.38867200
C	4.44953800	1.88097600	-9.68027900
C	4.28284000	3.19759500	-9.97439600
H	5.32968200	1.25766600	-9.69308300
H	4.98914100	3.94573600	-10.29812100
C	2.94524900	0.05132700	-8.81176700
C	2.33581300	4.80844700	-9.91710200
N	2.93960300	3.47918700	-9.79802300
N	3.20211500	1.39141900	-9.33297400
Au	0.35008000	2.31632300	-8.73013800
H	2.16716700	5.22061200	-8.92058100
H	1.38012800	4.72340300	-10.43730200
H	3.00879300	5.44957600	-10.48952100
H	3.73756400	-0.62032900	-9.14801900
H	1.98305900	-0.30137700	-9.18617000
H	2.91619700	0.08168200	-7.72013600
H	-3.96846200	1.35871100	-11.40470700
H	-4.58164800	0.55939800	-9.91806900
H	-3.09938700	-0.04335700	-10.69478800
C	-0.98290000	1.09218100	-5.65754700
C	-1.18821900	1.09370100	-4.26955600
C	-0.47337100	-0.07149100	-6.26117200
C	-0.86727200	-0.02266600	-3.49958400
H	-1.61866900	1.96975100	-3.80544500
C	-0.15501000	-1.18530500	-5.49270600
H	-0.32173100	-0.09548800	-7.33336900
C	-0.34521800	-1.16469400	-4.10697300
H	-1.02361600	0.00664100	-2.42571800
H	0.24260700	-2.07447900	-5.97476700
H	-0.09180400	-2.03540400	-3.50818600
N	0.90885200	3.95203600	-4.39191000
S	2.09885000	4.21572500	-5.50783000
S	1.24841000	4.42865000	-2.78034600
C	2.89887300	2.53099000	-5.66545300
C	-0.25789500	3.68508200	-1.93083400
F	3.52759500	2.19893500	-4.54761000
F	1.98183600	1.59671400	-5.95503500
F	3.78530100	2.58092200	-6.67791200
F	-1.38183500	3.88361200	-2.61621800
F	-0.07059000	2.37415200	-1.75485700
F	-0.34987500	4.27911000	-0.74234700
O	1.45679800	4.45356100	-6.80281900
O	3.15364300	5.09368900	-5.01873700
O	1.16482500	5.86795600	-2.59158500
O	2.39430400	3.66499200	-2.29417500

Gp4 $E_{M06(dichloroethane)}$ = -1376.067014

C	-0.77393700	2.02389000	-7.51828500
C	-0.13537600	2.87960600	-8.49708800
C	0.58180400	2.30515300	-9.68529600
O	0.89275900	1.14268300	-9.82333800
O	0.86076000	3.27056600	-10.58212200
C	1.54259200	2.82545500	-11.77633400
C	-1.98479900	3.95943200	-7.58216500
C	-2.93105900	4.96048300	-7.31208300
C	-2.85540300	6.12146600	-8.09181100
C	-1.88142900	6.26772300	-9.08678500
C	-0.93537900	5.26986900	-9.32802400
C	-0.98100600	4.09845200	-8.56106700
C	-3.97328100	4.82643900	-6.26920600
H	-3.58424000	6.90317800	-7.90331600
H	-1.86114500	7.17508500	-9.68242800
H	-0.17932200	5.38561500	-10.09416400
H	-3.98414400	3.86131800	-5.71216100
N	-1.81865000	2.70627000	-6.99332200
O	-4.78317700	5.69031200	-6.00653300
C	3.08544200	4.39547700	-6.14653400
C	4.94952500	4.53307500	-4.89149400
C	4.51824000	5.80022200	-5.12604300
H	5.80242200	4.16631800	-4.34180600
H	4.91456400	6.75294700	-4.81070300
C	4.19101500	2.22636200	-5.56291100
C	2.57453500	6.84802700	-6.32206800
N	3.37484900	5.69719900	-5.89984700
N	4.05652300	3.68368800	-5.52141600
Au	1.54062500	3.64972600	-7.23286400
H	1.88858200	6.53722000	-7.11047200
H	3.23797500	7.62574200	-6.70672000
H	2.00298100	7.23692700	-5.47495600
H	4.70638400	1.92070700	-6.47738500
H	3.20070600	1.76944500	-5.53137400
H	4.76402100	1.90038100	-4.69319400
H	1.67683700	3.72139900	-12.38139200
H	0.93600500	2.08668000	-12.30510900
H	2.50699000	2.38154300	-11.51704400
C	-0.49651400	0.65623300	-7.08265100
C	0.80762600	0.12669000	-7.09070800
C	-1.55686000	-0.15147000	-6.62437300
C	1.04293800	-1.16500100	-6.63376400
H	1.62842800	0.72642000	-7.46424100
C	-1.31560100	-1.44592200	-6.17201300
H	-2.58105600	0.20915900	-6.66910700
C	-0.01451600	-1.95355800	-6.16917500
H	2.05312300	-1.56286000	-6.64572000
H	-2.14413500	-2.06129800	-5.83565300
H	0.17379800	-2.96344000	-5.81743100
H	-2.34195800	2.37316200	-6.19453000

TS_{Gp4-Ap} $E_{M06(dichloroethane)}$ = -1376.047169

C	-0.92661500	2.21956400	-7.60122600
C	-0.10846000	2.48927100	-8.71618900
C	0.71619200	1.51559500	-9.46663000
O	1.69286400	0.96016100	-8.95622700
O	0.35233300	1.35721000	-10.72724700
C	1.17887500	0.47717500	-11.53510000
C	-1.25366500	4.40581600	-8.16649800
C	-1.61475300	5.76591800	-8.17773700
C	-1.06557900	6.55909200	-9.19346200
C	-0.19747000	6.02503700	-10.15720600
C	0.17166300	4.68095600	-10.12446300
C	-0.35112600	3.86383300	-9.11284400
C	-2.51621800	6.36376300	-7.16919600
H	-1.34353400	7.60805000	-9.21643700
H	0.19064700	6.66850000	-10.94047200
H	0.84787400	4.26922800	-10.86731400
H	-2.96923300	5.65249300	-6.44111600
N	-1.59370100	3.38543300	-7.29708500
O	-2.76781300	7.54964900	-7.10093000
C	3.05299400	4.12728800	-6.06851400
C	3.72008900	6.01998300	-5.05664300
C	4.55261900	5.02292800	-4.65573900
H	3.70343500	7.06960300	-4.80780500
H	5.39919100	5.03305400	-3.98699100
C	1.71940500	6.17489000	-6.59796600
C	4.75442600	2.55659900	-5.09916800
N	4.12990700	3.86647600	-5.28999900
N	2.80337900	5.45312700	-5.92434100
Au	1.98317800	2.89658900	-7.22793400
H	4.39755700	1.87818900	-5.87429200

H	4.49332800	2.15878100	-4.11491500
H	5.83874000	2.66008600	-5.17955500
H	0.75541900	5.75604400	-6.30395500
H	1.82758500	6.09179500	-7.68128800
H	1.76266800	7.22475900	-6.30611000
H	0.75441600	0.53063400	-12.53612000
H	1.12820300	-0.54018400	-11.14190200
H	2.21427500	0.82530400	-11.52404600
C	-1.23235200	0.98468800	-6.86792400
C	-0.25748300	0.00134300	-6.61825500
C	-2.54373900	0.77837200	-6.39620400
C	-0.59000300	-1.15041300	-5.90855200
H	0.75747300	0.13953200	-6.97052800
C	-2.86746000	-0.37442400	-5.68462000
H	-3.32500900	1.49860500	-6.62393500
C	-1.89084000	-1.34134100	-5.43598600
H	0.17330800	-1.89913000	-5.71863700
H	-3.88501600	-0.52230400	-5.33593900
H	-2.14325300	-2.24034000	-4.88179800
H	-2.17413900	3.48213500	-6.47659900

PhC≡CCO$_2$Me $E_{M06(dichloroethane)}$ = -536.056779

C	-4.03116500	4.96041900	5.97387600
C	-3.74882300	5.00461700	7.15353800
C	-3.49093500	5.09419000	8.56894700
O	-4.26301500	5.55905300	9.38404200
O	-2.27319800	4.59209300	8.87516600
C	-1.93695800	4.64432900	10.27221100
H	-0.94037400	4.20806900	10.34674900
H	-1.93410300	5.67840800	10.62906000
H	-2.65591000	4.06932100	10.86311100
C	-4.35494200	4.90529800	4.58815800
C	-3.44280100	4.35619600	3.66506400
C	-5.59130400	5.40012700	4.12750200
C	-3.76492500	4.30541900	2.31148900
H	-2.49125100	3.97565000	4.02294400
C	-5.90386000	5.34474700	2.77181600
H	-6.29170100	5.82251400	4.84115200
C	-4.99355000	4.79852600	1.86223500
H	-3.05730800	3.88083000	1.60497900
H	-6.85865600	5.72815400	2.42331000
H	-5.24112000	4.75717700	0.80510500

PAp $E_{M06(dichloroethane)}$ = -935.708470

C	-1.24723900	2.69263200	7.20797700
C	-2.01951300	3.27537600	8.20971700
C	-2.90147600	2.65282000	9.20002900
O	-3.50538500	3.27040300	10.06168000
O	-3.00513100	1.30830700	9.06195300
C	-3.87199500	0.66136400	10.00383800
C	-1.05040900	4.94511900	6.95197600
C	-0.71117200	6.24439000	6.52613600
C	-1.25900800	7.31192300	7.25059300
C	-2.10702500	7.09419200	8.34309400
C	-2.43643700	5.80278400	8.75717200
C	-1.89954500	4.70932400	8.06173100
C	0.16991500	6.49562300	5.37614600
H	-1.00338400	8.31774600	6.93249000
H	-2.51485800	7.94634700	8.87894200
H	-3.09057200	5.62510500	9.60226200
H	0.55048700	5.58419700	4.85712600
N	-0.68925800	3.70934000	6.45409000
O	0.49375300	7.59816800	4.97224300
H	-4.89491600	1.03701500	9.90853400
H	-3.82790200	-0.39999800	9.75587300
H	-3.52947200	0.83333400	11.02859200
C	-0.93217100	1.30381000	6.83950300
C	-0.93170800	0.92793800	5.48491700
C	-0.56234700	0.35578900	7.80719000
C	-0.57761600	-0.36731700	5.10756800
H	-1.24044300	1.64552500	4.72885300
C	-0.20839500	-0.93611500	7.42692900
H	-0.55360900	0.64201200	8.85211800
C	-0.21416600	-1.30288100	6.07773500
H	-0.59305500	-0.64569100	4.05749200
H	0.08043700	-1.65838300	8.18552900
H	0.06269800	-2.31208900	5.78568000
H	-0.00003200	3.54076800	5.73689100

Fp1 $E_{M06(dichloroethane)}$ = -1375.943630

C	-1.48708400	1.14423900	-0.08276500
C	-0.80388000	0.14027700	0.72239700
C	-1.57041800	-0.63568100	1.71584600
O	-1.80756200	-0.07019500	2.76664900
O	-1.84104300	-1.88707700	1.38744600
C	-2.64478200	-2.64136200	2.33341400
C	-2.94946600	-0.56786300	-1.07932300
C	-2.51854400	-1.60933700	-1.94220200
C	-3.33733500	-2.73705600	-2.11216400
C	-4.55538200	-2.85276800	-1.45116000
C	-4.97251500	-1.81975900	-0.60326300
C	-4.18308700	-0.68776300	-0.41508400
C	-1.21325500	-1.57387000	-2.60883700
H	-2.99722900	-3.53414200	-2.76925600
H	-5.17735200	-3.73011200	-1.59490600
H	-5.92504000	-1.89259900	-0.08609800
H	-4.51604300	0.12402900	0.22429400
H	-1.03203900	-2.40929800	-3.31569500
N	-2.25996200	0.62798100	-0.97737800
O	-0.35066000	-0.72298200	-2.42845800
C	3.04612000	-0.71884900	-0.24754400
C	5.18558600	-1.42346000	-0.28943800
C	4.89845500	-0.90272800	-1.51358800
H	6.09089200	-1.86425000	0.09832600
H	5.50714700	-0.80311300	-2.39884800
C	3.93876200	-1.74575900	1.86227500
C	2.87972200	0.17503900	-2.57941300
N	3.58531600	-0.47812300	-1.46983900
N	4.03784300	-1.30404400	0.47153900
Au	1.11309500	-0.27069300	0.30994600
H	2.79215600	1.24633700	-2.38118500
H	1.88507000	-0.25921600	-2.69388100
H	3.45479300	0.02143400	-3.49388300
H	4.63698600	-1.17715800	2.48206100
H	4.17313600	-2.81131700	1.92760900
H	2.92184200	-1.57612300	2.21576200
H	-2.76113700	-3.62469300	1.88197200
H	-3.61461200	-2.15480600	2.45909000
H	-2.12986400	-2.70450900	3.29405600
C	-1.09603400	2.55425100	-0.08397700
C	-1.45251500	3.39336200	-1.15307700
C	-0.38473600	3.07089200	1.01203400
C	-1.08560500	4.73436900	-1.12650100
H	-2.00279200	2.98042000	-1.99255000
C	-0.02689700	4.41687200	1.03530600
H	-0.13649200	2.42366500	1.84948200
C	-0.37315800	5.24660600	-0.03469600
H	-1.35249400	5.38435900	-1.95423700
H	0.51383800	4.81914900	1.88635400
H	-0.09272500	6.29581100	-0.01754300

TS_{Fp1-Ip} $E_{M06(dichloroethane)}$ = -1375.943047

C	-4.19128600	5.49595900	-5.86816500
C	-4.33973200	4.69474500	-7.12621800
C	-4.67681000	5.45338200	-8.35193700
O	-5.71053900	6.09977600	-8.30962500
O	-3.89526500	5.29107600	-9.41061100
C	-4.31814300	5.98832100	-10.61000200
C	-2.21356700	6.09802000	-6.68620300
C	-1.89597600	4.76679800	-7.13517000
C	-1.12179500	4.62132900	-8.31048000
C	-0.63938600	5.73089700	-8.97887100
C	-0.87918500	7.02629300	-8.46698600
C	-1.63092700	7.21299800	-7.31787600
C	-1.93057500	3.56759600	-6.22937900
H	-0.86797600	3.62221700	-8.65519900
H	-0.03403800	5.61005200	-9.87165500
H	-0.47533100	7.88943800	-8.98793900
H	-1.85498800	8.20299600	-6.93528500
H	-1.65860000	2.63154500	-6.75743900
N	-3.16663700	6.27951700	-5.71439500
O	-2.17977300	3.57039600	-5.04182100
C	-5.39030800	0.82739300	-6.38928100
C	-6.07999200	-1.31246400	-6.26106900
C	-5.66153200	-0.94009600	-5.02034700
H	-6.47725900	-2.24805300	-6.62311300
H	-5.62565400	-1.49094000	-4.09329200
C	-6.24690900	-0.19742900	-8.50667300
C	-4.73713700	1.18438500	-4.00163200
N	-5.24076600	0.37190100	-5.11766300
N	-5.90478200	-0.21552300	-7.08533700
Au	-4.90828300	2.75198300	-6.92388300
H	-5.45887500	1.96716600	-3.75516600
H	-3.78570400	1.64800300	-4.27268300
H	-4.59193700	0.53500900	-3.13712300
H	-7.32386200	-0.33789100	-8.63120700
H	-5.71011100	-0.99576900	-9.02542500
H	-5.95655100	0.76665900	-8.92451700
H	-3.55046900	5.76780300	-11.35026000
H	-4.37781400	7.06196100	-10.41738800
H	-5.29346900	5.61918700	-10.93495600
C	-5.17610300	5.29973500	-4.79511500
C	-4.73292500	5.27141100	-3.46123800
C	-6.53631100	5.09421000	-5.09243600
C	-5.64352400	5.02188700	-2.43779800
H	-3.67877900	5.41864800	-3.25316400
C	-7.44192700	4.85654700	-4.06059000
H	-6.87512200	5.15815200	-6.12213100
C	-6.99533800	4.81253400	-2.73584100
H	-5.30263000	4.99332200	-1.40714600
H	-8.49436100	4.71553100	-4.28727300
H	-7.70254400	4.62420500	-1.93303800

TS_{Fp1-Np} $E_{M06(dichloroethane)}$ = -1375.939841

C	-3.89166600	4.69644900	-4.98642900
C	-3.53732100	3.74596000	-3.94504600
C	-2.33836500	2.90438000	-4.22481700
O	-1.39612800	3.23387900	-4.92095500
O	-2.44810500	1.72489300	-3.59577400
C	-1.37832700	0.78572200	-3.85317400
C	-2.01488000	6.33795900	-4.28432900
C	-2.21355600	7.31236000	-3.25728900
C	-1.12626300	8.10256200	-2.86396200
C	0.13016900	7.95451600	-3.44804900
C	0.31413500	6.99518900	-4.45061700
C	-0.73927600	6.19096100	-4.87262000
C	-3.50256500	7.51041900	-2.58461600
H	-1.27698800	8.84346100	-2.08242700
H	0.95822000	8.57812700	-3.12752300
H	1.29000900	6.87072100	-4.91018700
H	-0.60804500	5.43924400	-5.63952800
H	-3.50674300	8.33556000	-1.84314900
N	-3.03949700	5.59954600	-4.75548300
O	-4.51658300	6.85309600	-2.77828200
C	-5.61034700	3.75843500	-0.43399000
C	-6.43479000	3.17634300	1.58367800
C	-7.10915900	4.28122800	1.16669300
H	-6.51908900	2.59437000	2.48838300
H	-7.90183600	4.84397200	1.63482100
C	-4.57932000	1.75571500	0.67355500
C	-7.08518200	5.73268800	-0.89062100
N	-6.58983100	4.62514100	-0.06723500
N	-5.52266700	2.87000900	0.59045700
Au	-4.52613100	3.79070600	-2.18399900
H	-7.84112900	5.36681900	-1.59089700
H	-6.25924100	6.18140800	-1.44428700
H	-7.53194400	6.48177900	-0.23392400
H	-3.84177500	1.94860200	1.45752500
H	-4.07111800	1.64986100	-0.28498400
H	-5.12211700	0.83449900	0.89957300
H	-1.65671400	-0.12084400	-3.31762200
H	-0.43263800	1.18661300	-3.47984100
H	-1.29133000	0.59381000	-4.92561200
C	-4.97390200	4.67617900	-5.95223900
C	-5.19149600	5.76679500	-6.81085100
C	-5.80325500	3.54467900	-6.01070900
C	-6.23530400	5.71850200	-7.72721800
H	-4.54303000	6.63602000	-6.74847700
C	-6.84705200	3.50342200	-6.93086800
H	-5.62664400	2.71188600	-5.33442000
C	-7.06114800	4.58827500	-7.78718200
H	-6.41065400	6.55596600	-8.39526200
H	-7.49169300	2.63165500	-6.98321900
H	-7.87539700	4.55498100	-8.50521400

Ip $E_{M06(dichloroethane)}$ = -1375.979608

C	-3.93123600	5.54316900	-5.71859300
C	-3.76219300	4.78665200	-6.98968300
C	-4.64485200	5.18272200	-8.14882400
O	-5.64327000	5.86485800	-8.06023400
O	-4.20435400	4.65738800	-9.31144300
C	-4.99215000	4.99271200	-10.47586100
C	-1.86241100	5.98792200	-6.24312100
C	-2.22156000	4.92215100	-7.21595900
C	-1.52493400	4.99383000	-8.51853400
C	-0.41795500	5.77004700	-8.63240300
C	0.04101900	6.58914100	-7.53789100
C	-0.64436300	6.69469500	-6.34884000
C	-1.65276200	3.58523400	-6.46780000
H	-1.83507100	4.32238500	-9.30748600
H	0.15481800	5.77170200	-9.55416800
H	0.95008000	7.16797000	-7.67747000
H	-0.33981300	7.37495000	-5.56110200
H	-1.94246000	3.57508200	-5.39849100
N	-2.80223500	6.17153300	-5.31179800
O	-1.01545200	2.72486000	-7.00184900
C	-4.94657600	0.76281900	-6.39587300
C	-6.08414600	-1.10267300	-5.84539200
C	-4.90674400	-1.48921200	-6.40334600
H	-6.90168500	-1.68153300	-5.44461400

H	-4.49795200	-2.47130200	-6.58340600
C	-7.20409600	1.09807300	-5.36321500
C	-2.91441400	-0.30868700	-7.39558100
N	-4.22003300	-0.33270900	-6.73055400
N	-6.08929700	0.28200800	-5.84470000
Au	-4.41134200	2.71601900	-6.67081900
H	-2.34834900	0.56392400	-7.06719000
H	-3.04666200	-0.26955300	-8.48022300
H	-2.36575500	-1.21327700	-7.12694800
H	-7.94815700	1.22448700	-6.15484100
H	-6.83028700	2.07560800	-5.05538600
H	-7.66363100	0.60349800	-4.50497900
H	-4.49423300	4.50059100	-11.31081100
H	-5.01690800	6.07534200	-10.62024000
H	-6.01295800	4.62133100	-10.35780000
C	-5.11681700	5.65268500	-4.88455100
C	-5.00576200	6.31080900	-3.63687600
C	-6.37287000	5.12633900	-5.26563100
C	-6.10669900	6.42279400	-2.79654500
H	-4.04727300	6.72454600	-3.34729500
C	-7.47031300	5.25030800	-4.42401100
H	-6.49529300	4.65629700	-6.23203300
C	-7.34068000	5.89276300	-3.18612400
H	-6.00671000	6.92607800	-1.83996100
H	-8.43414200	4.85811700	-4.73455700
H	-8.20211000	5.98492200	-2.53079800

TS_{Ip-Jp} $E_{M06(dichloroethane)}$ = -1375.975003

C	-4.02748700	5.64123800	-5.77506300
C	-3.77065700	4.93583300	-7.07580200
C	-4.65786900	5.24120900	-8.26185800
O	-5.69253600	5.86719800	-8.22110900
O	-4.14992200	4.71303300	-9.39896100
C	-4.90911700	4.99341500	-10.59672100
C	-1.90230000	5.99215200	-6.14698800
C	-2.31058600	5.17715200	-7.26757800
C	-1.42553800	4.99413500	-8.36362300
C	-0.14966900	5.50309600	-8.25666700
C	0.26881000	6.25696600	-7.11867200
C	-0.58659300	6.51972200	-6.07052400
C	-1.47132500	3.86827500	-5.80977100
H	-1.74917700	4.44069500	-9.23559900
H	0.55959100	5.34328000	-9.06292400
H	1.28385600	6.64122700	-7.09190000
H	-0.29501300	7.11655300	-5.21322300
H	-2.28083800	3.80107100	-5.06234200
N	-2.92633900	6.18607800	-5.25629400
O	-0.47165900	3.31772200	-6.02409400
C	-4.77441500	0.86215500	-6.44149500
C	-5.75963500	-0.95936700	-5.55224800
C	-4.98493500	-1.37724000	-6.58701200
H	-6.39203500	-1.51095000	-4.87391000
H	-4.81343900	-2.36312400	-6.99072100
C	-6.26586400	1.24259700	-4.45423700
C	-3.47405700	-0.27851300	-8.26158000
N	-4.38932900	-0.24719100	-7.12114700
N	-5.62241700	0.41619500	-5.47879800
Au	-4.23239200	2.81119300	-6.76044100
H	-3.20789800	0.74398100	-8.52951100
H	-3.96366200	-0.75931000	-9.11216000
H	-2.56991000	-0.83285900	-7.99625500
H	-7.26744200	0.85244100	-4.26174100
H	-6.34565000	2.27212300	-4.80535300
H	-5.68076200	1.21933500	-3.53067300
H	-4.35823800	4.51434700	-11.40571900
H	-4.97822700	6.07158800	-10.75911800
H	-5.91587900	4.57730800	-10.51108100
C	-5.28358900	5.70476300	-5.01823500
C	-5.29184700	6.39438300	-3.78804600
C	-6.47311900	5.08716300	-5.45429800
C	-6.44879300	6.45666400	-3.01800500
H	-4.38071900	6.87574000	-3.45209700
C	-7.62764600	5.15098700	-4.67925000
H	-6.50987900	4.58545000	-6.41237500
C	-7.61969300	5.83285500	-3.45842100
H	-6.43919100	6.99429000	-2.07466400
H	-8.53972500	4.68104000	-5.03558400
H	-8.52349700	5.88453400	-2.85805500

Jp $E_{M06(dichloroethane)}$ = -1375.983431

C	-3.93943900	5.60543400	-5.56997100
C	-3.94711200	5.13194300	-7.00552200
C	-4.90886300	5.49764900	-8.10176600
O	-4.82657800	5.05224000	-9.23285800
O	-5.81655200	6.38974700	-7.70111400
C	-6.78049700	6.80286000	-8.69702900
C	-1.81403800	5.34245900	-6.09504700
C	-2.56254400	5.09821300	-7.35194000
C	-1.85508300	4.98832300	-8.57142800
C	-0.52164400	5.34765100	-8.57399300
C	0.15833800	5.87953900	-7.41733700
C	-0.48404700	5.97405600	-6.22107400
C	-1.26902800	3.78129200	-5.76952500
H	-2.38048700	4.72574800	-9.48182300
H	0.02978800	5.29826500	-9.50919600
H	1.17429500	6.24361700	-7.53128200
H	-0.02059000	6.36906100	-5.32275500
H	-0.55953900	3.42771700	-6.53937400
N	-2.73483800	5.72525600	-5.08154100
O	-1.64139100	3.17166000	-4.82143400
C	-4.72911800	0.96197600	-6.54593400
C	-5.36253700	-1.17566800	-6.83979100
C	-4.99470100	-1.03046500	-5.53866100
H	-5.72450800	-2.03532100	-7.38208200
H	-4.97530800	-1.74023100	-4.72636400
C	-5.48248900	0.32058600	-8.85423300
C	-4.14676800	0.88600700	-4.11847500
N	-4.60939000	0.28776900	-5.37588400
N	-5.19426000	0.05904200	-7.44325500
Au	-4.30308000	2.92733000	-6.81280800
H	-3.14274900	1.29372800	-4.24714900
H	-4.13446100	0.11308900	-3.34902200
H	-4.82586600	1.68775000	-3.82002200
H	-4.82743200	-0.28738300	-9.48361900
H	-5.30960600	1.37651500	-9.06378500
H	-6.52632200	0.07572600	-9.06588700
H	-7.44214100	7.49690700	-8.18074800
H	-7.33344200	5.93616600	-9.06800700
H	-6.27313900	7.29275400	-9.53116700
C	-5.12062200	5.83168100	-4.71966900
C	-4.97108200	6.58552200	-3.54181000
C	-6.37648400	5.27523100	-5.01697200
C	-6.05382900	6.78509200	-2.69053800
H	-3.99999900	7.00888300	-3.30964200
C	-7.45515400	5.46611500	-4.15600600
H	-6.51618800	4.69278900	-5.92087200
C	-7.29850900	6.22464400	-2.99346800
H	-5.92793000	7.37742500	-1.78911300
H	-8.41917500	5.02640700	-4.39497800
H	-8.14245300	6.37996600	-2.32752700

TS_{Jp-Kp} $E_{M06(dichloroethane)}$ = -1375.981982

C	-3.95679200	5.54558000	-5.71647900
C	-3.97256900	5.14026700	-7.16448400
C	-5.02945300	5.61083200	-8.12162400
O	-6.03483000	6.21442200	-7.82395000
O	-4.71530400	5.26609700	-9.39458700
C	-5.65658900	5.70985000	-10.39692700
C	-1.86842300	5.60428300	-6.31929900
C	-2.56453100	5.27053600	-7.54412000
C	-1.83580200	5.17650300	-8.73489900
C	-0.46110000	5.44646000	-8.71021000
C	0.21810600	5.83862500	-7.53394600
C	-0.47010700	5.92922000	-6.32982600
C	-1.08928000	3.75524900	-6.19159400
H	-2.33551500	4.92311500	-9.66181100
H	0.10159600	5.37083200	-9.63621500
H	1.27961000	6.05908100	-7.57230700
H	0.00671400	6.22334900	-5.40019800
H	-0.62257100	3.52281000	-7.16434800
N	-2.73319100	5.77087600	-5.26217200
O	-1.31065400	3.16887200	-5.21066100
C	-4.72780400	1.02967900	-6.49413200
C	-5.18779500	-1.17406900	-6.51165900
C	-5.17308400	-0.76816800	-5.21415900
H	-5.36850100	-2.14381300	-6.94872900
H	-5.33654600	-1.31744900	-4.30007400
C	-4.85600800	-0.06751600	-8.74327800
C	-4.78005200	1.43653100	-4.03122100
N	-4.89057900	0.58598500	-5.22195400
N	-4.91210900	-0.05648400	-7.28258400
Au	-4.33377100	2.97395600	-6.95311200
H	-3.77055700	1.84822100	-3.96256100
H	-4.98850000	0.83058300	-3.14851500
H	-5.49992300	2.25617800	-4.09142400
H	-4.10576100	-0.78840000	-9.07834200
H	-4.58465900	0.92938200	-9.09111900
H	-5.83361500	-0.33979400	-9.14971800
H	-5.25184200	5.36231900	-11.34727800
H	-5.74010400	6.79925300	-10.38580600
H	-6.64073300	5.27295600	-10.21061400
C	-5.09127100	5.60223100	-4.78218000
C	-4.87254200	6.14049200	-3.49821000
C	-6.36526000	5.08903900	-5.09300500
C	-5.89575900	6.16306600	-2.55597400
H	-3.89277700	6.53637600	-3.25694100
C	-7.38286300	5.10282200	-4.14204700
H	-6.57122000	4.69545200	-6.07972400
C	-7.15329000	5.64032800	-2.87250300
H	-5.71379900	6.58888800	-1.57370200
H	-8.36076300	4.70573100	-4.39799500
H	-7.95197900	5.65799800	-2.13641000

Kp $E_{M06(dichloroethane)}$ = -1376.004752

C	-4.11580400	5.54307300	-5.82112900
C	-4.06899600	5.13269600	-7.22667100
C	-5.11511200	5.50141400	-8.23764700
O	-6.18356000	6.02062600	-8.00245100
O	-4.71031800	5.16429700	-9.48307400
C	-5.63797800	5.49420600	-10.54070500
C	-1.99880500	5.60193600	-6.31838900
C	-2.62742900	5.22909800	-7.55100300
C	-1.86807100	5.06430400	-8.68341900
C	-0.43511900	5.22017500	-8.63090500
C	0.21025100	5.50933400	-7.47375400
C	-0.52253200	5.70690700	-6.19097400
C	-0.03021200	4.73439200	-5.05844700
H	-2.34538800	4.81046800	-9.62336500
H	0.12895000	5.07977900	-9.54765400
H	1.29281800	5.56983800	-7.43693200
H	-0.27473700	6.69726500	-5.76728000
H	-0.68547300	4.75856500	-4.16640000
N	-2.85450800	5.77271700	-5.32196600
O	0.95289100	4.05347700	-5.14771700
C	-4.71327200	0.98273900	-6.54096600
C	-4.61463800	-1.26769400	-6.54851300
C	-5.65931600	-0.90603500	-5.75889400
H	-4.22515300	-2.24020400	-6.80693500
H	-6.36401600	-1.50270800	-5.20071800
C	-2.87376500	-0.06288800	-7.89398100
C	-6.72588800	1.26604800	-5.07011200
N	-5.70332300	0.47742900	-5.76135200
N	-4.04600600	-0.09643200	-7.02000500
Au	-4.36408400	2.95770400	-6.88495200
H	-6.31151900	2.23335500	-4.78297800
H	-7.03819900	0.72932900	-4.17236000
H	-7.58836100	1.42024000	-5.72439100
H	-2.01952800	-0.51592700	-7.38413000
H	-2.64256200	0.97451800	-8.13541400
H	-3.08633700	-0.61145200	-8.81506800
H	-5.15750700	5.16075700	-11.46012300
H	-5.81911400	6.57135800	-10.56540000
H	-6.58625200	4.97350700	-10.38656900
C	-5.24859500	5.69350100	-4.91872300
C	-5.03575900	6.33130700	-3.67551500
C	-6.53842500	5.19952700	-5.21613700
C	-6.07988100	6.48154200	-2.76986900
H	-4.04677100	6.70709600	-3.44232400
C	-7.57376500	5.34374100	-4.30139000
H	-6.72728500	4.71224900	-6.16323500
C	-7.35074300	5.98750200	-3.07798300
H	-5.90438300	6.98336600	-1.82328200
H	-8.56140000	4.96233500	-4.54305900
H	-8.16582900	6.10338400	-2.36940900

Kp1 $E_{M06(dichloroethane)}$ = -3203.233421

C	-4.11798900	5.86151800	-6.23804100
C	-4.22121900	5.42066400	-7.64196800
C	-5.32057700	5.83304500	-8.55920600
O	-6.34220000	6.41041100	-8.25517300
O	-5.04277600	5.46432400	-9.83850000
C	-6.02218300	5.86866900	-10.81068100
C	-2.05591300	5.72951800	-6.90049400
C	-2.80423000	5.42894100	-8.08111000
C	-2.14546500	5.24097400	-9.27457400
C	-0.71588100	5.34250700	-9.33707000
C	0.02959200	5.58826800	-8.22356800
C	-0.59051200	5.80031500	-6.89464800
C	0.08623000	4.88225900	-5.84656700
H	-2.70753700	5.02549600	-10.17636200
H	-0.23127600	5.21595200	-10.30037500
H	1.11293000	5.64601100	-8.28727900
H	-0.34956300	6.85236200	-6.54401200
H	1.12101400	5.17843000	-5.60277700
N	-2.82111200	5.96424600	-5.83818600
O	-0.42594200	3.89068700	-5.38938500
C	-4.32522000	1.43502800	-6.25512600
C	-4.45743200	-0.75669900	-5.75113200
C	-3.80807400	-0.13626500	-4.73017000
H	-4.72218000	-1.79193200	-5.89933500

H	-3.39533200	-0.52759600	-3.81353300
C	-5.46908800	-0.02277900	-7.93375100
C	-3.11572000	2.25019400	-4.22392500
N	-3.73540800	1.20552000	-5.05493500
N	-4.76760700	0.22542900	-6.67856100
Au	-4.41270500	3.28902100	-7.07750100
H	-2.30842700	2.74290000	-4.76930800
H	-2.71537000	1.78166800	-3.32362300
H	-3.86837400	2.99166800	-3.94633600
H	-4.89127300	-0.71456900	-8.55310800
H	-5.58473700	0.92468000	-8.46064600
H	-6.45578000	-0.44854600	-7.73109500
H	-5.64522600	5.51109100	-11.76956100
H	-6.12788600	6.95683400	-10.81984000
H	-6.99407600	5.42031900	-10.58607800
C	-5.16025100	6.13646600	-5.25481600
C	-4.79913200	6.85022000	-4.09047400
C	-6.49021400	5.69323200	-5.40579800
C	-5.75556000	7.12493500	-3.11787200
H	-3.78073900	7.20002400	-3.96835400
C	-7.43349500	5.96005500	-4.42089900
H	-6.77780400	5.14109300	-6.29118300
C	-7.07095400	6.68100500	-3.27688600
H	-5.46856900	7.68992500	-2.23599600
H	-8.45439300	5.60998200	-4.54482500
H	-7.81419900	6.89479600	-2.51308500
N	-0.52659900	8.46232800	-5.66416600
S	-0.69933500	8.11557600	-4.08367700
S	-1.08423600	9.80659200	-6.40311700
C	0.65580200	9.09663200	-3.24246000
C	-2.84567200	9.37521600	-6.87546200
F	0.41371400	10.40344300	-3.29193500
F	1.82892800	8.84229400	-3.83587500
F	0.72612400	8.70914600	-1.96119000
F	-3.56606600	9.00238600	-5.81571800
F	-2.85373200	8.36572900	-7.77307000
F	-3.42035700	10.44028500	-7.44163700
O	-0.25669400	6.71932100	-3.93331200
O	-1.94619400	8.55535800	-3.44757000
O	-1.21363100	10.97750800	-5.53564200
O	-0.39593100	9.89131200	-7.69205800

$TS_{Kp1\text{-}Gp2}$ $E_{M06(dichloroethane)}$ = -3203.224906

C	-4.11610900	5.78317700	-6.08126700
C	-4.20232400	5.38931600	-7.50597300
C	-5.25788400	5.90504500	-8.42123300
O	-6.25694200	6.51550300	-8.10655400
O	-4.97210800	5.59087100	-9.71435100
C	-5.90880700	6.09685400	-10.67951600
C	-2.04914600	5.57666500	-6.70236900
C	-2.77390000	5.37296200	-7.91056000
C	-2.08844700	5.26365700	-9.10688300
C	-0.66886600	5.36242800	-9.12890700
C	0.05244700	5.51278900	-7.97136200
C	-0.60096100	5.64678200	-6.67358700
C	0.12571500	4.88816100	-5.56248700
H	-2.63476700	5.12395600	-10.03275200
H	-0.15622500	5.30451800	-10.08400200
H	1.13830800	5.54993900	-8.00214200
H	-0.46861500	6.82457600	-6.33562100
H	1.17204700	5.21028500	-5.40884500
N	-2.84097700	5.81333500	-5.64191500
O	-0.35574500	3.96458100	-4.95064200
C	-4.39364400	1.34898700	-6.33903300
C	-4.56821900	-0.86116000	-5.93406500
C	-3.83670500	-0.31340600	-4.92738100
H	-4.87647900	-1.87897400	-6.11525200
H	-3.38383100	-0.76304400	-4.05764000
C	-5.68125700	0.01368700	-8.01365100
C	-3.04412100	2.02207900	-4.34238100
N	-3.73816500	1.04057100	-5.19091600
N	-4.90175100	0.17597600	-6.79097200
Au	-4.46331800	3.24549500	-7.06521300
H	-2.26519400	2.54307800	-4.90252500
H	-2.59075100	1.49269000	-3.50301700
H	-3.76095600	2.75612200	-3.96775000
H	-5.14467900	-0.62970700	-8.71682100
H	-5.83053600	0.99584600	-8.46287400
H	-6.65270100	-0.43000200	-7.77864100
H	-5.53080800	5.77325500	-11.65011600
H	-5.95994000	7.18804400	-10.63085200
H	-6.90688400	5.68788800	-10.49808900
C	-5.18618300	6.09940500	-5.13513000
C	-4.85708800	6.86089000	-3.99431200
C	-6.51210700	5.66056900	-5.30953600
C	-5.84015700	7.18001800	-3.06194700
H	-3.84033000	7.21276400	-3.86135600
C	-7.48439900	5.97117600	-4.36483600
H	-6.77563100	5.07750600	-6.18350400
C	-7.15269400	6.73470100	-3.24048700
H	-5.57797900	7.78069100	-2.19578300
H	-8.50347000	5.62217200	-4.50665600
H	-7.91670700	6.98266700	-2.50813200
N	-0.61203600	8.23080100	-5.74587200
S	-0.67351600	8.22763500	-4.10242000
S	-1.06438600	9.46710400	-6.71892400
C	0.63786600	9.48131800	-3.58021700
C	-2.91849600	9.26025200	-6.94869800
F	0.10800600	10.68914000	-3.43071800
F	1.61764400	9.52566000	-4.48725600
F	1.14456400	9.07455000	-2.40962200
F	-3.54192900	9.06858900	-5.78896100
F	-3.15790100	8.20399200	-7.74867600
F	-3.40078300	10.35637700	-7.53832600
O	-0.12593200	6.92050000	-3.72156800
O	-1.92462300	8.71161900	-3.51700700
O	-0.90409400	10.77528100	-6.08596300
O	-0.50755100	9.17129500	-8.03878900

$TS_{Fp\text{-}Lp}$ $E_{M06(dichloroethane)}$ = -1375.938101

C	-4.31393500	5.33298300	-6.33114500
C	-4.57016400	4.09972400	-7.05746000
C	-4.71517500	4.26823000	-8.53409900
O	-5.70554600	3.78052600	-9.05728100
O	-3.77616600	4.97808200	-9.12656000
C	-3.91442300	5.16054300	-10.55876700
C	-2.73621900	4.19302500	-4.82004800
C	-1.53470900	3.50772100	-5.13318200
C	-0.95074400	2.67541400	-4.17035400
C	-1.52609300	2.51123300	-2.91164400
C	-2.72665600	3.16849900	-2.61797600
C	-3.34185100	3.98699300	-3.56252800
C	-0.96313300	3.57034300	-6.49023500
H	-0.03260400	2.15027300	-4.42373000
H	-1.04829400	1.88216400	-2.16736300
H	-3.18858600	3.04882500	-1.64196300
H	-4.25586600	4.52203600	-3.32578200
H	0.01741900	3.06333500	-6.60908300
N	-3.24606500	5.19860100	-5.61227500
O	-1.51376800	4.10075100	-7.43927900

C	-5.12810100	0.22030100	-5.96794900
C	-5.80399200	-1.92242300	-6.15351400
C	-5.17031100	-1.79463100	-4.95674500
H	-6.27824400	-2.77458300	-6.61538200
H	-4.97433200	-2.51661300	-4.17920100
C	-6.38019000	-0.39876900	-8.05999500
C	-3.99639000	0.07523100	-3.74781500
N	-4.76939000	-0.47553800	-4.85878500
N	-5.76628800	-0.68075100	-6.76003100
Au	-4.78644100	2.19960900	-6.41575300
H	-4.25242100	-0.46289300	-2.83299600
H	-4.24102500	1.13014400	-3.62891900
H	-2.92502500	-0.01853000	-3.94377800
H	-6.01789400	-1.12103000	-8.79546700
H	-6.10814300	0.60826000	-8.37704900
H	-7.46803800	-0.46984000	-7.97870800
H	-2.99667500	5.65597700	-10.86970200
H	-4.78760700	5.78402100	-10.76519800
H	-4.02518100	4.19215800	-11.05194400
C	-4.92364600	6.63476600	-6.60803800
C	-6.15755700	6.70018300	-7.27988700
C	-4.30719100	7.81598800	-6.15784100
C	-6.75811500	7.93558900	-7.51089600
H	-6.65402300	5.79185500	-7.60904200
C	-4.90807000	9.04564200	-6.40085100
H	-3.35668300	7.75529300	-5.63766500
C	-6.13294800	9.10740600	-7.07688800
H	-7.71338800	7.98367300	-8.02430800
H	-4.42572400	9.95847100	-6.06506000
H	-6.60133700	10.07004700	-7.25996700

Lp $E_{M06(dichloroethane)}$ = -1375.983572

C	-4.08380100	5.24389600	-6.12483800
C	-3.73903000	4.20778000	-7.19468700
C	-4.44987400	4.38768800	-8.51278000
O	-5.66237500	4.33001500	-8.57459400
O	-3.63970600	4.56590300	-9.56365300
C	-4.30791500	4.66983100	-10.84181400
C	-2.81580800	4.08516700	-4.48490100
C	-1.63013600	3.68932600	-5.20015300
C	-0.62580800	2.91699200	-4.54445200
C	-0.84282800	2.42825000	-3.27664900
C	-2.04623400	2.75149300	-2.60402500
C	-2.99541500	3.57777800	-3.17836400
C	-1.40618300	4.03001100	-6.54981300
H	0.29458600	2.68840600	-5.07559700
H	-0.09286100	1.81674200	-2.78626000
H	-2.20817700	2.37667600	-1.59716900
H	-3.88019200	3.88607700	-2.63169000
H	-0.39815300	4.00448400	-6.96390600
N	-3.66502700	5.06427800	-4.91774800
O	-2.28267100	4.34759100	-7.43169000
C	-5.08287300	0.38709000	-6.09980800
C	-6.36973600	-1.46423800	-6.03759600
C	-5.37785500	-1.62597200	-5.12353200
H	-7.18210200	-2.11447100	-6.32317300
H	-5.16219300	-2.44052500	-4.44959600
C	-7.02280800	0.30832400	-7.69256500
C	-3.45839000	-0.22317900	-4.29954700
N	-4.59647600	-0.48361400	-5.17842700
N	-6.17452000	-0.22536100	-6.62456000
Au	-4.36118400	2.23999700	-6.58908200
H	-3.79654600	0.23759400	-3.36722100
H	-2.76338600	0.45268300	-4.79854100
H	-2.95264700	-1.16610900	-4.08111500
H	-6.86443100	-0.26158300	-8.61221500
H	-6.76923100	1.35474700	-7.86528300
H	-8.07076500	0.23644400	-7.39187900
H	-3.51081200	4.79928800	-11.57283600
H	-4.98443900	5.52800600	-10.84374300
H	-4.87926800	3.76043300	-11.04368100
C	-4.84343900	6.47176100	-6.41190000
C	-5.68793000	7.00095700	-5.41837900
C	-4.68284000	7.16874000	-7.62323200
C	-6.37696700	8.18792100	-5.64432700
H	-5.80454100	6.46141800	-4.48466400
C	-5.35493800	8.36934400	-7.83290100
H	-4.00142700	6.80007000	-8.38329800
C	-6.21086400	8.87532900	-6.85060300
H	-7.04255600	8.57946500	-4.88101900
H	-5.21048000	8.91181700	-8.76225500
H	-6.74570700	9.80451500	-7.02399600

TS_{Lp-Ap} $E_{M06(dichloroethane)}$ = -1375.961998

C	-3.86094800	5.13105100	-6.11237700
C	-3.31289900	4.78351700	-7.44402800
C	-3.78297900	5.39798000	-8.76432100
O	-4.19136600	4.76977300	-9.71804500
O	-3.60846400	6.71149700	-8.70324100
C	-3.97010500	7.45897000	-9.89263700
C	-2.32916700	3.77606800	-4.86337000
C	-1.87774400	2.91633000	-5.91972800
C	-1.20385100	1.71301100	-5.62526300
C	-0.85969000	1.42169500	-4.31732200
C	-1.21010200	2.30982800	-3.27783600
C	-1.94142500	3.45391600	-3.54109000
C	-2.07265500	3.35801700	-7.27733000
H	-0.90122400	1.05784500	-6.43772000
H	-0.29952000	0.51949600	-4.09272800
H	-0.92369900	2.07712200	-2.25669300
H	-2.27140500	4.11202600	-2.74418900
H	-1.76559800	2.75446700	-8.13319000
N	-3.27658700	4.76056300	-5.00467100
O	-1.90653100	4.72748800	-7.46781700
C	-6.00837900	1.46503300	-7.47952100
C	-7.64365700	0.00363900	-7.96956600
C	-7.93753600	0.56016400	-6.76332400
H	-8.16702600	-0.73691200	-8.55410100
H	-8.77149300	0.40276200	-6.09725900
C	-5.78075100	0.22909600	-9.64681500
C	-6.85584400	2.31238500	-5.28908800
N	-6.92273800	1.45483100	-6.47787700
N	-6.45784400	0.57573000	-8.39603500
Au	-4.37326000	2.66544700	-7.51695000
H	-6.90175000	3.36317100	-5.58606300
H	-5.92237800	2.12843400	-4.75288700
H	-7.69990000	2.07675300	-4.63990900
H	-6.52461100	0.12496200	-10.43936600
H	-5.23316100	-0.71011600	-9.53043900
H	-5.08868300	1.02986700	-9.90945500
H	-3.73575900	8.49587100	-9.65844500
H	-5.03677100	7.33338900	-10.09363100
H	-3.38806500	7.10513200	-10.74615400
C	-5.13327900	5.89182200	-5.99637800
C	-5.33099300	6.70249800	-4.86563600
C	-6.16173800	5.79533300	-6.95186100
C	-6.51836100	7.41227100	-4.70523800
H	-4.54192000	6.76975500	-4.12514900
C	-7.35479400	6.49730300	-6.77901300
H	-6.05613400	5.15618700	-7.82324200

C	-7.53511400	7.31215500	-5.65926500
H	-6.65072400	8.04555700	-3.83302000
H	-8.14271300	6.40553900	-7.52104700
H	-8.46108800	7.86475500	-5.53052100

PQ'p $E_{M06(dichloroethane)}$ = -935.650385

C	-3.40133300	4.94683400	6.12192900
C	-2.18346700	4.67319300	6.97041800
C	-2.39041300	4.00434400	8.30389000
O	-3.20437900	3.12211200	8.46701200
O	-1.55173600	4.46370700	9.24755600
C	-1.67133400	3.81499000	10.52754000
C	-2.21331800	4.50555100	4.14741700
C	-0.98780200	4.20660700	4.78537800
C	0.09906400	3.75536600	4.03477500
C	-0.00450300	3.62873000	2.64895200
C	-1.20741000	3.94840400	2.00931700
C	-2.30313300	4.37990500	2.75224800
C	-0.91587900	4.34919600	6.25060200
H	1.03242900	3.51468900	4.53867700
H	0.84948000	3.28914000	2.06992500
H	-1.28973200	3.85459500	0.93004400
H	-3.25028000	4.62003700	2.27954000
H	-0.15903000	3.76745900	6.77791500
N	-3.36788700	4.89330000	4.83229900
O	-1.14049500	5.64411000	6.83208100
H	-0.93699000	4.30143500	11.16964800
H	-2.68190300	3.94349800	10.92509900
H	-1.46016400	2.74577700	10.43639200
C	-4.65144500	5.37859200	6.78298200
C	-5.88743600	5.17903800	6.14571600
C	-4.62322300	6.03883200	8.02275600
C	-7.06631000	5.61459100	6.74295100
H	-5.90041500	4.67826200	5.18359300
C	-5.80491900	6.48267000	8.61445100
H	-3.67458900	6.23434100	8.51583400
C	-7.02972700	6.26671800	7.97997000
H	-8.01753700	5.44449600	6.24586000
H	-5.76774200	7.00099400	9.56864200
H	-7.95145300	6.60620300	8.44482300

$TS_{Ep1\text{-}Mp}$ $E_{M06(dichloroethane)}$ = -1375.925418

C	-4.38776100	5.90463300	-5.71332100
C	-4.45105100	5.05800900	-6.79643400
C	-3.88708400	5.55107100	-8.08376000
O	-2.71940500	5.39731800	-8.37606700
O	-4.81773500	6.11066300	-8.86812200
C	-4.35543500	6.53804900	-10.16872500
C	-3.11713400	7.93419900	-5.12619400
C	-3.46572900	9.31172300	-5.13349100
C	-2.69013500	10.26859400	-4.43908200
C	-1.59812800	9.81854900	-3.72918500
C	-1.26795400	8.43679600	-3.71122700
C	-2.00337700	7.48314200	-4.39501600
C	-4.62215000	9.42651500	-5.92181300
H	-2.96381100	11.31861500	-4.45867800
H	-0.98406600	10.51744400	-3.17155700
H	-0.40394400	8.11486300	-3.13729900
H	-1.73939600	6.43249400	-4.38638900
H	-5.12905400	10.34410800	-6.22316000
N	-3.89218300	7.17134900	-5.94687900
O	-5.08724000	8.32130300	-6.36454900
C	-5.99323700	1.26274700	-6.70809800
C	-6.62494300	-0.84406600	-7.21870500
C	-7.08768800	-0.56986900	-5.97074300
H	-6.70372200	-1.73400300	-7.82374100
H	-7.65880200	-1.17067300	-5.28006200
C	-5.28112000	0.38373100	-8.94546800
C	-7.04325600	1.42248300	-4.43837300
N	-6.68810300	0.72096500	-5.67271800
N	-5.96039400	0.28912900	-7.65407400
Au	-5.18881100	3.16129000	-6.77587900
H	-6.28539900	2.17416800	-4.21355100
H	-7.08782600	0.70019300	-3.62040300
H	-8.01521100	1.91161000	-4.54781200
H	-4.38612300	-0.24458500	-8.94554400
H	-4.99487100	1.42097300	-9.11898700
H	-5.95926400	0.05741800	-9.73779300
H	-5.23748400	6.92818000	-10.67533300
H	-3.93328400	5.69267200	-10.71818400
H	-3.59242900	7.31385600	-10.06416200
C	-4.82505100	5.56468500	-4.32902500
C	-4.34998600	4.40592500	-3.69538000
C	-5.70412200	6.41005100	-3.63719300
C	-4.76518900	4.08940300	-2.40077300
H	-3.64480300	3.76431100	-4.21620600
C	-6.11972100	6.09089900	-2.34422200
H	-6.08304000	7.30458500	-4.12373500
C	-5.65365700	4.92900400	-1.72373300
H	-4.38137700	3.19608600	-1.91573800
H	-6.81190700	6.74615800	-1.82334000
H	-5.97456600	4.68417000	-0.71543300

Mp $E_{M06(dichloroethane)}$ = -1375.945061

C	-3.00135900	4.47753000	-6.10010100
C	-3.36873100	3.92421500	-7.37918100
C	-2.66739900	4.49872800	-8.55109300
O	-1.72761700	3.86370000	-8.98723600
O	-3.17084100	5.62511300	-9.03174100
C	-2.49683500	6.16622600	-10.19868500
C	-1.74268600	6.21774100	-5.06924800
C	-0.36201500	6.45908700	-4.83286700
C	0.02925700	7.39701900	-3.87570800
C	-0.92798200	8.09899100	-3.14193000
C	-2.28751200	7.85146200	-3.36335700
C	-2.70042400	6.90865400	-4.30186600
C	0.61783500	5.62138700	-5.54016300
H	1.08833000	7.55696700	-3.69044700
H	-0.62001700	8.82197200	-2.39362700
H	-3.03618500	8.39565200	-2.79542000
H	-3.75486700	6.74004400	-4.49043000
H	1.67716400	5.93885800	-5.46560300
N	-2.11213600	5.44037300	-6.15169100
O	0.30456700	4.62646900	-6.17301600
C	-5.59607800	0.54681500	-7.80019300
C	-6.66366900	-1.36380300	-7.25702500
C	-6.71809800	-1.23326800	-8.61062800
H	-7.04514100	-2.13489500	-6.60575200
H	-7.16727300	-1.86143200	-9.36430500
C	-5.63550300	-0.06104500	-5.36857400
C	-5.92891800	0.46063200	-10.28491500
N	-6.05699100	-0.06134700	-8.92380100
N	-5.97796300	-0.26456100	-6.77821700
Au	-4.51083300	2.29083000	-7.62504000
H	-5.15323700	1.22625900	-10.30014800
H	-6.87802700	0.89439600	-10.61143600
H	-5.64504700	-0.35218200	-10.95703800
H	-4.67744400	-0.53650400	-5.14179300
H	-6.41883700	-0.50052300	-4.74786800
H	-5.56665300	1.00663800	-5.15734300

H	-3.08629100	7.03307800	-10.49257400
H	-2.46957600	5.42092800	-10.99712400
H	-1.47841600	6.45735400	-9.93224000
C	-3.53771900	3.88889600	-4.83760200
C	-2.63799200	3.36231100	-3.90047400
C	-4.91645800	3.83465800	-4.58769300
C	-3.11557900	2.77700400	-2.72798200
H	-1.57178600	3.39981700	-4.10652300
C	-5.38930800	3.26369800	-3.40463500
H	-5.61334300	4.24780100	-5.31217600
C	-4.48982300	2.73001600	-2.47667700
H	-2.41552400	2.36003900	-2.01009300
H	-6.45700700	3.24186000	-3.20536800
H	-4.85873300	2.28388700	-1.55765500

TS_{Mp-Np} $E_{M06(dichloroethane)}$ = -1375.946191

C	-3.83721900	5.06223300	-7.34329500
C	-3.94531400	4.02222100	-8.36447700
C	-4.21641100	4.46136200	-9.75357600
O	-5.39427200	4.51807900	-10.05630400
O	-3.17694800	4.69521800	-10.53635800
C	-3.49978800	5.07187200	-11.90147500
C	-1.48569100	5.77170300	-6.98818700
C	-1.00339700	5.23527900	-5.75991000
C	0.17296400	5.77390800	-5.21162400
C	0.86622800	6.80724900	-5.83458700
C	0.39831400	7.30577000	-7.05406700
C	-0.75192800	6.77788700	-7.63593200
C	-1.60907700	4.10426300	-5.03667700
H	0.54633700	5.36079700	-4.27742100
H	1.76874300	7.20893600	-5.38568300
H	0.93698100	8.10034700	-7.56148100
H	-1.11465600	7.14463700	-8.59033200
H	-1.05639800	3.81818500	-4.11838900
N	-2.62404300	5.32641700	-7.64743700
O	-2.61222800	3.48446600	-5.35745600
C	-4.00225200	0.10024200	-7.24580700
C	-4.07379300	-2.15381200	-7.21221400
C	-4.12573500	-1.72176900	-5.92405000
H	-4.07534200	-3.15029300	-7.62611800
H	-4.18965600	-2.26983000	-4.99684400
C	-3.92117500	-1.07118800	-9.46622700
C	-4.17484400	0.52174300	-4.78186900
N	-4.07693100	-0.34102800	-5.96311100
N	-3.99888300	-1.02435000	-8.00697700
Au	-3.94548400	2.07060200	-7.83961000
H	-3.55121200	1.40696600	-4.91430300
H	-3.83061300	-0.04001500	-3.91133300
H	-5.21369500	0.82737700	-4.62909100
H	-4.79395200	-1.59488400	-9.86501800
H	-3.00860000	-1.58975100	-9.77212800
H	-3.90491200	-0.05198800	-9.85114800
H	-2.53791700	5.20973200	-12.39251200
H	-4.07918400	5.99794600	-11.90812600
H	-4.07466400	4.27675400	-12.38193400
C	-4.76982900	5.46472400	-6.31721500
C	-6.07534300	4.94383500	-6.37292700
C	-4.40817800	6.37089300	-5.30261700
C	-7.00608800	5.30982300	-5.40504100
H	-6.34915800	4.27146600	-7.18125700
C	-5.34475100	6.73322300	-4.34269300
H	-3.40402000	6.78094200	-5.27292500
C	-6.63992900	6.19997600	-4.39089800
H	-8.01549900	4.91259700	-5.44472500
H	-5.07353300	7.43067100	-3.55626500
H	-7.36788700	6.48822600	-3.63808200

Np $E_{M06(dichloroethane)}$ = -1375.958352

C	-4.27711500	5.66029700	-6.75996700
C	-3.82196100	4.72460500	-7.78526100
C	-3.71511900	5.24963300	-9.18829400
O	-4.57875100	5.03178400	-10.01031100
O	-2.58829000	5.94393600	-9.41567900
C	-2.44173200	6.45232800	-10.76264600
C	-1.84324900	5.53783800	-5.93759500
C	-1.83009100	5.06247200	-4.60323000
C	-0.62006900	5.12613300	-3.89363600
C	0.54403100	5.61569300	-4.48176000
C	0.51744800	6.04031100	-5.81239900
C	-0.67209600	5.99927100	-6.54115700
C	-2.96941700	4.40231500	-3.93358400
H	-0.59752200	4.76587700	-2.86787200
H	1.46686400	5.65489400	-3.91212000
H	1.42200700	6.40996500	-6.28541600
H	-0.72028600	6.33112400	-7.57258100
H	-2.76368600	4.11726600	-2.88115900
N	-3.00023100	5.55913600	-6.72951900
O	-4.04806900	4.13482100	-4.43891700
C	-4.67463800	0.72986700	-7.16272700
C	-5.22959000	-1.21741700	-6.16281800
C	-5.07555700	-1.46875000	-7.48838100
H	-5.49661600	-1.86838600	-5.34474800
H	-5.17702500	-2.38279200	-8.05278600
C	-5.06781700	0.79747400	-4.68068900
C	-4.45789900	-0.12137800	-9.51319900
N	-4.73917700	-0.26567500	-8.08518500
N	-4.98127700	0.13285300	-5.98111800
Au	-4.22379500	2.71176200	-7.48308600
H	-4.47391000	0.93686300	-9.77426500
H	-5.22592200	-0.64522300	-10.08720800
H	-3.47523700	-0.54044300	-9.74748000
H	-4.36143600	0.33430200	-3.98599400
H	-6.08269600	0.69945500	-4.28551800
H	-4.82597000	1.85434100	-4.79106300
H	-1.47653900	6.95744000	-10.77916200
H	-3.25022700	7.15062900	-10.99212100
H	-2.46283000	5.62782300	-11.47924000
C	-5.39789400	6.26894100	-6.13895900
C	-6.66207500	6.04989200	-6.72319400
C	-5.25927200	7.07356200	-4.98893500
C	-7.78636100	6.63198700	-6.14887300
H	-6.73436900	5.43391500	-7.61507100
C	-6.38841500	7.65202000	-4.42831300
H	-4.27675900	7.22996200	-4.55456000
C	-7.64725000	7.42902400	-5.00683000
H	-8.76648300	6.47232200	-6.58644000
H	-6.30045800	8.27408500	-3.54334500
H	-8.52699200	7.88453500	-4.56139300

TS_{Np-Op} $E_{M06(dichloroethane)}$ = -1375.949706

C	-4.55827900	5.68818600	-7.19589200
C	-3.95530800	4.39360900	-7.45294700
C	-3.60637800	4.08737700	-8.88841000
O	-2.51991700	4.26528000	-9.38598200
O	-4.67008000	3.54946200	-9.51575700
C	-4.44570500	3.16863300	-10.89090200
C	-2.54864400	5.77188500	-5.75368500
C	-3.27144000	5.93404700	-4.54721200
C	-2.57664000	6.07936600	-3.32708300
C	-1.19096900	6.04051300	-3.30718400

C	-0.48854800	5.84751600	-4.50843100
C	-1.15678600	5.71697000	-5.72676600
C	-4.70597100	5.85328100	-4.53600000
H	-3.13990300	6.21323000	-2.40654600
H	-0.65224400	6.15542800	-2.37262300
H	0.59676700	5.80919800	-4.49299900
H	-0.62228500	5.58177800	-6.66123800
H	-5.21760400	5.93871000	-3.56687600
N	-3.20521500	5.66261300	-6.98718800
O	-5.43806800	5.65846200	-5.53088600
C	-4.54336000	0.97969200	-5.17652600
C	-4.24142900	-1.02852900	-4.18689100
C	-5.51879200	-0.63989900	-3.93924500
H	-3.70066300	-1.91447900	-3.89187700
H	-6.31315100	-1.12413700	-3.39258000
C	-2.27230800	-0.06634900	-5.40487600
C	-6.95116300	1.32350300	-4.56702500
N	-5.68483400	0.59255900	-4.54856700
N	-3.66006400	-0.02624900	-4.94546200
Au	-4.24542300	2.69668300	-6.27517000
H	-6.75693100	2.36837800	-4.81057200
H	-7.41726500	1.26125600	-3.58090100
H	-7.62290900	0.89662800	-5.31708000
H	-2.09706400	-0.99144600	-5.95986700
H	-1.59424800	-0.01861700	-4.54829500
H	-2.09086500	0.78609900	-6.05924100
H	-5.39274400	2.75475600	-11.23594400
H	-3.65050200	2.42121500	-10.95086100
H	-4.16360200	4.04205200	-11.48427700
C	-5.39349500	6.65104700	-7.88727000
C	-5.10428000	8.02341400	-7.81146400
C	-6.48747400	6.18778800	-8.63599900
C	-5.91280700	8.93131100	-8.48690000
H	-4.24310000	8.36165000	-7.24228700
C	-7.29319700	7.10410500	-9.30642500
H	-6.67555500	5.12086700	-8.69943100
C	-7.00723900	8.47125200	-9.22964500
H	-5.69293300	9.99344800	-8.44249500
H	-8.13840600	6.75709500	-9.89271900
H	-7.63556000	9.18310600	-9.75714200

Op $E_{M06(dichloroethane)}$ = -1375.961167

C	-4.15987700	5.72567400	-7.32206400
C	-3.75448600	4.31988900	-7.55171500
C	-3.84340400	3.86900400	-8.98490600
O	-4.81526300	3.25252200	-9.38045800
O	-2.78722400	4.19393800	-9.73346800
C	-2.86661200	3.78907900	-11.11753400
C	-2.06352100	5.48772100	-6.09093700
C	-2.72492900	5.87055300	-4.88605500
C	-2.01536800	5.94572100	-3.65775400
C	-0.67697000	5.61462300	-3.62910800
C	-0.03549900	5.21038900	-4.82267800
C	-0.70829500	5.15243800	-6.04010100
C	-4.11002900	6.09639700	-4.93918400
H	-2.53557700	6.25863000	-2.75606500
H	-0.11496100	5.66621900	-2.70289600
H	1.01744700	4.94481600	-4.79039100
H	-0.20646700	4.85624500	-6.95483400
H	-4.68339000	6.35250900	-4.04784700
N	-2.75034700	5.45352300	-7.29556500
O	-4.82724100	6.01914700	-5.99975800
C	-4.59246600	1.11511700	-5.06634600
C	-4.63462300	-0.43848700	-3.42561100
C	-5.53678500	-0.81401200	-4.36838900
H	-4.34715600	-0.90277600	-2.49496300
H	-6.19518500	-1.66747300	-4.41818700
C	-3.01367800	1.45669900	-3.15066700
C	-6.34574000	0.10936000	-6.55803400
N	-5.49680900	0.14640900	-5.36521900
N	-4.06731600	0.74553700	-3.86884900
Au	-4.14147400	2.75195300	-6.23085800
H	-6.01500900	0.87568600	-7.25975500
H	-7.38674300	0.29575700	-6.28015800
H	-6.26240500	-0.87205200	-7.03122800
H	-2.09462500	0.86366800	-3.14877700
H	-3.33045100	1.64121900	-2.12056500
H	-2.82722700	2.40770400	-3.65053500
H	-1.93306100	4.12180600	-11.57012600
H	-3.72380500	4.26657600	-11.59893100
H	-2.97065600	2.70348200	-11.19073600
C	-4.72222200	6.67043200	-8.31927200
C	-4.03030600	7.84192100	-8.64785800
C	-5.95332900	6.37839900	-8.92148200
C	-4.57501000	8.72767200	-9.57607600
H	-3.06369000	8.04127800	-8.19432800
C	-6.49454100	7.26940000	-9.84676800
H	-6.46365100	5.45100400	-8.67964900
C	-5.80755500	8.44313000	-10.17146600
H	-4.03928900	9.63500900	-9.83850700
H	-7.44589200	7.04577300	-10.31985300
H	-6.22982500	9.13378900	-10.89568700

TS_{Op-Pp} $E_{M06(dichloroethane)}$ = -1375.945076

C	-4.31352600	5.77463300	-7.40448800
C	-3.88025500	4.40074500	-7.66105700
C	-4.20518900	3.84144700	-9.02836100
O	-3.39095000	3.46961000	-9.84087300
O	-5.54239900	3.75733700	-9.18015000
C	-5.98265800	3.21958200	-10.44398900
C	-1.88810400	5.34155800	-6.57787800
C	-2.44797900	5.38700200	-5.24765200
C	-1.58724500	5.34588600	-4.10353900
C	-0.22889700	5.36078300	-4.28185000
C	0.31900300	5.44135600	-5.59506100
C	-0.48405000	5.46936200	-6.71570000
C	-3.78393300	5.72454900	-5.10011100
H	-2.02507800	5.35153100	-3.10902500
H	0.43660100	5.34425800	-3.42491700
H	1.39827200	5.46638700	-5.71358400
H	-0.07084700	5.49610300	-7.71793700
H	-4.24686700	5.88458200	-4.13162900
N	-2.62786200	5.16519800	-7.70199500
O	-4.56487700	6.11617000	-6.09060200
C	-4.66233200	1.22818100	-5.04762300
C	-5.66996700	-0.50672500	-4.01189100
C	-4.39056700	-0.44870800	-3.55928400
H	-6.47814400	-1.17831800	-3.76665400
H	-3.86265100	-1.06561300	-2.84869200
C	-7.06836100	0.80955100	-5.62604300
C	-2.38360800	0.98959700	-4.04083900
N	-3.79042000	0.62242400	-4.19969900
N	-5.81794800	0.52679000	-4.92176400
Au	-4.27708800	2.83435400	-6.28016900
H	-2.27162400	2.06438400	-4.19195200
H	-1.76708400	0.45609900	-4.76950700
H	-2.06085000	0.73167600	-3.02999500
H	-7.84360800	1.09061000	-4.90808500
H	-7.38594300	-0.07753700	-6.18002900
H	-6.90423800	1.63129600	-6.32321400

H	-7.07090400	3.20443500	-10.39080000
H	-5.58359400	2.21261700	-10.59033300
H	-5.64598900	3.86164600	-11.26234000
C	-4.77801400	6.78682800	-8.36056600
C	-4.30814200	6.77657800	-9.68736500
C	-5.70733600	7.76355900	-7.95943700
C	-4.77872400	7.71950400	-10.59589900
H	-3.55555500	6.05909000	-9.99358100
C	-6.18073800	8.69356100	-8.88145800
H	-6.07036700	7.78457400	-6.93804500
C	-5.71932500	8.67490100	-10.19998300
H	-4.40324400	7.71272300	-11.61459000
H	-6.90764500	9.43649100	-8.56765600
H	-6.08511200	9.40670600	-10.91408000

Pp $E_{M06(dichloroethane)}$ = -1375.952380

C	-4.40566800	3.11269300	-9.62647900
C	-3.71275100	1.90511200	-9.15566700
C	-4.22377100	0.58685000	-9.70477800
O	-3.53869100	-0.31288400	-10.12727100
O	-5.57559400	0.52764600	-9.59678100
C	-6.17549000	-0.68081300	-10.10224900
C	-1.58668000	2.98359500	-8.86239500
C	-2.09124600	3.93099100	-7.85788100
C	-1.15447600	4.51919200	-6.93882900
C	0.18559100	4.34702000	-7.12968300
C	0.69085700	3.57147600	-8.23329900
C	-0.15644200	2.93391900	-9.08609800
C	-3.42851400	4.24642700	-7.79265000
H	-1.52847500	5.16338900	-6.14738500
H	0.89152600	4.83430100	-6.46367400
H	1.76494400	3.48754200	-8.36676000
H	0.19684900	2.30212900	-9.89379200
H	-3.83638600	4.92914900	-7.05757000
N	-2.32396900	2.07719300	-9.45304800
O	-4.25669600	4.20711700	-8.91354700
C	-4.55006600	1.08007600	-5.05267300
C	-5.56103000	0.28318900	-3.19950600
C	-4.30450800	0.66160400	-2.84882600
H	-6.36286500	-0.13896200	-2.61369600
H	-3.79291600	0.62401800	-1.89953500
C	-6.92085600	0.30141200	-5.30984800
C	-2.30927600	1.59918400	-4.05406300
N	-3.70082400	1.15119300	-3.99519600
N	-5.69299500	0.54433900	-4.55312000
Au	-4.16554300	1.64197300	-6.99363100
H	-2.17725700	2.25823300	-4.91312300
H	-1.63986300	0.74006900	-4.15243400
H	-2.07102800	2.14617000	-3.13910400
H	-7.68669600	1.02856700	-5.02584000
H	-7.28007200	-0.70932700	-5.10173600
H	-6.70605800	0.39649300	-6.37468900
H	-7.24512200	-0.57271600	-9.92320200
H	-5.77600900	-1.55262200	-9.57804200
H	-5.97435800	-0.78553700	-11.17212000
C	-5.14876600	3.28957900	-10.85325200
C	-4.94180700	2.41624400	-11.94479300
C	-6.05849600	4.36423900	-10.98083500
C	-5.63921500	2.61313000	-13.12956700
H	-4.20684900	1.62135500	-11.87848900
C	-6.76678600	4.53625500	-12.16227100
H	-6.21512400	5.03644200	-10.14443700
C	-6.55811600	3.66319500	-13.23711100
H	-5.46351200	1.95323600	-13.97312500
H	-7.47897900	5.35037100	-12.25202000
H	-7.10828300	3.80614900	-14.16252800

TS_{Pp-Qp} $E_{M06(dichloroethane)}$ = -1375.952372

C	-0.22360700	2.04455700	-0.64764400
C	0.45983500	0.76510500	-0.88884000
C	0.02284900	-0.00553600	-2.11950200
O	0.75855500	-0.53585900	-2.91626900
O	-1.33162400	-0.07408400	-2.17073900
C	-1.86421900	-0.77560200	-3.31112100
C	2.52577600	1.43808900	0.13173500
C	1.91810400	1.65552600	1.45110000
C	2.76306300	1.60290100	2.61185500
C	4.11929800	1.54564200	2.46506700
C	4.72989600	1.52227900	1.16177300
C	3.96884100	1.49459700	0.03342200
C	0.56486900	1.88560900	1.57386700
H	2.31069000	1.69238100	3.59602400
H	4.75714600	1.55804900	3.34391900
H	5.81304600	1.50948700	1.09000000
H	4.40134800	1.42481700	-0.95876600
H	0.07971000	2.03223200	2.53102200
N	1.86074400	1.03689700	-0.92443600
O	-0.16196400	2.53201000	0.57045700
C	-0.65274700	-2.22690500	1.94979600
C	-1.76229900	-3.91643500	2.95205200
C	-0.52852300	-3.84618200	3.51630800
H	-2.59398900	-4.57542200	3.14765200
H	-0.07018000	-4.43983200	4.29202600
C	-3.00319300	-2.63857100	1.18116300
C	1.52813900	-2.44316600	3.16480600
N	0.13585400	-2.80277900	2.89368700
N	-1.81923800	-2.91925800	1.99270100
Au	-0.15217000	-0.65992600	0.71384000
H	1.68714900	-1.39369200	2.91308400
H	2.20227300	-3.06342300	2.56766500
H	1.73488700	-2.59495400	4.22638200
H	-3.76047400	-2.12913800	1.78370200
H	-3.40961600	-3.57819500	0.79968800
H	-2.71640500	-2.00237300	0.34321500
H	-2.94689400	-0.75251700	-3.18836700
H	-1.49358100	-1.80350100	-3.33352100
H	-1.57223700	-0.27192900	-4.23693300
C	-0.86298100	2.90675700	-1.61459200
C	-0.55609300	2.79022900	-2.98912000
C	-1.77362400	3.89899100	-1.18382800
C	-1.15789900	3.64148900	-3.90666900
H	0.18211400	2.07060700	-3.32616100
C	-2.38508800	4.72921500	-2.11322400
H	-2.00696500	3.99150000	-0.12886400
C	-2.07866000	4.60250300	-3.47373100
H	-0.90583400	3.56262200	-4.95935200
H	-3.09787400	5.47809900	-1.78280000
H	-2.55369900	5.25903200	-4.19680300

Qp $E_{M06(dichloroethane)}$ = -1375.973619

C	-4.30632400	5.87897100	-7.14465500
C	-3.25369700	4.91994100	-7.56323700
C	-3.66194100	3.91182900	-8.60170600
O	-4.81787100	3.53350400	-8.68124800
O	-2.65466400	3.47968400	-9.35090600
C	-2.98356600	2.43633700	-10.29645100
C	-1.53681200	5.62415200	-6.06279300
C	-2.31728600	5.82886800	-4.88418500
C	-1.68732900	6.36635900	-3.75707800
C	-0.33540000	6.70574800	-3.78374700

C	0.42878200	6.50829300	-4.94484200
C	-0.16090300	5.94971400	-6.06639500
C	-3.73759400	5.38711800	-4.83938400
H	-2.26565400	6.51807100	-2.84971500
H	0.12946400	7.12383300	-2.89574500
H	1.48043800	6.77606500	-4.95739600
H	0.40587700	5.75881800	-6.97178800
H	-4.22063300	5.78329500	-3.94552600
N	-2.02006500	4.98701000	-7.17990300
O	-4.45287100	6.18756400	-5.91010800
C	-4.52823500	1.29284400	-5.07574500
C	-4.50396900	-0.94114700	-4.74688100
C	-5.53702000	-0.66111400	-5.58391300
H	-4.14903400	-1.87841100	-4.34730300
H	-6.26031200	-1.30784200	-6.05569600
C	-2.75198300	0.39750900	-3.54902100
C	-6.50761900	1.44135500	-6.59132200
N	-5.53397700	0.70938200	-5.77652400
N	-3.89682400	0.26748300	-4.44828200
Au	-4.11482900	3.31476200	-4.99287900
H	-5.98872300	2.13737400	-7.25213300
H	-7.19539200	1.99111200	-5.94374900
H	-7.07076000	0.72371700	-7.19045000
H	-1.96996600	-0.30492000	-3.84819100
H	-3.05796000	0.18857200	-2.52007300
H	-2.36631800	1.41502600	-3.61256900
H	-2.05385300	2.22153800	-10.82105000
H	-3.75397700	2.78374700	-10.98936100
H	-3.34545000	1.55150700	-9.76645700
C	-5.08874400	6.62827000	-8.10424800
C	-4.70665200	6.69456800	-9.46331100
C	-6.23868300	7.32495100	-7.66706300
C	-5.46372700	7.43578200	-10.36070600
H	-3.80417500	6.19908800	-9.80608600
C	-6.99497100	8.05212300	-8.57523400
H	-6.53110300	7.26894500	-6.62450800
C	-6.60924500	8.10888700	-9.92059200
H	-5.16228000	7.49569400	-11.40147500
H	-7.88559700	8.57506200	-8.24172500
H	-7.20213000	8.68185400	-10.62748100

TS_{Qp-Ap} $E_{M06(dichloroethane)}$ = -1375.970052

C	-3.53066500	6.27894400	-7.87263700
C	-2.76777900	5.00512500	-8.11988900
C	-2.80853600	4.38228400	-9.49865900
O	-3.25598500	3.27385200	-9.71646300
O	-2.31790000	5.21545700	-10.41150900
C	-2.36205900	4.75695200	-11.78404300
C	-2.11306800	4.67647900	-5.88000000
C	-2.95018200	5.68425300	-5.32847100
C	-3.08757100	5.80286600	-3.93928300
C	-2.35676000	4.96862800	-3.09734900
C	-1.49409300	4.00150400	-3.63468200
C	-1.38094700	3.84845100	-5.01198100
C	-3.62827100	6.59997900	-6.26011100
H	-3.73847100	6.56913000	-3.52663000
H	-2.44383000	5.08032000	-2.02101200
H	-0.91914600	3.36292500	-2.97120900
H	-0.74257400	3.08773600	-5.44945400
H	-4.41541500	7.26450500	-5.89675500
N	-2.09155100	4.35752800	-7.23591300
O	-2.76830400	7.23983600	-7.18805300
C	-6.47849200	3.09531600	-6.53639500
C	-6.97894100	0.91506000	-6.65083000
C	-8.12859400	1.58787900	-6.37484800
H	-6.79315600	-0.13826300	-6.79154600
H	-9.13712200	1.23585200	-6.22336100
C	-4.55913400	1.56825200	-7.03880700
C	-8.75784300	3.99457900	-5.99426600
N	-7.80219200	2.93218400	-6.31045300
N	-5.97198300	1.85748900	-6.74759200
Au	-5.37081300	4.75435000	-6.60264400
H	-8.32706400	4.95549000	-6.27660600
H	-8.97889700	3.99207600	-4.92358700
H	-9.67670400	3.83105400	-6.56120400
H	-4.45232800	0.49272000	-7.18426200
H	-3.94125300	1.88513800	-6.19548700
H	-4.24089600	2.09465600	-7.94208100
H	-1.87107800	5.53722500	-12.36319900
H	-3.40306700	4.63675600	-12.09566200
H	-1.83610400	3.80482800	-11.88018000
C	-4.51929000	6.84006200	-8.85729700
C	-4.62604300	8.23091600	-8.98651400
C	-5.33642100	6.01060400	-9.64605800
C	-5.53842700	8.78426100	-9.88573200
H	-3.98521200	8.87344500	-8.39324500
C	-6.24199400	6.56980200	-10.54595500
H	-5.26749200	4.92967800	-9.57212600
C	-6.34869000	7.95803600	-10.66630100
H	-5.60869900	9.86374600	-9.98012300
H	-6.86299800	5.91861600	-11.15410600
H	-7.05511000	8.39155900	-11.36787500

PQp $E_{M06(dichloroethane)}$ = -935.645623

C	-3.36817900	6.29624200	7.86482500
C	-2.70516300	4.97476100	8.14607900
C	-2.63100400	4.48320900	9.57354200
O	-2.82263200	3.34328500	9.93005100
O	-2.32232500	5.50336500	10.39748900
C	-2.31761100	5.18338000	11.79843100
C	-2.23412200	4.55845500	5.90121500
C	-2.88997200	5.71662000	5.42465800
C	-3.02845100	5.91686800	4.05035600
C	-2.48264500	5.00347900	3.14666600
C	-1.80171900	3.87452100	3.61585700
C	-1.68412700	3.64961300	4.98499200
C	-3.42052500	6.67210000	6.41446100
H	-3.54831300	6.80102400	3.68902700
H	-2.58067200	5.17582100	2.07856600
H	-1.37315900	3.16696400	2.91185100
H	-1.18442000	2.76949700	5.37694800
H	-4.21419600	7.34783800	6.09567500
N	-2.16662100	4.21923800	7.25770800
O	-2.47230100	7.27428300	7.31283300
H	-2.03735000	6.10547500	12.30773800
H	-3.31417700	4.85784500	12.11137100
H	-1.59813300	4.38743200	12.00883000
C	-4.42716500	6.79228600	8.79744200
C	-4.45092000	8.13148400	9.19803100
C	-5.41190800	5.91118600	9.26434100
C	-5.44981000	8.58523200	10.06024700
H	-3.67878500	8.80187300	8.83514900
C	-6.40520400	6.36642700	10.13157000
H	-5.39809500	4.86834200	8.95567400
C	-6.42747300	7.70528000	10.53073200
H	-5.46039300	9.62673300	10.37061600
H	-7.16355500	5.67614600	10.49088400
H	-7.20260900	8.05998500	11.20462200

$TS_{Ep1L-FpL}$ $E_{M06(dichloroethane)}$ = -2348.612214

C	-3.02798900	5.02044400	6.56146800
C	-3.71890900	3.89803100	6.98356500
C	-3.90763700	3.60158900	8.43504300
O	-5.00588400	3.46627500	8.94248800
O	-2.72231400	3.44501500	9.04099200
C	-2.54961000	5.24191800	5.17293100
C	-2.65541300	6.50815900	4.57652700
C	-1.94192900	4.19715800	4.45922000
C	-2.18510300	6.71965300	3.28211500
H	-3.11152800	7.32394300	5.13012400
C	-1.45676000	4.41611900	3.17043000
H	-1.83309500	3.21873300	4.91757200
C	-1.58190700	5.67404900	2.57699200
H	-2.28419500	7.69999900	2.82510400
H	-0.98324000	3.59990900	2.63553600
H	-1.20454400	5.84296800	1.57231100
C	-2.61561700	2.88263100	10.41380300
C	-1.10416400	2.84952200	10.63285700
H	-0.68366300	3.85842500	10.56153200
H	-0.87840800	2.44885500	11.62605400
H	-0.61804200	2.21925600	9.88187400
C	-3.21210400	1.47412100	10.42301700
H	-4.29224100	1.50074900	10.27115900
H	-2.75801000	0.86365900	9.63528700
H	-3.00657900	0.99868000	11.38785200
C	-3.30133700	3.81411200	11.41566900
H	-3.11792800	3.44644700	12.43100600
H	-2.89228600	4.82609500	11.34111600
H	-4.37729100	3.85556700	11.24349300
C	-3.33868000	6.47858200	8.57617300
C	-2.39947300	6.96480500	9.53024900
C	-2.82188000	7.57570600	10.73174600
C	-4.17563600	7.67426200	10.97162100
C	-5.10764600	7.18152400	10.02150800
C	-4.72084200	6.59224700	8.83087500
C	-1.11102200	6.74353700	9.00985900
H	-2.08974700	7.94078900	11.44527100
H	-4.53770200	8.12309400	11.89022400
H	-6.16869500	7.26285100	10.23804000
H	-5.44058900	6.20816300	8.11831500
H	-0.17174800	7.08116200	9.45420900
N	-2.76353800	6.04810500	7.42423900
O	-1.05757700	6.14859600	7.88960200
C	-5.57630400	1.11077700	4.63807100
C	-5.93450800	-0.61645000	3.22643600
C	-7.10136600	-0.37431900	3.88219500
H	-5.67202900	-1.34524700	2.47609900
H	-8.06899600	-0.84649800	3.82169900
C	-3.63073800	0.40798300	3.29868000
C	-2.65126200	-0.13803100	4.14749200
C	-3.33364300	1.07717500	2.09573200
C	-1.31605000	-0.01142100	3.74177800
C	-1.98487500	1.16075600	1.73370300
C	-0.98703100	0.62296800	2.54680900
H	-0.52855100	-0.42709000	4.36293000
H	-1.70732300	1.65674800	0.80997300
H	0.05388700	0.69905100	2.24467100
C	-7.80213800	1.26830800	5.66698500
C	-8.53081400	2.39532900	5.25003400
C	-7.89473100	0.71647800	6.95637800
C	-9.40852000	2.96452500	6.18009100
C	-8.78749500	1.32470200	7.84608900
C	-9.53861500	2.43356700	7.46188600
H	-9.99079700	3.83697400	5.89907900
H	-8.88679500	0.93226600	8.85350700
H	-10.22582000	2.89070900	8.16833300
N	-6.85759100	0.68607600	4.74416300
N	-5.01383400	0.31063600	3.69914200
C	-8.35624200	3.01534200	3.86915800
H	-7.68546600	2.37701400	3.28482600
C	-7.03665700	-0.46022400	7.40560300
H	-6.47046100	-0.82529600	6.54234100
C	-4.42570200	1.74334800	1.26345800
H	-5.35492200	1.18050800	1.40740400
C	-2.99204000	-0.87010800	5.44115800
H	-4.06439400	-0.76377100	5.62965200
C	-4.13102400	1.74230600	-0.24499900
H	-3.29539600	2.40470600	-0.49754300
H	-3.89162900	0.73783500	-0.61043200
H	-5.00646000	2.10660500	-0.79294500
C	-4.67743900	3.18066000	1.76772800
H	-5.49955500	3.64068200	1.20688200
H	-4.93592300	3.19666700	2.83068300
H	-3.78327600	3.79932700	1.63861200
C	-2.69461700	-2.37620200	5.30763200
H	-3.24904500	-2.81735100	4.47194200
H	-1.62758700	-2.55501600	5.13277900
H	-2.97929500	-2.90487400	6.22442700
C	-2.26488400	-0.26569900	6.65705900
H	-1.17825900	-0.38472700	6.58098100
H	-2.48387100	0.80276200	6.75965700
H	-2.59104300	-0.76965400	7.57429200
C	-9.68923100	3.09689000	3.10358400
H	-10.15566900	2.10984500	3.01197300
H	-10.40311900	3.75914800	3.60584600
H	-9.52334500	3.49282900	2.09545100
C	-7.68667900	4.39951700	3.97598800
H	-8.31965600	5.10057600	4.53232800
H	-6.72169200	4.33234000	4.49143800
H	-7.51333600	4.81786100	2.97802000
C	-7.89207500	-1.63392800	7.91559400
H	-8.46200300	-1.35822100	8.80973600
H	-8.60550400	-1.96705200	7.15380700
H	-7.25182500	-2.48302900	8.17989800
C	-6.01200600	-0.01101500	8.46502600
H	-5.35670600	-0.84618300	8.74005500
H	-5.39240500	0.81114400	8.09428600
H	-6.51399200	0.33977300	9.37397000
Au	-4.65179400	2.54852200	5.77084200

$TS_{Ep1L\text{-}MpL}$ $E_{M06(dichloroethane)}$ = -2348.614853

C	-3.49938500	5.21328100	6.71182700
C	-3.88151400	3.93797900	7.05577700
C	-3.60954500	3.49874500	8.45357900
O	-4.40585100	3.72171700	9.34664100
O	-2.46208200	2.82500300	8.53540800
C	-3.75508900	5.86763500	5.39836400
C	-5.04477700	5.86985800	4.84682300
C	-2.71294700	6.50041500	4.70575500
C	-5.28243700	6.48186500	3.61611300
H	-5.85674600	5.38984200	5.38478600
C	-2.95219600	7.10762500	3.47307800
H	-1.70919500	6.49295300	5.12229000
C	-4.23767500	7.09977000	2.92545800
H	-6.28479800	6.47498700	3.19878300
H	-2.13467900	7.58183800	2.93755500
H	-4.42333200	7.57429200	1.96628500
C	-1.97021400	2.27585600	9.82404000
C	-0.65962100	1.60524300	9.41583100
H	0.02347100	2.33573600	8.97069700

H	-0.17704400	1.16290500	10.29321500
H	-0.84575700	0.81441700	8.68303800
C	-2.97007100	1.25486400	10.37039200
H	-3.90780500	1.73188600	10.65867000
H	-3.17914800	0.48985300	9.61633800
H	-2.53884400	0.76239300	11.24859000
C	-1.72263300	3.43469100	10.79286400
H	-1.23827100	3.05729900	11.69963100
H	-1.05855400	4.17352700	10.33054200
H	-2.65916100	3.92143600	11.07089400
C	-2.88112900	7.24775300	7.97539100
C	-1.62399700	7.81987800	8.31378000
C	-1.52711900	9.15199200	8.78075100
C	-2.68811600	9.88696800	8.87117600
C	-3.93878600	9.31255500	8.51173300
C	-4.06237900	8.00869400	8.06610400
C	-0.66474200	6.82020300	8.10030000
H	-0.56263600	9.57494600	9.04278100
H	-2.65714000	10.91609800	9.21246700
H	-4.83337900	9.92347500	8.58952900
H	-5.01830100	7.57224500	7.80268600
H	0.39963400	6.85873000	8.33285600
N	-2.80738400	5.92693000	7.66914200
O	-1.12664600	5.72371200	7.62432900
C	-5.67878800	1.09492700	4.73271500
C	-5.94756900	-0.68450800	3.36605800
C	-7.16463700	-0.38695100	3.89505500
H	-5.63357100	-1.45130700	2.67590600
H	-8.13433800	-0.83962600	3.76153500
C	-3.63125100	0.27653000	3.64428500
C	-2.79135300	-0.48547600	4.47516100
C	-3.15657600	1.12053700	2.62587600
C	-1.41481400	-0.40528300	4.23547400
C	-1.77101200	1.16357500	2.42960000
C	-0.91008100	0.40620600	3.22115100
H	-0.73120900	-0.97822100	4.85481500
H	-1.36304800	1.80352100	1.65303100
H	0.16190700	0.45363500	3.05103100
C	-7.99858700	1.36546700	5.50998300
C	-8.83287800	2.30029500	4.86781000
C	-8.07414900	1.07026800	6.88247400
C	-9.79241800	2.94327000	5.65695600
C	-9.05621500	1.74086000	7.62293400
C	-9.90499600	2.66392700	7.01882600
H	-10.45795600	3.67187400	5.20665800
H	-9.15524900	1.53539600	8.68418100
H	-10.65990500	3.17200000	7.61231300
N	-6.97880100	0.71215600	4.72442800
N	-5.05170100	0.23598800	3.89397600
C	-8.64992300	2.65515000	3.39484300
H	-8.20457600	1.79260100	2.88677600
C	-7.16043200	0.05430700	7.55869400
H	-6.37071500	-0.22304800	6.85407100
C	-4.08297100	1.99377700	1.78936700
H	-5.11688900	1.76704100	2.06956600
C	-3.32866300	-1.33263900	5.62217400
H	-4.42244300	-1.29599300	5.59760200
C	-3.94158200	1.69951800	0.28501100
H	-2.93714100	1.94264300	-0.07924800
H	-4.13045700	0.64281200	0.06591500
H	-4.65629900	2.30131300	-0.28757900
C	-3.84629600	3.48508600	2.09423500
H	-4.55170100	4.10724700	1.53252300
H	-3.98007500	3.70200000	3.15881300
H	-2.83173700	3.79175500	1.81499500
C	-2.91938700	-2.81018600	5.48559500
H	-3.25771200	-3.22975200	4.53182700
H	-1.83179400	-2.93254000	5.53767800
H	-3.35958500	-3.40226900	6.29573300
C	-2.88623300	-0.75238800	6.97923000
H	-1.79651600	-0.80060300	7.08952600
H	-3.18760500	0.29537800	7.08208400
H	-3.33263100	-1.32454900	7.80132400
C	-9.97127000	2.96765500	2.67412000
H	-10.70557400	2.16755200	2.81578200
H	-10.41781500	3.90382700	3.02730800
H	-9.79089900	3.08110500	1.59970700
C	-7.65766700	3.82784300	3.25393900
H	-8.04708100	4.71834500	3.76261600
H	-6.68470600	3.58813900	3.69267800
H	-7.50248700	4.07758400	2.19758900
C	-7.94115100	-1.22785500	7.90625600
H	-8.75142900	-1.01561100	8.61315900
H	-8.38702800	-1.67715300	7.01161300
H	-7.27682300	-1.96819000	8.36649100
C	-6.46324300	0.63816000	8.80070700
H	-5.74101100	-0.08474000	9.19679000
H	-5.92793800	1.56382500	8.56692800
H	-7.17820300	0.85989500	9.60081200
Au	-4.81171200	2.56202600	5.87769800

Ay $E_{M06(trifluoromethylbenzene)}$ = -1431.062971

C	-3.49174800	4.48103100	6.45207800
C	-2.80394900	4.80614200	7.48021000
C	-5.09465400	0.85861400	7.79594700
C	-5.70153900	-1.30663000	7.95193000
C	-6.31408800	-0.63464300	8.96152500
H	-5.72162100	-2.35083000	7.68075400
H	-6.97611400	-0.97838100	9.74114900
C	-4.15292500	-0.71092700	6.07290100
C	-6.41945700	1.75225600	9.73603400
N	-5.92962800	0.68990200	8.85312700
N	-4.95740900	-0.37613900	7.24788600
Au	-4.26153300	2.61420100	7.16497500
H	-5.72425400	2.59100500	9.72567300
H	-7.40414600	2.09000200	9.40135100
H	-6.49381300	1.36000400	10.75247900
H	-3.46707900	-1.52517900	6.31950800
H	-4.80551000	-1.01670600	5.25071200
H	-3.57870900	0.16570400	5.77330200
N	-2.34335000	5.12755200	8.63856000
C	-1.00923600	4.73032000	9.15555400
H	-1.08746200	3.77682200	9.68421100
H	-0.33956200	4.63441700	8.30045800
H	-0.64862600	5.50005300	9.83743400
S	-3.56956900	5.67217600	9.87430200
O	-4.67375800	4.71909700	9.80198900
O	-2.79422500	5.88317200	11.08824900
C	-4.08579900	7.23396700	9.14363200
H	-4.45708000	7.03929800	8.13537600
H	-4.88644300	7.62224100	9.77848900
H	-3.23009300	7.91106700	9.13986200
C	-3.76364800	5.11508200	5.16699600
C	-3.16443800	6.35103600	4.84747400
C	-4.63444700	4.51832400	4.23865600
C	-3.43310000	6.97013700	3.63208400
H	-2.47912500	6.81266400	5.55398500
C	-4.90396400	5.14412800	3.02316000
H	-5.10085900	3.56748500	4.47879500
C	-4.30487200	6.36818900	2.71741800

H	-2.96273000	7.91928800	3.39339000
H	-5.57973900	4.67586900	2.31404500
H	-4.51293400	6.85264600	1.76808400

$TS_{Ay\text{-}Ey1}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.555509

C	-2.53076500	3.17198800	8.51294100
C	-2.16124400	4.10884200	7.68307600
C	-1.65200400	6.10741200	9.83027600
C	-0.59782200	6.40315000	10.75939300
C	-0.88935900	7.00519700	12.01618100
C	-2.20259400	7.28018700	12.29505700
C	-3.24897300	6.97466500	11.36147200
C	-3.00815900	6.39464200	10.14018200
C	0.53621300	5.96120900	10.11256800
H	-0.09607100	7.23247600	12.72036300
H	-2.46938600	7.73774700	13.24228300
H	-4.27187500	7.20854100	11.64189700
H	-3.79882500	6.14859000	9.43972400
H	1.58670700	5.94771900	10.36769900
N	-1.15472800	5.56154100	8.71147200
O	0.22322600	5.45631100	8.91703000
C	-5.58528800	1.06901300	6.66693000
C	-7.10192700	-0.43974800	5.95404000
C	-7.37818600	0.74136200	5.34054600
H	-7.58621700	-1.40178500	5.89111900
H	-8.14732900	1.00710300	4.63222300
C	-5.39868500	-1.24294100	7.61541500
C	-6.35379400	3.05196900	5.35461100
N	-6.44210900	1.65464500	5.79125700
N	-5.99904600	-0.21940400	6.76224700
Au	-4.02816500	2.02821800	7.58517700
H	-5.49828900	3.19240600	4.69069900
H	-7.27288300	3.31174900	4.82692100
H	-6.23461700	3.70382300	6.22147800
H	-6.09276600	-1.51719900	8.41469900
H	-5.16134300	-2.12613100	7.01688500
H	-4.48265400	-0.84435700	8.05152700
N	-2.25439600	4.58313700	6.45290500
C	-1.18058000	4.40718300	5.46042600
H	-0.83140700	3.37405300	5.51739100
H	-1.58719600	4.59300300	4.46500700
H	-0.35098700	5.09119800	5.66900100
S	-3.57769300	5.66865900	6.08646300
O	-4.52547900	5.52526700	7.19071600
O	-3.95834500	5.38262300	4.70462000
C	-2.80837100	7.29404600	6.17534200
H	-2.38291200	7.41273200	7.17309800
H	-2.03762900	7.35821800	5.40471500
H	-3.59476000	8.02976700	5.98948600
C	-2.11472800	2.98591800	9.90975000
C	-0.75818100	2.82645300	10.23502100
C	-3.07388100	2.96473900	10.93435000
C	-0.36850400	2.67503700	11.56549800
H	-0.01844100	2.81941400	9.44100900
C	-2.67636200	2.83717400	12.26471100
H	-4.12499900	3.06814400	10.68052000
C	-1.32408000	2.69156700	12.58476000
H	0.68251400	2.54059400	11.80602200
H	-3.42499200	2.84156300	13.05172300
H	-1.01845700	2.57779400	13.62071000

$TS_{Ay\text{-}Ey2}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.538697

C	-1.77919400	2.72765800	8.00672400
C	-1.18174800	3.76219700	8.45142800
C	-3.20116000	2.20694700	10.79717400
C	-2.68784700	2.06524000	12.13486400
C	-3.42686100	2.55761700	13.24973700
C	-4.62230500	3.17815700	12.99309500
C	-5.11725900	3.33690500	11.65238600
C	-4.43826000	2.86857000	10.55692700
C	-1.48173400	1.42874100	11.94474600
H	-3.05273700	2.43930600	14.26152300
H	-5.21725200	3.56527200	13.81440900
H	-6.06168900	3.85354300	11.51017400
H	-4.80302800	3.00560400	9.54604600
H	-0.70487900	1.07636100	12.60876500
N	-2.37519200	1.65959000	9.90434600
O	-1.28359700	1.20411600	10.64182300
C	0.04383500	6.20503000	5.31288500
C	0.94593900	7.15402400	3.47837800
C	0.41536700	8.14840500	4.23769500
H	1.46836200	7.18410600	2.53481100
H	0.37566300	9.21484400	4.07922200
C	1.16664000	4.66100900	3.68770800
C	-0.86136800	8.27156900	6.40684500
N	-0.12947200	7.54992400	5.35988500
N	0.70662700	5.96839500	4.15245100
Au	-0.56549100	4.87918900	6.74459200
H	-0.69967400	7.79452500	7.37411700
H	-0.49332000	9.29858800	6.44383600
H	-1.93080300	8.27324400	6.17956500
H	0.94225800	4.55599300	2.62361500
H	2.24406000	4.56207900	3.84728700
H	0.64480500	3.88279000	4.24503400
N	-0.99316900	4.27963500	9.75921800
C	0.43159400	4.36796900	10.14915000
H	0.99876200	5.04962200	9.50561300
H	0.49917900	4.70340800	11.18655900
H	0.84536800	3.35993300	10.08332100
S	-1.85583800	5.78978300	9.91233900
O	-3.12371900	5.60404000	9.20643300
O	-0.96723500	6.90906200	9.56244000
C	-2.15722100	5.83034600	11.68440700
H	-2.77021700	4.97112400	11.95426800
H	-1.20727100	5.83313000	12.22074600
H	-2.69167700	6.76460200	11.87315400
C	-2.37092500	1.89024200	7.02134200
C	-1.97934500	0.54408600	6.88242300
C	-3.37675400	2.42574000	6.18760500
C	-2.57732700	-0.24840000	5.90967100
H	-1.22730500	0.13772400	7.55034400
C	-3.95950600	1.62487300	5.21070200
H	-3.67025000	3.46341600	6.31384200
C	-3.56202900	0.29061300	5.07239200
H	-2.28085400	-1.28709300	5.80125200
H	-4.72706800	2.03577500	4.56204200
H	-4.02445900	-0.33388500	4.31354400

Ey1 $E_{M06(trifluoromethylbenzene)}$ = -1830.582200

C	-2.51029900	3.47696600	8.68598700
C	-1.90899500	4.56340900	8.14185300
C	-1.55581300	6.17311500	10.07064800
C	-0.37952700	6.74257200	10.65690100
C	-0.47650700	7.53712800	11.83498300
C	-1.72579600	7.71789600	12.36773400
C	-2.89154700	7.14371500	11.75956100
C	-2.84008900	6.37449000	10.62060300
C	0.65100200	6.33130000	9.83693500
H	0.40917300	7.97352800	12.28359500
H	-1.84904000	8.31233600	13.26698700

H	-3.85640800	7.33101300	12.22091900
H	-3.71343400	5.95602800	10.13907500
H	1.71745200	6.51365700	9.83708200
N	-1.19724800	5.47760700	8.97959900
O	0.20291100	5.57141200	8.84065200
C	-5.38830900	1.26436100	6.71838400
C	-6.61917200	-0.48362600	5.98376700
C	-7.22294200	0.65402400	5.55217600
H	-6.87836300	-1.52157600	5.84330900
H	-8.11893000	0.80288300	4.96980500
C	-4.56112400	-1.03200200	7.30500300
C	-6.80446300	3.11970900	5.80735300
N	-6.45505200	1.71161000	6.00678300
N	-5.49996400	-0.09116200	6.69801100
Au	-3.93213100	2.39060300	7.66178400
H	-5.89930900	3.72602600	5.80131800
H	-7.31198000	3.22242700	4.84565200
H	-7.46997000	3.45659300	6.60747900
H	-5.11089000	-1.75465200	7.91352000
H	-4.00130900	-1.55964600	6.52742000
H	-3.86740300	-0.48028400	7.93942600
N	-1.97944300	5.01714100	6.79671600
C	-1.49991200	4.11734200	5.73087500
H	-2.18003300	3.27852800	5.55340700
H	-1.37865700	4.68276400	4.80296700
H	-0.52212700	3.74022900	6.03661000
S	-3.40088400	5.90629800	6.42351200
O	-3.93632700	6.38198000	7.70389000
O	-4.24246100	5.14466600	5.49027200
C	-2.73267500	7.31501200	5.52294600
H	-2.07487600	7.87015100	6.19291200
H	-2.19168700	6.95797500	4.64471200
H	-3.58369000	7.92726800	5.21555100
C	-2.18859900	3.08828200	10.07790300
C	-0.85591800	2.91717300	10.49826300
C	-3.21867000	2.88307400	11.01355200
C	-0.56442600	2.56669500	11.81629800
H	-0.05167100	3.03527500	9.77708100
C	-2.92323900	2.55929000	12.33677400
H	-4.25176000	2.99044600	10.69396700
C	-1.59578600	2.39818900	12.74329800
H	0.46888100	2.41972100	12.11876300
H	-3.73136300	2.41924600	13.04922500
H	-1.36810300	2.12780100	13.77025300

Ey2 $E_{M06(trifluoromethylbenzene)}$ = -1830.577895

C	-1.83537300	2.68403200	8.75372600
C	-1.34791100	3.95283700	8.77394100
C	-3.32676300	2.47667800	10.80859800
C	-3.40251600	1.49658700	11.85174500
C	-4.37361200	1.62488300	12.88647700
C	-5.21372600	2.70615500	12.82970900
C	-5.12317700	3.67196100	11.77207700
C	-4.19873300	3.58674100	10.75563800
C	-2.42467100	0.57581700	11.53509800
H	-4.43662600	0.88891800	13.68059900
H	-5.96968500	2.84383800	13.59579800
H	-5.81633800	4.50797400	11.77665800
H	-4.11069100	4.33197500	9.97383200
H	-2.09740400	-0.35126700	11.98604500
N	-2.34977400	2.12038500	9.96058500
O	-1.77915300	0.92613400	10.42394800
C	-0.40953400	6.17126500	5.43387300
C	-0.03606400	6.84354600	3.30911800
C	0.12900000	7.92351600	4.11611900
H	0.05110400	6.73858600	2.23872600
H	0.38570700	8.94615200	3.88665800
C	-0.62092600	4.42669800	3.64390400
C	-0.04570300	8.37863600	6.57790600
N	-0.10255500	7.49435400	5.41178900
N	-0.36656800	5.78003400	4.13235100
Au	-0.85901100	5.02802500	7.08825500
H	-0.20238700	7.79931500	7.48771300
H	0.93418700	8.86170200	6.61955200
H	-0.82593600	9.14062400	6.49805400
H	-1.42641000	4.44692800	2.90475600
H	0.28507200	4.02042800	3.18482100
H	-0.91727800	3.79420200	4.48106800
N	-1.14928600	4.51445500	10.10983000
C	0.24672800	4.29379600	10.55866600
H	0.97108600	4.75323200	9.87571400
H	0.38731500	4.69935000	11.56335900
H	0.41433800	3.21536900	10.59748400
S	-1.62408900	6.17300900	10.18720300
O	-2.93130900	6.24857900	9.52331000
O	-0.53494600	7.07212800	9.77860300
C	-1.88206600	6.37054700	11.96025000
H	-2.62066800	5.63668600	12.28499800
H	-0.93904400	6.25601800	12.49621700
H	-2.26090400	7.38695400	12.09214300
C	-1.95128000	1.79575000	7.57419600
C	-0.88040200	1.65505100	6.67689500
C	-3.13684800	1.08118300	7.33646400
C	-1.00843100	0.84748000	5.54623200
H	0.05241100	2.17166400	6.87891400
C	-3.26111700	0.27228900	6.20858300
H	-3.97311200	1.17710500	8.02489700
C	-2.19898700	0.15737200	5.30695100
H	-0.16985000	0.74199000	4.86355400
H	-4.18833200	-0.26417600	6.02929300
H	-2.29589200	-0.47662300	4.43046900

$TS_{Ey1-Fy1}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.571279

C	-2.30210900	2.78713700	8.91585200
C	-1.73539400	3.98392200	8.50802700
C	-1.57665800	5.22234000	10.65766100
C	-0.47566600	5.62173300	11.46734300
C	-0.67388300	6.09644900	12.78848400
C	-1.96211900	6.14872200	13.26474300
C	-3.05730600	5.75602400	12.44087800
C	-2.89711900	5.29748200	11.14861000
C	0.67001900	5.46273600	10.68470000
H	0.17281600	6.40003200	13.39564100
H	-2.15780900	6.49724500	14.27314900
H	-4.06237700	5.82496000	12.84689100
H	-3.72638200	5.02669400	10.50736500
H	1.69643800	5.72366000	10.94071300
N	-1.20267100	4.86988700	9.40832900
O	0.46081200	4.98592800	9.50737300
C	-5.32940300	1.04714000	6.71815000
C	-6.65740500	-0.44321500	5.66152900
C	-7.24907600	0.77649500	5.56449500
H	-6.95923800	-1.40971900	5.28894400
H	-8.17405400	1.07868500	5.09865500
C	-4.53490800	-1.33073900	6.66136100
C	-6.71021700	3.10227500	6.38068500
N	-6.42158100	1.67487400	6.21306300
N	-5.48550200	-0.25860900	6.37493000
Au	-3.79157200	1.91614300	7.79194000
H	-5.81341400	3.68431700	6.16703800

H	-7.50094500	3.38118900	5.68197900
H	-7.04279600	3.29768900	7.40356600
H	-3.82616600	-0.98402900	7.41363200
H	-5.07326600	-2.20083900	7.04519300
H	-3.99329800	-1.60761800	5.75229400
N	-1.79407500	4.49459300	7.18096800
C	-1.24573100	3.68490200	6.07919300
H	-1.90023500	2.85473300	5.79611000
H	-1.08492800	4.32235200	5.20584300
H	-0.27834500	3.29899100	6.40688800
S	-3.19734300	5.40320500	6.81344900
O	-3.88233300	5.66334200	8.08493300
O	-3.90837400	4.76182700	5.69799000
C	-2.50092300	6.94774900	6.20784400
H	-1.92732600	7.40072000	7.01773800
H	-1.86506200	6.73556800	5.34608400
H	-3.33688000	7.58640500	5.91310800
C	-1.90865000	2.20110600	10.20030600
C	-2.88251300	1.68159100	11.07890000
C	-0.55164300	2.12886800	10.58357700
C	-2.51682000	1.16070600	12.31649900
H	-3.92844400	1.71481500	10.78766600
C	-0.18702400	1.56950100	11.80548700
H	0.21195200	2.48587400	9.90010700
C	-1.16830900	1.09828600	12.68238000
H	-3.28137100	0.78724600	12.99149500
H	0.86305300	1.49724600	12.07444900
H	-0.88328700	0.66965800	13.63876800

$TS_{Ey1\text{-}My1}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.568904

C	-3.81137500	5.09126300	6.74654800
C	-2.89615000	4.70156100	7.70331800
C	-2.08617000	5.57783300	9.87873200
C	-2.35208100	5.17344600	11.21727300
C	-1.55806400	5.63812500	12.29392200
C	-0.50594100	6.47531300	11.99930700
C	-0.23908600	6.86112800	10.65494500
C	-1.00429700	6.43339400	9.58400100
C	-3.47158300	4.33736900	11.15153200
H	-1.77374900	5.32893400	13.31156100
H	0.13388700	6.84656400	12.79270500
H	0.60212700	7.52066000	10.46146800
H	-0.79771100	6.72408000	8.56007400
H	-4.03539400	3.89333800	11.97040000
N	-3.01717600	5.13030400	9.00274700
O	-3.90183100	4.12633000	9.95704100
C	-3.69810200	3.93859100	2.79729500
C	-3.25873900	2.89716400	0.84305500
C	-4.11179300	3.92071400	0.57593000
H	-2.81093400	2.16127100	0.19349900
H	-4.54451300	4.25889500	-0.35278200
C	-2.17928500	1.95621600	2.91340900
C	-5.21392000	5.73246000	1.91393700
N	-4.37277700	4.54402100	1.78360700
N	-3.01482400	2.92635400	2.20422500
Au	-3.72462500	4.46238600	4.79761100
H	-5.44992200	5.88793300	2.96685800
H	-4.68780700	6.61018100	1.52794200
H	-6.14002800	5.58432800	1.35303200
H	-1.44844300	1.54595700	2.21355800
H	-1.65550600	2.45688300	3.72721600
H	-2.79919100	1.14503100	3.30660500
N	-1.82633700	3.77135300	7.48139400
C	-2.19883600	2.35272600	7.33487700
H	-2.75424400	2.16951700	6.40849800
H	-1.30262100	1.72750300	7.34553200
H	-2.82020100	2.08309300	8.19235000
S	-0.54162300	4.31235600	6.49346300
O	-0.63564000	5.77461800	6.43645400
O	-0.48013300	3.50605700	5.26802000
C	0.89234400	3.87402400	7.49373600
H	0.83786900	4.42601300	8.43316400
H	0.89186200	2.79676100	7.66996900
H	1.77842700	4.16028100	6.92219700
C	-4.83830300	6.08764500	7.08964400
C	-6.17883400	5.86282700	6.71670600
C	-4.51529700	7.29392300	7.74436800
C	-7.17085500	6.78405000	7.04326600
H	-6.43411800	4.94665300	6.19158500
C	-5.50377900	8.23292200	8.02846100
H	-3.47923000	7.50966700	7.98524300
C	-6.83617800	7.97510100	7.69450300
H	-8.20362300	6.58149000	6.77450700
H	-5.23445000	9.16904500	8.50940900
H	-7.60667900	8.70488900	7.92561000

Fy1 $E_{M06(trifluoromethylbenzene)}$ = -1830.619450

C	-2.37928100	2.71355200	8.98009000
C	-2.23816700	4.18497200	8.83961700
C	-2.49941900	4.67241700	11.13859500
C	-1.56663800	5.01482200	12.14844400
C	-1.89208900	4.77366800	13.49346300
C	-3.10653100	4.19764700	13.85149800
C	-4.02765200	3.87515700	12.84939700
C	-3.73438000	4.11574100	11.50774900
C	-0.25248000	5.60323700	11.83646700
H	-1.16869300	5.03950500	14.26098100
H	-3.34092400	4.01309400	14.89484500
H	-4.98914700	3.44384300	13.11383700
H	-4.46905200	3.92028800	10.73270300
H	0.29382900	5.99625200	12.72012100
N	-2.26172400	5.02307900	9.80589100
O	0.25170800	5.67039300	10.72596300
C	-5.96474900	1.46548600	7.41471500
C	-7.81709200	0.30567700	6.85561300
C	-7.81652300	1.45807400	6.13203600
H	-8.51935700	-0.51299200	6.88368800
H	-8.52232700	1.83847100	5.41013100
C	-6.28970900	-0.75622700	8.53501900
C	-6.30216600	3.46846300	5.95266100
N	-6.67781000	2.15338200	6.48650700
N	-6.67581700	0.32850500	7.63543200
Au	-4.16747400	2.05644700	8.24270800
H	-5.31206600	3.42175400	5.49662200
H	-7.03267600	3.75800200	5.19632100
H	-6.28246200	4.20454700	6.75607400
H	-5.48997700	-0.40676600	9.18816800
H	-7.14907700	-1.04777500	9.14356000
H	-5.94055100	-1.61732100	7.95809600
N	-2.26055100	4.67852500	7.52439500
C	-1.68436700	3.89808800	6.41528400
H	-2.35728000	3.11683300	6.04718500
H	-1.44521000	4.57344600	5.59394100
H	-0.75850100	3.44336700	6.77540000
S	-3.58052100	5.73360500	7.14961000
O	-4.69877400	5.40108800	8.04193600
O	-3.74564500	5.64126800	5.69669700
C	-2.93650400	7.34766500	7.60083400
H	-2.64670900	7.29707900	8.65131300
H	-2.07839800	7.56041200	6.96096200

H	-3.73842300	8.07143400	7.43541600
C	-1.32801500	1.97072800	9.56557500
C	-1.47655000	0.56734500	9.78637500
C	-0.09498500	2.59365900	9.93561300
C	-0.45440800	-0.16908700	10.35605800
H	-2.40919100	0.09183300	9.49971500
C	0.92336300	1.84577900	10.50124800
H	0.03626300	3.66132700	9.79043400
C	0.74516300	0.47025900	10.71220600
H	-0.57212600	-1.23447300	10.52564800
H	1.85615300	2.32443100	10.78166000
H	1.54820200	-0.11164600	11.15632900

My1 $E_{M06(trifluoromethylbenzene)}$ = -1830.617012

C	-3.37612200	6.10137200	6.40776500
C	-2.36017400	5.56801300	7.36203300
C	-2.48133800	4.69756700	9.65213400
C	-2.79537900	3.32391900	9.84312600
C	-2.54651500	2.72940100	11.09401000
C	-1.96714100	3.44312000	12.13475400
C	-1.65042500	4.79203600	11.93577500
C	-1.91975700	5.41685600	10.72033300
C	-3.33519400	2.46877000	8.78062700
H	-2.80458200	1.68165200	11.23158400
H	-1.77156000	2.96597200	13.08930800
H	-1.20344500	5.36875900	12.74061600
H	-1.71231700	6.47375300	10.58447500
H	-3.70951600	1.48465300	9.13105800
N	-2.86569100	5.39960500	8.51663500
O	-3.36290000	2.73925800	7.58511100
C	-4.44909300	3.15641400	3.77632900
C	-4.26017600	1.19623800	2.68086200
C	-5.33891600	1.84824400	2.16900300
H	-3.83102200	0.23813000	2.43242400
H	-6.03258900	1.56920800	1.39121400
C	-2.55079600	1.69968500	4.47810500
C	-6.47849600	4.04081600	2.60396400
N	-5.43711600	3.04747600	2.85215900
N	-3.72979000	2.01131100	3.66179400
Au	-3.99956100	4.66856100	5.09687000
H	-6.28405700	4.91357600	3.22720400
H	-6.46396700	4.33640800	1.55163400
H	-7.45827500	3.62541300	2.85530900
H	-2.16573700	0.72530100	4.17290300
H	-1.78580300	2.46390900	4.32277400
H	-2.83723000	1.67754200	5.53158600
N	-1.10018600	5.16528600	6.91132600
C	-0.37198900	4.05397400	7.55401100
H	-1.01931600	3.17980800	7.60284100
H	0.49789200	3.80027700	6.94717500
H	-0.04457900	4.34385500	8.55400100
S	-0.55451500	5.66760600	5.36503200
O	-1.46452100	6.74587200	4.95952100
O	-0.34690000	4.48324800	4.53250300
C	1.04783800	6.40261700	5.73648900
H	0.88914300	7.24803500	6.40743500
H	1.70737000	5.65608600	6.18164000
H	1.45522200	6.73914400	4.77974000
C	-3.88390000	7.41878400	6.60395300
C	-5.04483900	7.83537000	5.90099200
C	-3.23934500	8.35411600	7.45940900
C	-5.54640200	9.11905900	6.05572800
H	-5.53755300	7.12632800	5.24358800
C	-3.73629500	9.63828900	7.60314900
H	-2.34711200	8.05419800	7.99718900
C	-4.89166400	10.02019700	6.90464000
H	-6.43873900	9.42650000	5.51995400
H	-3.23559900	10.34954900	8.25244400
H	-5.28057900	11.02781200	7.02192800

TS_{Fy1-Gy} $E_{M06(trifluoromethylbenzene)}$ = -1830.601665

C	-2.79281600	2.65088300	9.46287800
C	-2.57223200	4.07335000	9.00478900
C	-2.58978800	4.55151200	11.13237400
C	-1.83176000	4.98966300	12.25247300
C	-1.79948700	4.15472100	13.36287500
C	-2.52925300	2.93716100	13.44163500
C	-3.37364200	2.58059200	12.41955800
C	-3.44397900	3.38896700	11.23863700
C	-0.99825700	6.22393700	12.23889300
H	-1.16919700	4.43828200	14.20380100
H	-2.45444500	2.33197500	14.33913500
H	-4.01194400	1.70562900	12.50059700
H	-4.42980700	3.48843500	10.79058800
H	-0.46785100	6.41103500	13.19789200
N	-2.41331000	5.04205500	9.88604500
O	-0.88475600	6.98487600	11.30197300
C	-6.17144500	1.34375000	7.44181100
C	-7.88680800	0.26904000	6.44539200
C	-7.91941000	1.56421100	6.03408500
H	-8.52880600	-0.56579500	6.21074100
H	-8.59088600	2.07571400	5.36207200
C	-6.44346200	-1.08459900	7.99038600
C	-6.51115400	3.61610900	6.43764300
N	-6.86550300	2.20891500	6.65610000
N	-6.80752000	0.15321200	7.30505500
Au	-4.48721400	1.85766900	8.51344600
H	-5.70432200	3.70076100	5.70468700
H	-7.39038200	4.14590300	6.06750800
H	-6.18866700	4.07334000	7.37331800
H	-5.47212700	-0.94976900	8.46653000
H	-7.19169800	-1.32827300	8.74990300
H	-6.37986000	-1.89942800	7.26493700
N	-2.58175700	4.38518900	7.67950600
C	-2.23391400	3.43027200	6.61415500
H	-3.12149100	3.00205300	6.14300400
H	-1.64498300	3.94949900	5.85612000
H	-1.63393500	2.63401400	7.05651400
S	-3.43818200	5.84999800	7.19264500
O	-4.62131900	5.93969300	8.04790500
O	-3.56659500	5.70663800	5.74366100
C	-2.27973800	7.16355600	7.59695600
H	-2.03609400	7.08888000	8.65893600
H	-1.39814500	7.03648900	6.96583700
H	-2.78849900	8.10274700	7.36398000
C	-1.59465700	1.84948100	9.79102600
C	-1.72572000	0.47958400	10.09754600
C	-0.30269100	2.41757000	9.80713000
C	-0.61272200	-0.29154000	10.41344600
H	-2.71554300	0.03145500	10.08740800
C	0.81358100	1.63845700	10.10301800
H	-0.17005600	3.47112200	9.57765000
C	0.66295600	0.28413800	10.41172200
H	-0.73385700	-1.34473700	10.64912000
H	1.80183600	2.08864100	10.09252800
H	1.53381600	-0.32173900	10.64362200

Gy $E_{M06(trifluoromethylbenzene)}$ = -1830.635779

C	-2.48769600	2.61847100	9.70135800
C	-2.29903000	3.86169000	8.96671500

C	-2.80892000	4.63337300	10.92805700
C	-2.89813300	5.49159400	12.08214600
C	-2.58925300	4.91063200	13.29054600
C	-2.20038000	3.52537000	13.43627000
C	-2.25888400	2.66975000	12.38639900
C	-2.86862500	3.14787700	11.10817300
C	-3.11137000	6.95598000	11.97874600
H	-2.57350900	5.53971200	14.17910000
H	-1.85460700	3.18608100	14.40752500
H	-1.98617100	1.62256900	12.47577100
H	-3.95039200	2.94001200	11.27302700
H	-3.16738000	7.47502100	12.95975800
N	-2.59462200	5.00036400	9.69495200
O	-3.21898600	7.56893100	10.93611100
C	-6.17045700	1.75777000	7.70724800
C	-7.86403600	0.69426600	6.66731400
C	-8.20205600	2.00643500	6.76916500
H	-8.38924200	-0.14191500	6.23247100
H	-9.08368900	2.53681500	6.44446700
C	-5.89322200	-0.70968800	7.32234200
C	-7.13157300	4.07067600	7.74407700
N	-7.15226400	2.64356500	7.40588400
N	-6.61474500	0.55952900	7.24898500
Au	-4.39975600	2.17814500	8.64480600
H	-6.13450100	4.47480700	7.57098200
H	-7.84552200	4.58985000	7.10252000
H	-7.41608800	4.20967800	8.79057100
H	-4.94004000	-0.54813000	7.82591500
H	-6.48287500	-1.43781800	7.88557900
H	-5.70823300	-1.08889800	6.31382300
N	-1.89598600	4.06527600	7.69056200
C	-1.49481000	2.94828700	6.82433200
H	-2.33195900	2.25488700	6.66852100
H	-1.17650600	3.35199200	5.86493300
H	-0.66955500	2.41495800	7.29374400
S	-2.70835200	5.43139100	6.82363200
O	-4.12973200	5.34574600	7.16113900
O	-2.25803900	5.27705200	5.44425000
C	-1.98119400	6.92393700	7.51832200
H	-2.35000100	7.06001200	8.53476100
H	-0.89596800	6.81313700	7.48152100
H	-2.30431900	7.72549700	6.84802800
C	-1.49588200	1.48662700	9.68663700
C	-1.89440400	0.14685500	9.79801300
C	-0.12097900	1.77931900	9.68996900
C	-0.94655500	-0.87478200	9.88198700
H	-2.95379500	-0.09556300	9.82027400
C	0.82727200	0.75813000	9.76178100
H	0.20690400	2.81508100	9.63452800
C	0.41672300	-0.57336600	9.85614800
H	-1.27442500	-1.90711500	9.96392000
H	1.88504900	1.00450000	9.74950500
H	1.15327500	-1.36908100	9.91388100

Gy1 $E_{M06(trifluoromethylbenzene)}$ = -3657.877893

N	-3.93148800	0.87781200	-7.00558800
S	-2.59398200	0.16595500	-6.40870900
S	-4.90193800	0.25183700	-8.14461900
C	-1.36855600	0.15222700	-7.85149800
C	-6.20418500	-0.64768000	-7.14318200
F	-1.37713800	-1.02832600	-8.45749400
F	-1.68419000	1.11004100	-8.73257900
F	-0.15044900	0.39696700	-7.36102000
F	-5.65663600	-1.45063000	-6.22593500
F	-6.98991600	0.24760100	-6.50441400
F	-6.97513600	-1.37319300	-7.95585200
O	-2.04290400	1.13838600	-5.45393800
O	-2.75561300	-1.23264900	-5.99964900
O	-4.27325700	-0.77476300	-8.97536100
O	-5.63855700	1.36958000	-8.74037300
C	-5.02958000	3.83713800	-5.14615300
C	-4.04003900	4.22870100	-4.15154600
C	-2.80556800	3.94872900	-5.90879200
C	-1.73214600	3.92697200	-6.84573600
C	-2.06875300	4.04249300	-8.18289900
C	-3.41410000	4.17212300	-8.64361500
C	-4.46157700	4.05382100	-7.77282700
C	-4.16461500	3.67243500	-6.38644100
C	-0.32259900	3.79009000	-6.41803300
H	-1.25131900	4.04435300	-8.89911800
H	-3.59804200	4.32265100	-9.70219400
H	-5.49201400	4.05506400	-8.11014400
H	-4.08620600	2.52612300	-6.61259900
H	-0.18052900	3.64333900	-5.33025300
N	-2.75158500	4.20452000	-4.60658000
O	0.61979900	3.80435200	-7.18953800
C	-5.23969900	-0.10139800	-3.41014500
C	-5.98838600	-2.14569000	-2.81695800
C	-4.64873900	-2.11630900	-2.59940700
H	-6.71626900	-2.92797700	-2.66866200
H	-3.97405800	-2.86909200	-2.22309200
C	-7.69555500	-0.53468600	-3.68912300
C	-2.80637800	-0.44101800	-2.85236500
N	-4.20850300	-0.85549000	-2.95782200
N	-6.33663200	-0.89803100	-3.30548100
Au	-5.13753300	1.78035500	-4.20050500
H	-2.21050300	-1.02709500	-3.55280100
H	-2.46981700	-0.59791600	-1.82434200
H	-2.71713700	0.61225100	-3.10391700
H	-8.38281000	-0.79332600	-2.87916800
H	-7.98122800	-1.05989000	-4.60279900
H	-7.73448500	0.53905200	-3.87056900
N	-4.24922300	4.58747900	-2.83361800
C	-5.61413300	4.66187400	-2.28995800
H	-6.16252600	5.44912800	-2.80411800
H	-5.55039700	4.89521700	-1.22926100
H	-6.14393000	3.70974600	-2.42453700
S	-3.02446400	4.05831400	-1.66877400
O	-3.60716600	4.34589100	-0.35618100
O	-2.59532600	2.70011900	-2.00037300
C	-1.67622300	5.21334000	-1.95251500
H	-2.05148000	6.21942000	-1.75875900
H	-1.34607900	5.08920800	-2.98239100
H	-0.89765400	4.94388500	-1.23435500
C	-6.37228100	4.46075400	-5.37923700
C	-6.55033900	5.84455600	-5.21881100
C	-7.42755000	3.70917000	-5.92003200
C	-7.76760700	6.45113200	-5.53227000
H	-5.72220800	6.44912500	-4.85606000
C	-8.63952900	4.31830000	-6.24803300
H	-7.28615000	2.64830400	-6.10307400
C	-8.81947400	5.68835800	-6.04338700
H	-7.88758500	7.52173400	-5.38924400
H	-9.44307200	3.71926900	-6.66785200
H	-9.76587300	6.15966800	-6.29326600

$TS_{Gy1\text{-}Gy2}$ $E_{M06(trifluoromethylbenzene)}$ = -3657.872826

N	-3.87852200	0.97609000	-7.01213600
S	-2.55274700	0.23277700	-6.37847000
S	-4.83703500	0.30226800	-8.15533300

C	-1.30205800	0.19647200	-7.80614000
C	-6.15034800	-0.59604100	-7.16302900
F	-1.26339100	-1.01384400	-8.34743600
F	-1.63479400	1.09541800	-8.73729500
F	-0.10504800	0.50610200	-7.30467600
F	-5.61765800	-1.38343500	-6.22682200
F	-6.95829300	0.29912600	-6.55830400
F	-6.88911500	-1.33571100	-7.99201500
O	-2.01434800	1.18836000	-5.40645100
O	-2.77351200	-1.16187100	-5.99306500
O	-4.15998400	-0.73329200	-8.93204200
O	-5.57311100	1.39155000	-8.79617500
C	-5.00972900	3.80225700	-5.16760900
C	-3.99185800	4.21440300	-4.19088000
C	-2.80916900	3.94130000	-5.98101900
C	-1.76119000	3.92986600	-6.93759700
C	-2.12608100	3.99665300	-8.27780000
C	-3.47460200	4.07350000	-8.70570700
C	-4.50089800	3.96910400	-7.79368100
C	-4.16787400	3.66761300	-6.41817100
C	-0.34083800	3.84927300	-6.53721100
H	-1.32218400	4.00063000	-9.00875600
H	-3.69593600	4.17801300	-9.76245100
H	-5.53883400	3.94892500	-8.10580000
H	-4.04229000	2.42389700	-6.68356000
H	-0.17126600	3.75011200	-5.44783500
N	-2.72700900	4.19930400	-4.66673300
O	0.58605600	3.85819700	-7.32850600
C	-5.28303100	-0.10572100	-3.40889200
C	-6.07423200	-2.12783500	-2.79057200
C	-4.73654300	-2.11844000	-2.55921300
H	-6.81767900	-2.89398600	-2.63517400
H	-4.08003300	-2.87569200	-2.16027900
C	-7.73896100	-0.50313900	-3.72199800
C	-2.86155700	-0.48078900	-2.82878900
N	-4.27024500	-0.87167700	-2.93479300
N	-6.39471800	-0.88223900	-3.30335200
Au	-5.14914300	1.76744600	-4.22012500
H	-2.27224400	-1.08730800	-3.51776400
H	-2.53070100	-0.62906500	-1.79771700
H	-2.75243600	0.56764700	-3.09271400
H	-8.45366800	-0.78262300	-2.94356500
H	-7.99627600	-1.00077800	-4.65959300
H	-7.76888700	0.57580400	-3.87282900
N	-4.19002900	4.55985600	-2.86329400
C	-5.54990000	4.65676500	-2.31111200
H	-6.08333700	5.46269300	-2.81236400
H	-5.47476500	4.87617800	-1.24811300
H	-6.10287100	3.71912600	-2.45253400
S	-2.96602100	4.01353700	-1.71727900
O	-3.53044700	4.29656500	-0.39501100
O	-2.55030800	2.65313400	-2.05954000
C	-1.60754000	5.15427000	-2.00876100
H	-1.96613500	6.16250200	-1.79555200
H	-1.29999700	5.03955000	-3.04698000
H	-0.81859800	4.86561100	-1.30969800
C	-6.34132700	4.46392700	-5.38009800
C	-6.47106600	5.85569600	-5.24255400
C	-7.43713400	3.73894500	-5.87297100
C	-7.67632300	6.49628000	-5.53279200
H	-5.61448200	6.43904700	-4.91234100
C	-8.63836900	4.38082100	-6.17901600
H	-7.33617600	2.67010800	-6.03514300
C	-8.76758800	5.75957000	-5.99811500
H	-7.75721200	7.57276700	-5.40713400
H	-9.47358400	3.80033200	-6.56176500
H	-9.70515200	6.25716000	-6.22983500

Gy2 $E_{M06(trifluoromethylbenzene)}$ = -1830.243463

C	-5.06002000	3.87659200	-4.95066300
C	-3.78081700	4.29388300	-4.28883700
C	-3.15687300	3.82884800	-6.31099200
C	-2.38505500	3.61881800	-7.46908700
C	-3.05897300	3.28661300	-8.65728000
C	-4.44911200	3.16772600	-8.69257300
C	-5.21478000	3.35471300	-7.53130100
C	-4.56400800	3.65861400	-6.33968400
C	-0.91761600	3.74712600	-7.45094500
H	-2.46059600	3.13331700	-9.55034500
H	-4.94530600	2.92528400	-9.62859900
H	-6.29783700	3.26076400	-7.55586300
H	-0.48613600	4.00730600	-6.46274600
N	-2.71338700	4.21819200	-5.05420400
O	-0.19669100	3.58419800	-8.42363900
C	-5.10097500	-0.06624600	-3.42399000
C	-5.17090600	-2.31756400	-3.23669200
C	-4.85918800	-1.81243200	-2.01425600
H	-5.29818800	-3.33474000	-3.57294200
H	-4.66055300	-2.30477700	-1.07510700
C	-5.63388600	-1.34800600	-5.50726000
C	-4.49510800	0.50964100	-1.07658900
N	-4.82232200	-0.43581500	-2.14798300
N	-5.31667800	-1.23312900	-4.08699200
Au	-5.12262800	1.85110300	-4.15238600
H	-4.29868600	-0.05373000	-0.16252100
H	-5.33859200	1.18472500	-0.91434000
H	-3.61575600	1.09121500	-1.35799900
H	-6.59718300	-1.85048100	-5.63474900
H	-4.85249100	-1.91803500	-6.01784300
H	-5.68601000	-0.34673900	-5.93555900
N	-3.64059600	4.62223300	-2.92797300
C	-4.84409800	4.87967300	-2.12446200
H	-5.37187600	5.72872200	-2.55870900
H	-4.53955300	5.12218700	-1.10790400
H	-5.51899700	4.01352300	-2.10971400
S	-2.35542300	3.81102300	-2.09287900
O	-2.58610400	4.05365900	-0.66270300
O	-2.22925300	2.42268100	-2.56341900
C	-0.90698400	4.73178200	-2.62205400
H	-1.01289400	5.75590000	-2.26061100
H	-0.88348900	4.68735900	-3.71140700
H	-0.04314400	4.24054400	-2.16758500
C	-6.30343700	4.73036000	-4.83721300
C	-6.19802600	6.10363000	-5.12272800
C	-7.56611000	4.22130500	-4.50995800
C	-7.30968900	6.94174100	-5.05892900
H	-5.22611200	6.50950100	-5.39438000
C	-8.68613400	5.05610000	-4.45431200
H	-7.66815900	3.16261800	-4.28830600
C	-8.56214200	6.41944200	-4.72203700
H	-7.20004500	8.00127500	-5.27579300
H	-9.65538500	4.63738500	-4.19534200
H	-9.43140900	7.06975700	-4.67194600

Gy3 $E_{M06(trifluoromethylbenzene)}$ = -3657.909305

N	-0.45424600	3.99437700	-2.85103700
S	0.79137800	4.83598700	-2.05377100
S	-0.71470200	2.36507000	-2.71724600
C	2.35409100	4.33778800	-3.02885100
C	-1.99102000	2.26653800	-1.35278700

F	3.29403300	4.02458000	-2.13464200
F	2.12944400	3.28714900	-3.81426400
F	2.75947100	5.37175300	-3.75209400
F	-1.53235900	2.79416300	-0.23163400
F	-3.11939500	2.88977700	-1.71731000
F	-2.27811300	0.96475400	-1.15627800
O	0.56482500	6.24500100	-2.30775800
O	0.95012600	4.27048400	-0.72280000
O	0.45153000	1.66742000	-2.19852800
O	-1.40367600	1.92886800	-3.93032900
C	-4.57362200	4.22804700	-5.26485500
C	-3.61527400	4.80309300	-4.29342800
C	-2.36276400	4.36150300	-6.01290100
C	-1.27157500	4.20352200	-6.89095600
C	-1.54454000	3.76932000	-8.20189300
C	-2.84356900	3.49313900	-8.63124600
C	-3.92238100	3.62233300	-7.74682600
C	-3.67680300	4.04492000	-6.44331300
C	0.11879300	4.49984100	-6.52307000
H	-0.71393200	3.65973200	-8.89613500
H	-3.01978100	3.17899300	-9.65610300
H	-4.93743300	3.40085500	-8.06707300
H	-1.01022500	4.48060400	-3.62930300
H	0.84413000	4.35658300	-7.35682900
N	-2.35365600	4.79370400	-4.69230000
O	0.51315700	4.87549900	-5.43251400
C	-4.18224500	0.23868200	-3.91280400
C	-3.12372000	-1.73597000	-3.65320700
C	-3.90208200	-1.54402600	-2.55607000
H	-2.46644600	-2.54805300	-3.92161500
H	-4.05739400	-2.15469500	-1.68063100
C	-2.59050400	-0.39892900	-5.72475800
C	-5.40670700	0.30641600	-1.74553400
N	-4.55222100	-0.33479200	-2.73944300
N	-3.31690100	-0.64056700	-4.47682900
Au	-4.53682600	2.14272200	-4.56824900
H	-6.15679000	0.90914500	-2.25928500
H	-4.80363100	0.94949000	-1.10096900
H	-5.90190100	-0.46188800	-1.14758100
H	-2.27738300	-1.35846500	-6.14166900
H	-1.72495600	0.23474000	-5.52450200
H	-3.25019800	0.10829700	-6.43042000
N	-4.00471700	5.30793800	-3.05826500
C	-5.21116900	4.84131100	-2.36710100
H	-6.06519800	5.50009400	-2.55113400
H	-5.00248400	4.77056800	-1.29627300
H	-5.45957300	3.84256800	-2.73023400
S	-3.03864900	6.44379200	-2.18967600
O	-2.55061100	5.78418300	-0.97630400
O	-2.15062000	7.11017700	-3.12859100
C	-4.30096600	7.64694200	-1.70426700
H	-4.99740100	7.21170400	-0.98742100
H	-4.81663900	7.99045400	-2.60298200
H	-3.74923300	8.46863100	-1.24159400
C	-5.90550500	4.90156200	-5.45856700
C	-5.99016500	6.30318500	-5.38020300
C	-7.07304100	4.18549900	-5.75771600
C	-7.20459300	6.96199300	-5.57121800
H	-5.09005000	6.87770500	-5.17544100
C	-8.28784600	4.84319800	-5.96392800
H	-7.02442300	3.10126600	-5.81877900
C	-8.36080900	6.23343500	-5.86318800
H	-7.24594800	8.04623900	-5.50290500
H	-9.17951200	4.26585800	-6.19479900
H	-9.30735200	6.74536800	-6.01428300

$TS_{Gy3\text{-}Gy4}$ $E_{M06(trifluoromethylbenzene)}$ = -3657.905985

N	-0.61842900	4.34331800	-2.65237200
S	0.56220400	5.25448200	-1.84238100
S	-0.98260900	2.82614300	-2.13078700
C	0.78957300	6.69838100	-3.05778600
C	-0.31169500	1.77039600	-3.52264400
F	1.88291400	6.52308100	-3.77953400
F	-0.27246900	6.86067200	-3.85637500
F	0.92773000	7.79373000	-2.30619900
F	-0.91816400	2.07953200	-4.68004200
F	0.99637400	1.93735200	-3.64942500
F	-0.57755800	0.48223700	-3.24368700
O	-0.03967500	5.85806200	-0.65451500
O	1.83925200	4.55707200	-1.77997200
O	-2.43423800	2.65198200	-2.20163200
O	-0.23259000	2.45478200	-0.93886800
C	-4.47368600	4.31356100	-5.25364100
C	-3.60187300	4.82102000	-4.19609400
C	-2.24092000	4.54149100	-5.90766200
C	-1.12702300	4.43306300	-6.76920300
C	-1.37414000	4.15698800	-8.12725100
C	-2.66412500	3.95250800	-8.62013300
C	-3.75780600	3.98297500	-7.75101700
C	-3.53945800	4.26070100	-6.40215200
C	0.27345100	4.51590400	-6.34186100
H	-0.52436900	4.09229500	-8.80324500
H	-2.81581300	3.75509100	-9.67736300
H	-4.76626900	3.79307500	-8.10831500
H	-1.28367400	4.70473600	-3.55864300
H	1.00261300	4.48867100	-7.18319000
N	-2.30738300	4.87467700	-4.55490800
O	0.67289500	4.57246100	-5.19224800
C	-3.79489800	0.28899100	-4.04634400
C	-2.76201000	-1.70891900	-3.84865500
C	-3.36223900	-1.43616100	-2.66117100
H	-2.17207800	-2.55345400	-4.16862700
H	-3.40255300	-1.99844700	-1.74143800
C	-2.47339500	-0.47804300	-6.02098500
C	-4.67513700	0.48473000	-1.70839200
N	-3.99574600	-0.21384500	-2.80239300
N	-3.04480700	-0.64505900	-4.68856900
Au	-4.25851100	2.16572700	-4.68223500
H	-5.35109400	1.23199500	-2.12091900
H	-3.93648900	0.99692900	-1.08876900
H	-5.23569800	-0.24432000	-1.11817700
H	-2.42460200	-1.44968700	-6.51832800
H	-1.47252000	-0.04618500	-5.94193200
H	-3.10665200	0.19878900	-6.59540900
N	-4.00051900	5.33101700	-2.96379300
C	-3.10028800	6.21667300	-2.19419800
H	-2.51378700	5.66803900	-1.45886400
H	-3.69661400	6.97472400	-1.67999800
H	-2.43984800	6.71236300	-2.90269700
S	-5.31532200	4.72887900	-2.02256800
O	-5.85867800	3.51180300	-2.62563900
O	-4.86160700	4.73078300	-0.63389100
C	-6.54413700	6.03434800	-2.20725500
H	-6.87703900	6.06885400	-3.24377800
H	-6.09734500	6.98192200	-1.90076000
H	-7.36749200	5.77366900	-1.53785200
C	-5.84254300	4.90409400	-5.45147900
C	-5.93097600	6.27319300	-5.75927700
C	-7.02939900	4.16799900	-5.34833100
C	-7.16740900	6.89278200	-5.94042400

H	-5.01478500	6.85184600	-5.85020800
C	-8.26988800	4.78383300	-5.53120100
H	-6.97685900	3.11488000	-5.09392500
C	-8.34438500	6.14748600	-5.82236900
H	-7.21246700	7.95365900	-6.17239100
H	-9.17932700	4.19618800	-5.43840000
H	-9.31043600	6.62596900	-5.95935300

Gy4 $E_{M06(trifluoromethylbenzene)}$ = -1830.701042

C	-4.84113300	3.80957900	-4.73773700
C	-3.54979900	4.07217700	-4.11964600
C	-3.07495000	3.41698900	-6.23993200
C	-2.41142800	3.03284400	-7.41204900
C	-3.21900700	2.72231600	-8.51869000
C	-4.61304600	2.79887200	-8.44913300
C	-5.25576000	3.16209100	-7.26036500
C	-4.47526400	3.45577000	-6.14158000
C	-0.93624400	2.95434200	-7.51404100
H	-2.71996500	2.43149400	-9.43748300
H	-5.20556300	2.57469200	-9.33067300
H	-6.33848300	3.21756600	-7.19945700
H	-0.36960600	3.24364400	-6.60028400
N	-2.55136100	3.80904800	-5.00065300
O	-0.34606500	2.60013300	-8.51366300
C	-5.32895900	-0.23976800	-3.47976200
C	-5.38582800	-2.48807000	-3.62974300
C	-5.74321800	-2.15310900	-2.36278800
H	-5.28588900	-3.45123400	-4.10584400
H	-6.02411400	-2.76606300	-1.52032800
C	-4.67223000	-1.24144800	-5.68924300
C	-6.05062200	-0.01670200	-1.08513800
N	-5.70208500	-0.77100900	-2.28841100
N	-5.13922300	-1.30370300	-4.30258300
Au	-5.08302200	1.72290900	-3.98516900
H	-5.46809800	-0.38950600	-0.23913500
H	-7.11780900	-0.12416200	-0.87311700
H	-5.81724400	1.03519800	-1.24877400
H	-5.21718700	-1.97830400	-6.28316000
H	-3.60045700	-1.45324200	-5.73466400
H	-4.86243100	-0.24568600	-6.09103400
N	-3.32236000	4.54033400	-2.85042800
C	-4.42368500	4.65009800	-1.87399400
H	-5.00377700	5.56181300	-2.02984000
H	-3.99475400	4.63736800	-0.87346100
H	-5.08091500	3.78536300	-1.99634800
S	-1.74016300	5.08456200	-2.33798400
O	-1.78438500	5.14526500	-0.88677600
O	-0.75846200	4.25591000	-3.04422100
C	-1.68390400	6.75048700	-3.01505600
H	-2.48429400	7.33630800	-2.55896600
H	-1.79747500	6.69133200	-4.09970800
H	-0.70682300	7.16572900	-2.75436300
C	-6.00714100	4.73880000	-4.51612600
C	-5.78472500	6.12519100	-4.56253400
C	-7.31802100	4.27723800	-4.34150500
C	-6.83851900	7.02510800	-4.40955000
H	-4.77637100	6.49940100	-4.72703400
C	-8.37716900	5.17670100	-4.19899200
H	-7.51330500	3.20850700	-4.31442500
C	-8.14030800	6.55161000	-4.22506800
H	-6.64608600	8.09361200	-4.44393100
H	-9.38696200	4.80018400	-4.06413400
H	-8.96345200	7.25021000	-4.10907600
H	-1.58134500	3.73599500	-4.70830200

$TS_{Gy4\text{-}Ay}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.688524

C	-4.80172900	4.39096800	4.92993800
C	-3.58861200	4.53937200	4.24672100
C	-3.08348700	3.36947200	6.11900300
C	-2.45764000	2.61984700	7.13064300
C	-3.26012500	2.20264200	8.20151100
C	-4.62313800	2.52349200	8.26712800
C	-5.24128900	3.24186300	7.24297700
C	-4.47344100	3.65138200	6.14462200
C	-1.02422400	2.26157300	7.08905400
H	-2.78401100	1.62989300	8.99110600
H	-5.20485500	2.20845800	9.12785500
H	-6.29752300	3.48760000	7.28938000
H	-0.44059300	2.69602800	6.24494700
N	-2.56874700	3.93153200	4.96217900
O	-0.47894900	1.53892400	7.89852700
C	-5.15341100	0.09003200	3.57774700
C	-5.05948000	-2.06011800	4.22770700
C	-5.42812800	-2.04235500	2.91949200
H	-4.89751900	-2.88328000	4.90603600
H	-5.66099600	-2.84589500	2.23815800
C	-4.45404800	-0.31486600	5.94621000
C	-5.87730100	-0.26906200	1.19761800
N	-5.47916900	-0.71362800	2.53473500
N	-4.89879800	-0.74240400	4.61780000
Au	-5.03026300	2.09197200	3.58796500
H	-5.32576000	-0.84214200	0.44890300
H	-6.95141400	-0.41986100	1.06036300
H	-5.64159600	0.78980100	1.08915700
H	-4.99649700	0.58296100	6.24195300
H	-4.66058900	-1.11421700	6.65954600
H	-3.38313300	-0.10010800	5.93722100
N	-3.30450900	5.29791600	3.10163300
C	-1.94182800	5.84624100	2.94834200
H	-1.21521200	5.09115900	2.62785900
H	-1.95312700	6.64012100	2.19920500
H	-1.64549900	6.28302100	3.90406100
S	-4.05592400	4.87016700	1.59729000
O	-5.18546900	3.97757900	1.91714600
O	-3.01643800	4.44478200	0.66228200
C	-4.75480700	6.43732700	1.07224300
H	-5.50144000	6.73144100	1.81159400
H	-3.95668600	7.17680500	0.98528400
H	-5.21096000	6.25886300	0.09548600
C	-6.04901100	5.15164900	4.68723000
C	-5.99359800	6.53162100	4.43198600
C	-7.30370700	4.52658600	4.75122600
C	-7.16420600	7.26191500	4.22365900
H	-5.03001800	7.03211400	4.41071200
C	-8.47396400	5.25818400	4.54658100
H	-7.36106100	3.45861800	4.94743200
C	-8.40789100	6.62652800	4.27644700
H	-7.10637400	8.33075000	4.03716000
H	-9.43681500	4.75800800	4.59434300
H	-9.31857800	7.19597600	4.11681300
H	-1.64709600	3.75614000	4.59110500

PhC ≡ CNMeMs $E_{M06(trifluoromethylbenzene)}$ = -990.701103

C	-2.69395800	3.33151700	8.63747900
C	-2.99311900	3.65662800	7.50656700
N	-3.32711000	4.03683500	6.25601900
C	-2.42770000	3.69018100	5.14118200
H	-2.25345200	2.61244500	5.17679100
H	-2.92185700	3.94629100	4.20434500

H	-1.46621100	4.21501500	5.21450500
S	-4.27622500	5.47929700	6.13527000
O	-5.37533800	5.34770400	7.08339200
O	-4.49617400	5.69013200	4.70509100
C	-3.15576300	6.75700800	6.74917300
H	-2.83458800	6.47496500	7.75393400
H	-2.30561000	6.83481300	6.06820400
H	-3.71557600	7.69459800	6.77199700
C	-2.38544100	2.94277500	9.97349300
C	-1.10498100	2.45866500	10.30724400
C	-3.36217100	3.04447400	10.98487900
C	-0.81543100	2.08128800	11.61645900
H	-0.34840800	2.38083000	9.53212600
C	-3.05802900	2.67694300	12.29334000
H	-4.35081100	3.41327800	10.72932500
C	-1.78719300	2.19166200	12.61469600
H	0.17448700	1.70450500	11.85955500
H	-3.81867900	2.76361500	13.06455600
H	-1.55602700	1.90095400	13.63570300

PAy $E_{M06(trifluoromethylbenzene)}$ = -1390.350938

C	-6.11237600	1.69266600	5.59284200
C	-5.39235200	0.75700800	4.87006500
C	-3.86906500	1.83992700	6.10567400
C	-2.68514700	2.29320200	6.72155800
C	-2.80330900	3.35206900	7.62907200
C	-4.04631300	3.94300500	7.90420700
C	-5.21188100	3.48103600	7.29249200
C	-5.14210900	2.40481600	6.39388200
C	-1.39542100	1.67479900	6.41298100
H	-1.90791100	3.72251700	8.12298100
H	-4.10056700	4.77286000	8.60231100
H	-6.16601000	3.95400300	7.50456300
H	-0.52082100	2.10637500	6.94511100
N	-4.04146700	0.85767200	5.17506400
O	-1.24866900	0.74598800	5.62788000
N	-5.88050800	-0.19544000	3.95583600
C	-5.38295900	-0.10270500	2.56936000
H	-4.30496600	-0.29291000	2.48843300
H	-5.92097700	-0.82318000	1.95300800
H	-5.59311800	0.91026900	2.21606400
S	-6.01094000	-1.79550000	4.59027800
O	-4.85298200	-2.09453800	5.44189000
O	-6.34349600	-2.65799200	3.45353100
C	-7.45919200	-1.61254000	5.64451000
H	-7.25552300	-0.85043500	6.39736600
H	-8.30426900	-1.31946000	5.02111100
H	-7.62606600	-2.58492700	6.11342600
C	-7.57096400	1.87548200	5.57839500
C	-8.31032000	1.78029800	4.38567400
C	-8.26744400	2.10989900	6.77788700
C	-9.69792200	1.91068500	4.39523500
H	-7.78838900	1.60477000	3.45126600
C	-9.65570800	2.24889200	6.78422200
H	-7.71603700	2.15591800	7.71254400
C	-10.37757800	2.14807100	5.59348500
H	-10.25029800	1.83516000	3.46225800
H	-10.17365800	2.42619500	7.72308200
H	-11.45898400	2.25289300	5.59776300
H	-3.31199200	0.20403500	4.91956100

Fy2 $E_{M06(trifluoromethylbenzene)}$ = -1830.616154

C	-2.40188500	2.56650900	8.88789800
C	-2.23086900	4.02117100	8.69685400
C	-2.51506200	4.58037600	11.03894500
C	-3.74533200	4.36587700	11.71665700
C	-3.74723300	4.25033900	13.11791000
C	-2.57563500	4.33495100	13.86058500
C	-1.37032300	4.56582100	13.19215200
C	-1.34190100	4.69727900	11.80515200
C	-5.04143200	4.26678700	11.03170500
H	-4.69729800	4.08842800	13.62225000
H	-2.59931400	4.23988300	14.94120700
H	-0.44443400	4.65596200	13.75320600
H	-0.41003000	4.92227300	11.29766800
H	-5.91388200	4.22703800	11.71777200
N	-2.42348400	4.83309900	9.67090800
O	-5.21240900	4.22626000	9.82326900
C	-6.02321400	1.45589200	7.32904500
C	-7.80099900	0.34611400	6.49660500
C	-8.06809600	1.67855500	6.41530300
H	-8.38663700	-0.51326700	6.20927700
H	-8.93109900	2.20323800	6.03598800
C	-5.89907000	-1.04777600	7.35156600
C	-6.83514400	3.80206000	7.01098500
N	-6.97155600	2.34028700	6.92842500
N	-6.54255600	0.22970600	7.05606800
Au	-4.20639800	1.96009500	8.16267600
H	-6.04949800	4.14446200	6.33674100
H	-7.78766800	4.25177600	6.72708800
H	-6.57047800	4.08893700	8.02842800
H	-4.83274400	-0.87899200	7.50388400
H	-6.33239800	-1.49021000	8.25331300
H	-6.03870800	-1.72784700	6.50802700
N	-2.03312600	4.48938500	7.40269100
C	-1.58565000	3.55858100	6.34815200
H	-2.41705200	3.01585500	5.88748900
H	-1.06024900	4.12570700	5.58066400
H	-0.89265900	2.84214300	6.79546400
S	-2.95579700	5.86841400	6.83257600
O	-4.33498300	5.72477700	7.29343000
O	-2.64308300	5.93392300	5.40639100
C	-2.17980400	7.25172900	7.67626200
H	-2.29648500	7.10281500	8.74940300
H	-1.12957000	7.28261600	7.38156400
H	-2.70336100	8.14861200	7.33515300
C	-1.41350900	1.82720200	9.58281900
C	-1.68620900	0.49576800	10.01415300
C	-0.12531300	2.37722200	9.85590100
C	-0.72891500	-0.23606900	10.69512900
H	-2.66588300	0.07582100	9.80920400
C	0.83410200	1.63353500	10.52211300
H	0.10293700	3.38026100	9.51176000
C	0.53002900	0.33176900	10.94654700
H	-0.94564300	-1.24474000	11.03169800
H	1.81595900	2.05296800	10.71659200
H	1.28244200	-0.24789200	11.47402200

$TS_{Fy2\text{-}Iy}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.603002

C	-3.85786500	5.21751700	-8.53422100
C	-2.63886200	5.65917500	-7.75548100
C	-3.37126500	7.64996000	-8.23169900
C	-3.93912600	7.00846400	-9.40351300
C	-5.21387500	7.48583100	-9.87189800
C	-5.82652000	8.53747900	-9.24708500
C	-5.17185400	9.22040400	-8.17787200
C	-3.94057500	8.81640600	-7.69381400
C	-2.94597800	6.66210600	-10.52580000
H	-5.62558700	7.03957600	-10.77122500
H	-6.78443500	8.90637000	-9.59950000

H	-5.66606300	10.07418200	-7.72259200
H	-3.47294500	9.29824200	-6.84195800
H	-1.90423300	6.52984900	-10.18064400
N	-2.40401700	6.94366900	-7.57677500
O	-3.27861300	6.55625400	-11.67983500
C	-2.62834400	2.33036900	-11.27132100
C	-1.15703800	1.08103700	-12.43674200
C	-2.40620500	0.68660200	-12.80001300
H	-0.18601300	0.73618200	-12.75638000
H	-2.73673500	-0.06114900	-13.50408000
C	-0.20601300	2.76976300	-10.82038400
C	-4.74617900	1.37789000	-12.20751000
N	-3.29383200	1.46114200	-12.07251900
N	-1.31170600	2.08934900	-11.50275100
Au	-3.34285100	3.74401500	-9.95681100
H	-5.05811300	0.33201000	-12.15395800
H	-5.06033800	1.80644300	-13.16337300
H	-5.20735800	1.93404200	-11.39109100
H	0.71300000	2.59367800	-11.38158800
H	-0.08814400	2.38872600	-9.80298300
H	-0.39814300	3.84222100	-10.77601900
N	-1.74606000	4.73326000	-7.28489600
C	-2.14298900	3.37359100	-6.87039000
H	-3.21849700	3.37853100	-6.69063600
H	-1.62432000	3.12579200	-5.94201000
H	-1.90033200	2.62545400	-7.62664000
S	-0.05003300	4.97755800	-7.65017300
O	0.55372300	3.66238800	-7.44954600
O	0.01233400	5.64385000	-8.95250700
C	0.48886400	6.11572700	-6.37049400
H	0.38446100	5.61640000	-5.40547700
H	-0.14051000	7.00414700	-6.43854200
H	1.53684000	6.34847400	-6.57619700
C	-5.13528300	5.11268100	-7.78323400
C	-6.27826200	4.57923800	-8.41204400
C	-5.24459800	5.52738200	-6.44015800
C	-7.48301200	4.46510300	-7.72692900
H	-6.20786100	4.25974100	-9.44814900
C	-6.44660600	5.39168200	-5.74775100
H	-4.38229800	5.94792900	-5.93049800
C	-7.57006700	4.86517200	-6.38882300
H	-8.35330700	4.05367200	-8.22965200
H	-6.50605300	5.69904200	-4.70780300
H	-8.50690900	4.76231700	-5.84939200

Iy $E_{M06(trifluoromethylbenzene)}$ = -1830.626625

C	-3.79235100	6.44841100	-7.12452800
C	-2.62676800	5.78652800	-7.67867300
C	-4.05114500	5.51350000	-9.29192200
C	-4.82349000	6.28042100	-8.26539500
C	-5.60976500	7.41517800	-8.85942500
C	-6.00159200	7.31779300	-10.15177500
C	-5.54141700	6.23296800	-11.00354700
C	-4.59063600	5.33703900	-10.60222800
C	-6.01712500	5.41701500	-7.68529600
H	-5.96587500	8.20018400	-8.19980100
H	-6.66269900	8.06433800	-10.58095300
H	-5.92429300	6.18540300	-12.01908300
H	-4.15471800	4.61078900	-11.27936700
H	-6.53829400	5.94565300	-6.86476800
N	-2.84987700	5.16321300	-8.89621900
O	-6.36280700	4.33781700	-8.09680000
C	-4.28549200	2.97413300	-4.61525500
C	-3.87669500	1.18400500	-3.31639500
C	-5.19886200	1.16737100	-3.63421000
H	-3.28254600	0.50503800	-2.72505600
H	-5.98341900	0.47822900	-3.36356600
C	-1.91172800	2.65671200	-3.90579300
C	-6.73987400	2.64638700	-4.97564300
N	-5.43086900	2.27187600	-4.43506800
N	-3.33379100	2.30192400	-3.92379100
Au	-4.02022800	4.63729100	-5.76461900
H	-6.62825600	3.00760900	-5.99946200
H	-7.19319400	3.42456000	-4.35526000
H	-7.38278500	1.76465300	-4.97720400
H	-1.41762000	2.08568500	-3.11850700
H	-1.80676800	3.72266200	-3.69460700
H	-1.46174400	2.43299700	-4.87443800
N	-1.36585200	5.72289400	-7.16274100
C	-1.00656400	6.49578500	-5.96194700
H	0.03427000	6.29259600	-5.71836100
H	-1.64084800	6.22037000	-5.11003100
H	-1.13521600	7.55610800	-6.17516300
S	-0.51050200	4.16102500	-7.35389200
O	0.59118000	4.23179900	-6.39655600
O	-1.50681800	3.09412800	-7.25314300
C	0.13495700	4.26224700	-9.02592400
H	0.80350800	5.12336900	-9.07495100
H	-0.71276100	4.35786700	-9.70320300
H	0.68593900	3.33282100	-9.19227100
C	-3.78753100	7.78169400	-6.42897200
C	-4.39753000	8.00146300	-5.18814400
C	-3.22294700	8.87712200	-7.10704400
C	-4.42504900	9.28063900	-4.62608100
H	-4.84543200	7.16785000	-4.65426900
C	-3.24100900	10.15183500	-6.54219400
H	-2.76389300	8.72345000	-8.08118900
C	-3.84309100	10.35664000	-5.29741400
H	-4.89849000	9.43229300	-3.66046300
H	-2.78729600	10.98338900	-7.07361000
H	-3.85993700	11.34886300	-4.85664300

TS_{Iy-Jy} $E_{M06(trifluoromethylbenzene)}$ = -1830.616339

C	-4.04847300	5.97268700	-7.24543000
C	-2.72827600	5.64008900	-7.85711800
C	-4.03503500	5.61454200	-9.58730200
C	-4.92249500	5.83698000	-8.46792000
C	-6.24314100	6.32760400	-8.70586300
C	-6.71031300	6.31946200	-9.99546700
C	-5.86712300	5.93335100	-11.08541000
C	-4.54148200	5.59175100	-10.90812200
C	-5.09966700	3.84629000	-8.60102500
H	-6.86332800	6.63988500	-7.87193100
H	-7.72942200	6.62580500	-10.20873900
H	-6.28443800	5.93495900	-12.08807400
H	-3.88918600	5.35041000	-11.74030200
H	-4.08497000	3.44848500	-8.42028100
N	-2.75562400	5.39675500	-9.17259500
O	-6.13173200	3.36235600	-8.85348200
C	-4.64047300	2.73107500	-4.54731600
C	-4.17828000	0.96252100	-3.23217000
C	-5.48981200	1.27308800	-3.05348100
H	-3.57064100	0.18447900	-2.79699800
H	-6.24697000	0.82195700	-2.43119600
C	-2.29168000	1.88460500	-4.64084800
C	-7.05713500	3.01986200	-3.94604100
N	-5.75553000	2.35923500	-3.87006500
N	-3.67451300	1.86503400	-4.15085300
Au	-4.37952100	4.27921800	-5.87389000
H	-7.06961200	3.67676700	-4.81611500

H	-7.23461600	3.60815200	-3.04131900
H	-7.84124700	2.26667100	-4.05312000
H	-1.75930800	1.03030800	-4.22103400
H	-1.79416800	2.80598300	-4.33147700
H	-2.28262100	1.82567300	-5.72934800
N	-1.54448700	5.43204100	-7.17791900
C	-1.35862500	5.94585200	-5.81140200
H	-0.32765100	5.76829500	-5.51072300
H	-2.03133000	5.46117400	-5.09180200
H	-1.55969700	7.01637900	-5.81904100
S	-0.78365100	3.87796000	-7.51063100
O	0.08703500	3.62329700	-6.36326900
O	-1.84303800	2.91298800	-7.84201300
C	0.19571700	4.21548900	-8.97510200
H	0.93883500	4.97058400	-8.71320500
H	-0.48825600	4.56859600	-9.74740500
H	0.67528300	3.27397500	-9.25475900
C	-4.23301000	7.29469200	-6.52121000
C	-5.21728800	7.48117300	-5.53933300
C	-3.46346600	8.40327400	-6.91333500
C	-5.41382800	8.73264700	-4.95288600
H	-5.83185200	6.64127100	-5.22614800
C	-3.64962400	9.65093700	-6.31722700
H	-2.71773000	8.29045400	-7.69695000
C	-4.62560200	9.82009400	-5.33312300
H	-6.17981900	8.85417000	-4.19234300
H	-3.03711300	10.49171100	-6.62997700
H	-4.77301400	10.79111400	-4.87014600

Jy $E_{M06(trifluoromethylbenzene)}$ = -1830.622927

C	-4.49443600	5.99414200	-7.70396900
C	-3.15018800	5.44953700	-8.13299500
C	-4.58954400	4.24576600	-9.28074900
C	-5.38977400	5.27238700	-8.52871500
C	-6.75241700	5.50147400	-8.88213900
C	-7.19481400	5.00706200	-10.08108200
C	-6.32682900	4.30753200	-11.01455500
C	-5.04360500	4.02759100	-10.69142900
C	-5.03260300	2.82402900	-8.64201700
H	-7.36885400	6.16173500	-8.28203400
H	-8.21178000	5.22327300	-10.39687300
H	-6.71576600	4.06408700	-11.99814500
H	-4.35902300	3.51401000	-11.35879500
H	-6.10443000	2.60370400	-8.80526000
N	-3.20640700	4.49108100	-9.00833200
O	-4.27679100	2.10517400	-8.05644300
C	-5.14416400	3.52461600	-4.25060000
C	-4.79341700	1.95911600	-2.67585500
C	-5.73252400	2.81909700	-2.19740000
H	-4.35719700	1.07454300	-2.23871800
H	-6.27054700	2.83110100	-1.26236800
C	-3.43570300	1.78092300	-4.79831400
C	-6.83683600	4.91861500	-3.04434100
N	-5.93708900	3.77222100	-3.17899000
N	-4.44490900	2.40672700	-3.93678000
Au	-4.95921300	4.62289100	-5.95307500
H	-7.27839900	5.14506400	-4.01580300
H	-6.28663900	5.78995700	-2.67914900
H	-7.63128100	4.66542200	-2.34027300
H	-3.19992200	0.79410500	-4.39775700
H	-2.53121600	2.39393700	-4.81445900
H	-3.82470400	1.67951400	-5.81170000
N	-1.94273300	5.93334600	-7.65910600
C	-1.80783800	6.61177300	-6.35883200
H	-0.79943100	6.44009900	-5.98165200
H	-2.52557100	6.16733000	-5.66574500
H	-1.98632900	7.68710100	-6.42482300
S	-0.69214700	6.24750700	-8.83477400
O	-1.34597000	6.78544500	-10.02712800
O	0.31108700	7.01481500	-8.10091600
C	-0.04812300	4.60925700	-9.19955500
H	-0.88047800	3.99521700	-9.54386300
H	0.39865900	4.21077800	-8.28704400
H	0.70948500	4.73939400	-9.97656500
C	-4.71985700	7.43713200	-7.35939700
C	-5.68863700	7.86468000	-6.44041200
C	-3.97928800	8.40097800	-8.06611900
C	-5.90300300	9.22557700	-6.21524400
H	-6.27819600	7.13266300	-5.89364000
C	-4.19070300	9.75928200	-7.83167000
H	-3.24264800	8.09041600	-8.80241100
C	-5.14925700	10.17645200	-6.90459200
H	-6.65560100	9.54052300	-5.49812700
H	-3.60750300	10.49139200	-8.38229600
H	-5.31012000	11.23514300	-6.72469200

TS_{Jy-Ky} $E_{M06(trifluoromethylbenzene)}$ = -1830.618415

C	-3.89062100	6.19328500	-7.28017500
C	-2.64678900	5.61537900	-7.91145500
C	-4.17547700	5.26239100	-9.41311800
C	-4.83706500	6.03720900	-8.36306200
C	-6.13623600	6.51981700	-8.57964000
C	-6.71387900	6.32862000	-9.83010300
C	-6.01126800	5.73698600	-10.92471600
C	-4.72760700	5.27283500	-10.75814300
C	-5.05056600	3.68077800	-9.13167100
H	-6.65228800	7.07714600	-7.80420100
H	-7.72304400	6.69197400	-10.00368700
H	-6.49172500	5.68559100	-11.89611900
H	-4.15291100	4.82129400	-11.56049600
H	-6.13935000	3.86316400	-9.11732300
N	-2.82225600	5.09707400	-9.10704400
O	-4.43436900	2.69326800	-8.99588900
C	-4.59391700	2.85576100	-4.69859600
C	-4.15543900	1.15116200	-3.29570600
C	-5.50192200	1.19535300	-3.47396300
H	-3.54232500	0.49184900	-2.70136600
H	-6.29204900	0.58461100	-3.06572700
C	-2.17950100	2.45260500	-4.16957900
C	-7.08849400	2.61249400	-4.80348600
N	-5.75349700	2.25070900	-4.33433400
N	-3.61585300	2.17772300	-4.04905000
Au	-4.32041500	4.43363100	-5.96868200
H	-7.04678900	3.60317100	-5.25709900
H	-7.77855100	2.63322900	-3.95665200
H	-7.43803100	1.88524900	-5.54208900
H	-1.65357100	1.90742600	-3.38474700
H	-1.99981700	3.52173600	-4.04396600
H	-1.82446300	2.14342100	-5.15232300
N	-1.42323000	5.48751800	-7.27280700
C	-1.13448900	6.25507600	-6.04990900
H	-0.11720800	6.03185400	-5.73416400
H	-1.82807600	6.00581900	-5.23748600
H	-1.21881400	7.31775100	-6.27603400
S	-0.69189700	3.89566000	-7.37137800
O	0.31419300	3.87051900	-6.30796000
O	-1.75874600	2.88889600	-7.38217100
C	0.11288500	3.93030100	-8.97513500
H	0.87091500	4.71502300	-8.95412500
H	-0.65772900	4.12707700	-9.72061900

H	0.57062000	2.94767600	-9.11427400
C	-3.91838200	7.52744400	-6.56443700
C	-4.51288400	7.73269200	-5.31338700
C	-3.36292200	8.63171000	-7.23465300
C	-4.53861800	9.00606700	-4.73860400
H	-4.95135400	6.89445200	-4.77945800
C	-3.37755200	9.90031900	-6.65679200
H	-2.90812500	8.48777500	-8.21226800
C	-3.96689200	10.09103300	-5.40415900
H	-5.00087800	9.14552500	-3.76562000
H	-2.93410300	10.73883600	-7.18601000
H	-3.98081300	11.07825900	-4.95202600

Ky $E_{M06(trifluoromethylbenzene)}$ = -1830.643525

C	-4.01511000	6.16461700	-7.01915300
C	-2.77722000	5.59602900	-7.55196600
C	-4.17698200	5.25114100	-9.16187000
C	-4.92702600	5.97633800	-8.16800600
C	-6.20444300	6.38981400	-8.43419200
C	-6.82643900	6.06769900	-9.69749500
C	-6.18237600	5.32796800	-10.63736600
C	-4.84391000	4.71513100	-10.37151100
C	-5.17080100	3.19830600	-10.04154800
H	-6.74869400	6.98483200	-7.70498100
H	-7.82101400	6.45478400	-9.89613400
H	-6.65749900	5.08728500	-11.58322800
H	-4.19049200	4.68505700	-11.24667800
H	-5.73801900	3.06175200	-9.10030700
N	-2.92852000	5.02485600	-8.80241600
O	-4.84680100	2.29727300	-10.75985500
C	-4.81595800	2.59983500	-4.76957400
C	-4.52300300	0.75396100	-3.51527700
C	-5.85771200	0.89273400	-3.73095600
H	-3.96950100	0.00791200	-2.96675000
H	-6.69443600	0.29224700	-3.40951500
C	-2.45182300	2.03960400	-4.17860000
C	-7.31816100	2.51368200	-4.96663500
N	-6.01948500	2.03252500	-4.50032100
N	-3.90063300	1.80844500	-4.15784500
Au	-4.41419400	4.27943900	-5.85464100
H	-7.18647600	3.49002700	-5.43338400
H	-7.99991300	2.60821800	-4.11777300
H	-7.73606700	1.81387600	-5.69574500
H	-1.96429800	1.24012300	-3.61932800
H	-2.22634000	2.99844500	-3.70589900
H	-2.09224200	2.04630800	-5.20812200
N	-1.54954000	5.54250700	-6.96336600
C	-1.32275000	6.18251700	-5.65745200
H	-0.29918700	5.98321000	-5.34671200
H	-2.01809400	5.79075100	-4.90349300
H	-1.47449400	7.25612500	-5.75986000
S	-0.61791600	4.03910300	-7.24277300
O	0.44007500	4.07255300	-6.23603800
O	-1.57136300	2.92777300	-7.27568400
C	0.09114500	4.30257000	-8.87045800
H	0.72443800	5.18978900	-8.81939900
H	-0.73039500	4.41979000	-9.57582100
H	0.68733100	3.41182900	-9.08548300
C	-4.11361500	7.45042800	-6.24140300
C	-4.88316800	7.57747900	-5.07818300
C	-3.47541800	8.59279400	-6.75474200
C	-4.99783800	8.81107600	-4.43204400
H	-5.38891500	6.70700900	-4.66922200
C	-3.58094500	9.82194200	-6.10543100
H	-2.89123900	8.51209500	-7.66889700
C	-4.34353300	9.93400700	-4.93956900
H	-5.59499900	8.89022500	-3.52823500
H	-3.07265300	10.69156800	-6.51179000
H	-4.42802100	10.89083100	-4.43308800

Ky1 $E_{M06(trifluoromethylbenzene)}$ = -3657.883485

C	-3.89901500	5.76472100	-7.19383600
C	-3.01823400	4.79765200	-7.87946100
C	-4.85269900	4.61148600	-8.99436300
C	-5.10628200	5.67627800	-8.05990900
C	-6.27092700	6.38430400	-8.12044100
C	-7.26535300	6.06524800	-9.11948700
C	-7.07814000	5.06685400	-10.01666800
C	-5.82611800	4.24703800	-10.04324000
C	-6.17445100	2.74976100	-10.12745900
H	-6.45069200	7.20204800	-7.42713800
H	-8.17480400	6.65808400	-9.14799100
H	-7.82904500	4.84800100	-10.77072000
H	-5.30592000	4.45157300	-11.00079500
H	-6.63956800	2.46661900	-11.09001800
N	-3.66023400	4.07153600	-8.85618000
O	-5.98549200	1.94955700	-9.24360200
C	-4.84836100	2.67446100	-4.44755600
C	-5.32546100	1.27631300	-2.74388700
C	-5.22365800	0.53063800	-3.87640900
H	-5.54102100	0.99517800	-1.72491200
H	-5.32882700	-0.53116700	-4.03517100
C	-5.11453600	3.71893300	-2.19044900
C	-4.70522000	1.00953600	-6.30941900
N	-4.93360500	1.40198500	-4.90931500
N	-5.09132500	2.59068000	-3.11457500
Au	-4.39271900	4.26659300	-5.64120700
H	-5.35360800	1.58051300	-6.97512300
H	-4.93284600	-0.05308800	-6.40850900
H	-3.66666300	1.19654200	-6.58661600
H	-6.11917800	3.84508100	-1.77644200
H	-4.83130100	4.62035700	-2.73430700
H	-4.40277400	3.54797900	-1.37801700
N	-1.71792100	4.55055700	-7.62987300
C	-0.97899800	5.30895600	-6.61638600
H	-0.00033100	4.85066400	-6.48839000
H	-1.52736100	5.28741500	-5.66680400
H	-0.86335100	6.34214500	-6.94572100
S	-0.99932400	3.02047400	-8.20034800
O	0.37956700	3.07988200	-7.71292000
O	-1.87749200	1.93350700	-7.76606400
C	-1.00155200	3.17793700	-9.98544400
H	-0.48196200	4.10199000	-10.23684000
H	-2.03231900	3.20994500	-10.32987300
H	-0.46905400	2.29784900	-10.35389500
C	-3.46930200	7.14903700	-6.78095500
C	-3.75444300	7.67509100	-5.51498500
C	-2.83566900	7.97307900	-7.72794400
C	-3.40531100	8.98883900	-5.19123800
H	-4.25116500	7.04921300	-4.77769600
C	-2.47912100	9.28075700	-7.40081500
H	-2.61422100	7.58009500	-8.71494600
C	-2.76253800	9.79424500	-6.13206100
H	-3.63322700	9.37874500	-4.20258200
H	-1.98346600	9.89911100	-8.14424800
H	-2.48591800	10.81449600	-5.88032100
N	-3.36565300	4.86608900	-11.84476200
S	-3.75408000	4.17233800	-13.26010900
S	-2.42468900	6.17223400	-11.68502700
C	-2.43442300	2.85209900	-13.37064100

C	-3.70506600	7.52740900	-11.60944800
F	-1.22245500	3.39489300	-13.18724200
F	-2.63088500	1.92813200	-12.41514400
F	-2.47496000	2.25601600	-14.56333300
F	-4.37864900	7.60941300	-12.75659000
F	-4.57851200	7.26778800	-10.61438100
F	-3.11457400	8.70083100	-11.35035200
O	-5.00350900	3.42853000	-13.02139100
O	-3.61504000	4.98754800	-14.46520400
O	-1.53973400	6.49841600	-12.80223600
O	-1.87440300	6.15895400	-10.31644400

$TS_{Ky1\text{-}Gy2}$ $E_{M06(trifluoromethylbenzene)}$ = -3657.871145

C	-3.84024800	5.83650000	-7.12927700
C	-2.91962100	4.83378900	-7.71709000
C	-4.70729000	4.55744400	-8.88166000
C	-4.99105500	5.69894700	-8.06258800
C	-6.13602100	6.43248300	-8.26503300
C	-7.05387100	6.05503500	-9.29173300
C	-6.82603500	4.94980800	-10.06814200
C	-5.61169900	4.15348300	-9.93602000
C	-5.76227800	2.68675400	-10.26719400
H	-6.33596800	7.31017400	-7.65554400
H	-7.94559600	6.65488200	-9.44577300
H	-7.53566700	4.65816900	-10.83808600
H	-4.86066300	4.56902000	-10.91401500
H	-6.49236900	2.48961600	-11.07406700
N	-3.49645700	4.04049700	-8.64956100
O	-5.16942000	1.78748500	-9.71180100
C	-4.90448800	2.68405000	-4.51872700
C	-5.34363300	1.10897800	-2.96571200
C	-5.27751900	0.49124100	-4.17533000
H	-5.53188900	0.71855600	-1.97780500
H	-5.39634500	-0.54625200	-4.44588700
C	-5.07674000	3.47501600	-2.15561900
C	-4.83581600	1.23469300	-6.55841900
N	-5.01008900	1.46904600	-5.11484100
N	-5.11395800	2.45599300	-3.19778100
Au	-4.42125600	4.36224400	-5.57613800
H	-5.53764500	1.84748100	-7.12406900
H	-5.03339900	0.18168500	-6.76398100
H	-3.81926400	1.48789400	-6.86375600
H	-6.01410600	3.46611200	-1.59223600
H	-4.94701600	4.44894900	-2.62829400
H	-4.23990200	3.28742100	-1.47645400
N	-1.60921000	4.63751200	-7.41016500
C	-0.95570800	5.38755000	-6.33350800
H	0.06287700	5.01832600	-6.22688200
H	-1.50384300	5.25283800	-5.39227800
H	-0.93436500	6.44672000	-6.59111500
S	-0.87024200	3.10207300	-7.88021000
O	0.53434400	3.25541900	-7.49261300
O	-1.66094100	2.00819700	-7.30900600
C	-0.96497200	3.09737500	-9.68179400
H	-0.83731400	4.12268500	-10.03221000
H	-1.93685400	2.71165300	-9.97660900
H	-0.13825400	2.45933200	-10.00408600
C	-3.41943800	7.23135700	-6.74768100
C	-3.56250800	7.73696000	-5.44981500
C	-2.89853600	8.07647200	-7.74440700
C	-3.18184800	9.04594900	-5.14377500
H	-3.97046700	7.09497300	-4.67326300
C	-2.51420500	9.38137500	-7.43858600
H	-2.78878800	7.69943900	-8.75602400
C	-2.65257900	9.87116200	-6.13660400
H	-3.29839300	9.41762200	-4.12903100
H	-2.10635200	10.01609600	-8.22086300
H	-2.35220200	10.88834200	-5.89985100
N	-3.92868500	4.94887600	-11.94291800
S	-4.15816800	4.07405600	-13.32425900
S	-2.79999800	6.13970600	-11.76491700
C	-2.90134400	2.71166600	-13.06204500
C	-3.89616600	7.64616900	-11.84763900
F	-1.69044900	3.23614700	-12.83934800
F	-3.25671600	1.98470000	-11.99406100
F	-2.85565700	1.92604500	-14.13692900
F	-4.48327200	7.73450600	-13.03854700
F	-4.83461800	7.55372800	-10.89395100
F	-3.15777500	8.73761000	-11.62381000
O	-5.46400600	3.43154200	-13.15642000
O	-3.79951300	4.75568700	-14.55948000
O	-1.84440800	6.22627900	-12.86232400
O	-2.33112700	6.12411100	-10.37519300

$TS_{Fy1\text{-}Ly}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.593215

C	-3.78805100	4.50091200	9.31136100
C	-2.79387600	4.83366700	8.24412600
C	-0.81427200	5.54804500	9.50188700
C	-1.18037000	6.11981600	10.75628900
C	-0.19767800	6.37716900	11.73763500
C	1.12931200	6.03361400	11.53515100
C	1.49983600	5.47091400	10.30413000
C	0.55393900	5.25814600	9.30762700
C	-2.52624200	6.53939700	11.05774100
H	-0.50231000	6.84816700	12.66939300
H	1.87279300	6.22607800	12.30179200
H	2.54039500	5.22384700	10.11310300
H	0.84759200	4.86657500	8.33938600
H	-2.65255100	7.22788200	11.91026000
N	-1.60063400	5.29511100	8.39047600
O	-3.55057300	6.21415100	10.44536800
C	-2.16674200	1.60222000	11.77840000
C	-0.66394000	0.41033300	12.96766600
C	-1.88548300	-0.14879100	13.17388300
H	0.30880200	0.14664700	13.35287300
H	-2.18353100	-1.00197700	13.76334600
C	0.20324800	2.39075700	11.67730700
C	-4.21899600	0.28351500	12.35505900
N	-2.79282000	0.59679700	12.44153100
N	-0.85501700	1.47729100	12.10768000
Au	-2.99315900	3.03257100	10.54335600
H	-4.38176800	-0.54716700	11.66273000
H	-4.58887400	0.01293900	13.34650200
H	-4.75517400	1.16398900	12.00046100
H	1.15669700	1.85915100	11.68629900
H	-0.00544600	2.73719000	10.66528900
H	0.25806200	3.25545000	12.34345400
N	-3.01680800	4.19156200	6.99868500
C	-1.80719000	3.63537800	6.34219200
H	-1.19625100	3.17888500	7.12189600
H	-2.12064600	2.87672800	5.62900400
H	-1.21962200	4.40459500	5.83352000
S	-4.34962300	4.46790100	5.88134900
O	-5.61165000	4.12609200	6.52089000
O	-3.94166100	3.80791100	4.64625600
C	-4.25977100	6.24809300	5.60843600
H	-4.46758000	6.77342600	6.53942200
H	-3.26370300	6.48570500	5.23060000
H	-5.02002800	6.48265300	4.85924600
C	-5.21806000	4.73932400	9.21355000

C	-5.74919100	5.98179500	8.79652800
C	-6.11513700	3.69963800	9.53285200
C	-7.11643600	6.16351500	8.67476400
H	-5.07282000	6.81219800	8.62544500
C	-7.48568500	3.86783400	9.36094100
H	-5.72549700	2.74082300	9.85970900
C	-7.98880100	5.09822700	8.93656700
H	-7.51162200	7.12828900	8.37161700
H	-8.16189300	3.04474000	9.56972400
H	-9.05999100	5.23569400	8.82181400

Ly $E_{M06(trifluoromethylbenzene)}$ = -1830.618517

C	-3.44126900	4.64803700	-9.37757200
C	-2.57027200	4.53728400	-8.10266000
C	-0.48135100	4.97566800	-9.16549600
C	-0.79490200	6.00107600	-10.11934400
C	0.21725100	6.50246400	-10.99011300
C	1.46686100	5.92734600	-11.00833000
C	1.75974600	4.87610500	-10.10602600
C	0.82208400	4.42712000	-9.19419300
C	-2.07609800	6.57905700	-10.20635100
H	-0.02404800	7.32305100	-11.66083500
H	2.23066300	6.29043400	-11.68782900
H	2.75571100	4.44205800	-10.10175400
H	1.06956200	3.67724300	-8.45028000
H	-2.19969700	7.55771700	-10.67235300
N	-1.28329200	4.60386000	-8.12871700
O	-3.19202600	6.08801400	-9.81779500
C	-2.19309400	1.97155900	-12.35064400
C	-0.89256900	0.75762400	-13.74086500
C	-2.18387800	0.40670700	-13.97809300
H	0.02669300	0.41905500	-14.19278400
H	-2.60963000	-0.30061600	-14.67264900
C	0.25672900	2.38187800	-12.18316200
C	-4.42068200	1.05307200	-13.03354000
N	-2.96522800	1.16369000	-13.12111300
N	-0.91918100	1.71648600	-12.74308800
Au	-2.78649100	3.29358000	-10.88561800
H	-4.69847200	0.20138400	-12.40600000
H	-4.83185300	0.91756900	-14.03622300
H	-4.82176100	1.97096200	-12.60280000
H	1.14824300	2.00944600	-12.69019000
H	0.33039300	2.17196300	-11.11463200
H	0.17904000	3.46124600	-12.32864900
N	-3.20169400	4.41666400	-6.87832100
C	-4.10097000	3.28000300	-6.58605900
H	-5.10321800	3.62791000	-6.32615500
H	-3.66756000	2.69139500	-5.77075600
H	-4.16958200	2.63956400	-7.46384600
S	-2.40462000	5.14440300	-5.49236000
O	-1.66214700	4.12320600	-4.75844400
O	-1.78397900	6.37217900	-5.98024200
C	-3.86969100	5.59380900	-4.54130100
H	-4.37495100	4.69562100	-4.18447500
H	-4.52357100	6.20039300	-5.16990900
H	-3.50053100	6.17633400	-3.69362300
C	-4.93103300	4.68096500	-9.09435100
C	-5.48536300	5.73739000	-8.34941800
C	-5.77711100	3.64659900	-9.51289500
C	-6.84098400	5.75285500	-8.03098100
H	-4.84549800	6.55021700	-8.01979900
C	-7.13453700	3.65145100	-9.18253600
H	-5.37089300	2.81884300	-10.08754100
C	-7.67069900	4.70396300	-8.44147600
H	-7.25238800	6.58198300	-7.46216200
H	-7.77144500	2.83541600	-9.51139900
H	-8.72705600	4.71294300	-8.18944000

$TS_{Ly\text{-}Ly1}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.601306

C	-2.92827200	6.17212500	-6.51892200
C	-1.82259700	6.30334700	-7.46193100
C	-2.88429000	7.53422600	-9.23598700
C	-4.21492500	6.96758100	-9.12560100
C	-5.09966600	7.01416000	-10.23990500
C	-4.76685500	7.76668500	-11.33767100
C	-3.52567800	8.46946500	-11.38388100
C	-2.60966500	8.35998800	-10.36861700
C	-4.58143600	6.44074500	-7.87120300
H	-6.06740200	6.52577400	-10.16603700
H	-5.46253100	7.85901100	-12.16583000
H	-3.29408000	9.07365300	-12.25589100
H	-1.63668100	8.83649300	-10.42814100
H	-5.59878500	6.11566800	-7.65181300
N	-1.84431400	7.16303300	-8.47125800
O	-3.96035400	7.06999300	-6.77941900
C	-3.59639300	2.20122900	-8.12702800
C	-3.32872500	0.18512200	-9.08986800
C	-3.56224100	-0.02256600	-7.76642400
H	-3.14018800	-0.51098100	-9.89217000
H	-3.61768400	-0.93387600	-7.19167900
C	-3.16727300	2.20298900	-10.59287300
C	-4.02654400	1.44872100	-5.77762000
N	-3.72123400	1.22555700	-7.19066800
N	-3.35032000	1.55289100	-9.29121700
Au	-3.72278200	4.23327100	-7.81466500
H	-3.51320200	2.34627600	-5.42879800
H	-3.67796900	0.59035600	-5.20066200
H	-5.10454100	1.56817800	-5.63727800
H	-2.65098000	1.50885600	-11.25799300
H	-2.56066200	3.09979100	-10.46682900
H	-4.14044100	2.46016700	-11.01974600
N	-0.67762600	5.49480900	-7.41166900
C	-0.39626100	4.56923800	-6.30227600
H	-0.17159200	5.13582700	-5.40120800
H	0.46908100	3.96729000	-6.57122300
H	-1.24332200	3.90047500	-6.11056100
S	-0.13183200	4.92338400	-8.99395000
O	0.67586100	3.73225800	-8.73324700
O	-1.29549400	4.82872500	-9.88656600
C	0.94686300	6.24916100	-9.54579100
H	1.77080900	6.32395400	-8.83418800
H	0.35970300	7.16541600	-9.58212100
H	1.31294700	5.95941500	-10.53395900
C	-2.81793400	5.90349900	-5.05845300
C	-3.77473500	5.12022000	-4.39671200
C	-1.84209800	6.57752100	-4.30845800
C	-3.72324900	4.96856600	-3.01262600
H	-4.55917200	4.63573900	-4.97144400
C	-1.79830300	6.43002700	-2.92155400
H	-1.13214800	7.22999000	-4.80944500
C	-2.72994700	5.61727300	-2.27297700
H	-4.46272100	4.35270400	-2.50921000
H	-1.04088100	6.95744900	-2.34954600
H	-2.69164400	5.50046600	-1.19414400

Ly1 $E_{M06(trifluoromethylbenzene)}$ = -1830.631268

C	-2.27758600	-0.29019500	-0.45971400
C	-1.60307100	-0.25535300	0.86997300
C	-1.43699600	2.12620000	1.06440000
C	-1.07454700	2.46802800	-0.26663500

C	-1.02818700	3.82033600	-0.62176700
C	-1.32354500	4.81717200	0.30701700
C	-1.68149500	4.47678600	1.61870100
C	-1.72298100	3.14262700	1.99783500
C	-0.69093500	1.40170800	-1.23523400
H	-0.75032800	4.09097500	-1.63706300
H	-1.27495200	5.86064200	0.01048100
H	-1.91601200	5.25379700	2.33951500
H	-1.98166800	2.85165100	3.01090200
H	-0.64910900	1.82270900	-2.24091300
N	-1.40901500	0.82759200	1.54221900
O	-1.91369000	0.51808200	-1.37962500
C	2.88689000	-0.67574600	-0.72185900
C	5.01970300	-1.22590900	-0.21349600
C	4.52341200	-2.20706800	-1.01182200
H	5.98909600	-1.10821100	0.24560700
H	4.97774700	-3.11075900	-1.38775200
C	4.15156200	0.93736000	0.72085700
C	2.33945500	-2.62078400	-2.19967500
N	3.21655000	-1.85737200	-1.30779600
N	4.00303800	-0.30040600	-0.04373200
Au	1.08234600	0.32491600	-0.90137200
H	2.41877800	-2.23884000	-3.22095800
H	1.30743500	-2.53675400	-1.85697000
H	2.64490300	-3.66921500	-2.18127800
H	4.61565500	0.71699800	1.68540100
H	3.16556800	1.37357300	0.88228800
H	4.77483900	1.64631000	0.16883000
N	-1.48375500	-1.48358000	1.53984800
C	-1.42073000	-1.49285000	3.00868800
H	-0.48521200	-1.06376400	3.38196400
H	-1.53735500	-2.52363700	3.34832800
H	-2.24922000	-0.89433000	3.39180100
S	-0.77978000	-2.82048300	0.72995900
O	-1.46725800	-4.01795500	1.19464800
O	-0.74485700	-2.45332500	-0.69290500
C	0.91297000	-2.85800100	1.35187100
H	0.89446100	-3.06830700	2.42228100
H	1.38966600	-1.90170100	1.13300700
H	1.41681800	-3.67011800	0.82206100
C	-3.47085300	-1.07416600	-0.72335900
C	-3.89749100	-1.22475900	-2.06290600
C	-4.22913200	-1.65591300	0.31670500
C	-5.04262900	-1.95300600	-2.35019900
H	-3.31016100	-0.78587400	-2.86110500
C	-5.38389100	-2.36798300	0.01819400
H	-3.92413100	-1.54095100	1.34862700
C	-5.78819700	-2.52450900	-1.31144300
H	-5.35671100	-2.08147900	-3.38112600
H	-5.96807500	-2.80589600	0.82101700
H	-6.68425400	-3.09410000	-1.53973200

$TS_{Ly1\text{-}Ay}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.624471

C	-2.75174500	6.52300400	-6.64308800
C	-1.58856800	6.43200400	-7.59123600
C	-2.76370300	7.13545900	-9.52640000
C	-4.07081000	7.05662600	-8.97260900
C	-5.20009100	7.15528400	-9.80139000
C	-5.04137900	7.40521000	-11.15862400
C	-3.75350800	7.54309600	-11.70489300
C	-2.63013700	7.40010200	-10.90302500
C	-4.18970200	6.88862800	-7.52614000
H	-6.19271500	7.07345200	-9.36670500
H	-5.91518300	7.51305300	-11.79368400
H	-3.63726300	7.74981500	-12.76440800
H	-1.62920100	7.46677200	-11.31680300
H	-5.16191300	6.69090900	-7.06908300
N	-1.61210800	6.82459300	-8.82212900
O	-3.40209900	7.76012300	-6.74915800
C	-3.99045000	2.50610500	-8.21322500
C	-3.85742200	0.61924500	-9.41650600
C	-4.20151200	0.27359300	-8.14664400
H	-3.68418600	0.01289300	-10.29163500
H	-4.39768400	-0.69006800	-7.70336600
C	-3.31161100	2.79247600	-10.59732200
C	-4.65194700	1.52911500	-6.00505200
N	-4.27551200	1.44834800	-7.41777500
N	-3.73528500	1.99642500	-9.43961400
Au	-3.86115600	4.43494800	-7.70462900
H	-4.12017200	2.35869900	-5.53548200
H	-4.37009800	0.59669700	-5.51275600
H	-5.73016400	1.68281000	-5.90937000
H	-3.27426800	2.14066500	-11.47111000
H	-2.32735100	3.21898800	-10.39850600
H	-4.03367300	3.59313100	-10.77205900
N	-0.43720000	5.79038200	-7.10892600
C	0.36562700	6.38281200	-6.02503800
H	-0.30784600	6.89562800	-5.33545400
H	1.08647800	7.10798400	-6.42070100
H	0.88490300	5.59179300	-5.48439700
S	0.26597400	4.56502000	-8.07095200
O	1.10600200	3.79396800	-7.15764300
O	-0.84202000	3.92453500	-8.78996300
C	1.30974700	5.42352900	-9.25783000
H	2.08625200	5.95912600	-8.70734700
H	0.67180900	6.10799200	-9.81759800
H	1.75909600	4.66471100	-9.90309000
C	-2.79674000	5.91356500	-5.26675600
C	-2.19487300	4.67556300	-4.96018500
C	-3.49572200	6.59930800	-4.26225700
C	-2.29998300	4.14611000	-3.67636500
H	-1.63079900	4.13838600	-5.71292500
C	-3.59713900	6.06017900	-2.97858400
H	-3.95337800	7.55578400	-4.48732500
C	-3.00366300	4.83299200	-2.68168500
H	-1.81924500	3.19859500	-3.45065300
H	-4.13747600	6.60587800	-2.21094300
H	-3.07963600	4.41723700	-1.68136000

PQ'y $E_{M06(trifluoromethylbenzene)}$ = -1390.298196

C	-1.91843000	7.04959400	7.62375600
C	-2.75662000	6.10222400	6.79902200
C	-0.33167900	5.41664000	8.16594000
C	-0.94842500	4.39392600	7.41332100
C	-0.43721400	3.09508600	7.45466900
C	0.70176100	2.80913300	8.20822300
C	1.33062500	3.82718800	8.93412800
C	0.81602100	5.12111100	8.91661600
C	-2.16069500	4.73658000	6.65042900
H	-0.92887900	2.31032500	6.88454800
H	1.10121000	1.79921700	8.22544600
H	2.21936800	3.60739600	9.51904500
H	1.27938500	5.92320800	9.48267700
H	-2.85212900	3.92651100	6.41986400
N	-0.81809100	6.72578000	8.20871000
O	-2.07220800	5.71365300	5.59149400
N	-2.36285300	8.38628400	7.75394100
C	-1.77476800	9.16377200	8.86103400
H	-0.70556600	9.36031100	8.72165600
H	-2.32132000	10.10121300	8.94632000

H	-1.89623400	8.57463100	9.77159200
S	-2.47587300	9.27348300	6.25655000
O	-2.59459300	10.68029700	6.63737000
O	-3.47025100	8.63353300	5.40421200
C	-0.85342800	8.99401600	5.50867900
H	-0.07633500	9.30569600	6.20968800
H	-0.76873700	7.93142400	5.26994800
H	-0.81997400	9.60053600	4.60084900
C	-4.24747500	6.22669700	6.75551800
C	-4.93920700	5.94633800	5.57391400
C	-4.95972900	6.54213500	7.91726800
C	-6.33248700	5.98507400	5.55394900
H	-4.37424100	5.72497800	4.67477500
C	-6.35379800	6.58247100	7.89424700
H	-4.42658300	6.76538400	8.83713200
C	-7.04437400	6.30346300	6.71290200
H	-6.86283900	5.77692300	4.62855600
H	-6.89958000	6.83373000	8.79971000
H	-8.13029700	6.33856100	6.69485500

$TS_{My1\text{-}Oy}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.598972

C	-2.45744500	5.58772200	7.88173000
C	-1.83871300	6.16346000	6.69339700
C	0.05328000	4.90626400	7.64214800
C	0.24986900	4.10667900	6.48670200
C	1.27577200	3.13468000	6.45801600
C	2.07222000	2.93497000	7.57199800
C	1.85014100	3.71162200	8.72402200
C	0.86034200	4.69163000	8.76203000
C	-0.64563200	4.22686000	5.38159900
H	1.42032700	2.54172100	5.55819000
H	2.86002200	2.18945300	7.55972800
H	2.47209300	3.55491700	9.60065600
H	0.70695600	5.30378500	9.64443300
H	-0.47928900	3.60721800	4.49112700
N	-0.90298400	5.92442900	7.68838300
O	-1.65311500	4.97521800	5.34990900
C	-3.96539600	1.72977800	7.76101500
C	-4.52790600	-0.41448000	8.19822500
C	-5.21600000	-0.02910900	7.09278000
H	-4.51243000	-1.35201300	8.73229500
H	-5.91912800	-0.56472800	6.47376900
C	-2.89055700	0.66661500	9.76175800
C	-5.40696700	2.06952500	5.73076600
N	-4.85949000	1.28484200	6.83871800
N	-3.76783900	0.67424200	8.59310400
Au	-3.14886900	3.61953100	7.84986300
H	-6.48914400	2.16984100	5.84896000
H	-4.95229800	3.06064000	5.73292800
H	-5.18762500	1.57088400	4.78288000
H	-3.47710400	0.47752200	10.66486300
H	-2.13023400	-0.11125300	9.64978800
H	-2.40594100	1.63949400	9.84417700
N	-2.00358700	7.32783600	6.02802000
C	-0.85888800	7.96173400	5.35750600
H	0.00875900	7.84927700	6.01208600
H	-0.66993600	7.50567600	4.38197200
H	-1.06202900	9.02454900	5.21835200
S	-3.60923800	7.65350000	5.39982900
O	-4.42697000	6.49545200	5.74970700
O	-3.41050400	8.08515800	4.02079700
C	-4.09365000	9.06847600	6.39867900
H	-4.14094900	8.76396500	7.44445100
H	-3.36422400	9.86569200	6.24274200
H	-5.07567500	9.37989300	6.03346300
C	-3.12819700	6.57874200	8.79507900
C	-2.41692000	7.59166600	9.45268800
C	-4.52242100	6.51769900	8.95304600
C	-3.08313600	8.52284400	10.25130300
H	-1.34048600	7.64775000	9.33046400
C	-5.18819200	7.45828700	9.73942100
H	-5.08676000	5.74866200	8.43541700
C	-4.47143400	8.46415100	10.39356200
H	-2.51553100	9.29699400	10.76013500
H	-6.26804000	7.40189600	9.84310700
H	-4.98945700	9.19106100	11.01231500

Oy $E_{M06(trifluoromethylbenzene)}$ = -1830.605842

C	-2.46077300	5.56133800	7.51431800
C	-1.68045200	5.98031000	6.32831900
C	-0.00037900	4.79547700	7.64436400
C	0.31278200	3.95629600	6.53455200
C	1.30964400	2.95057900	6.64146500
C	1.95320400	2.75992800	7.84587400
C	1.60939800	3.56989500	8.95260100
C	0.65464100	4.57754200	8.86125300
C	-0.46979300	4.08390200	5.37446500
H	1.54516200	2.33652100	5.77613100
H	2.71696500	1.99684800	7.94923900
H	2.11483900	3.40856900	9.90066500
H	0.41184900	5.20729700	9.71035800
H	-0.30747800	3.44660600	4.50357800
N	-0.91486200	5.82635500	7.51663200
O	-1.44184900	4.90555400	5.23817600
C	-3.99968900	1.71405100	7.76762000
C	-4.43536900	-0.41563100	8.38696300
C	-5.35133500	-0.06777700	7.44658100
H	-4.29236100	-1.33700000	8.93005200
H	-6.16381700	-0.62677000	7.00867100
C	-2.51972800	0.73311800	9.53434100
C	-5.85834800	1.99454000	6.10625200
N	-5.06717800	1.23618700	7.07621000
N	-3.61420800	0.68544700	8.56751700
Au	-3.18959600	3.60820600	7.64517400
H	-5.28948100	2.86666800	5.78287700
H	-6.07252400	1.36213800	5.24150100
H	-6.79700300	2.32230200	6.56165000
H	-2.91460800	0.85793100	10.54663900
H	-1.94524000	-0.19483900	9.47801200
H	-1.87166300	1.57631500	9.29326700
N	-1.69872200	7.21470400	5.69479800
C	-0.43202000	7.75423000	5.17820300
H	-0.11192300	7.24712600	4.26212300
H	-0.55148400	8.81702000	4.96198000
H	0.31920700	7.64212000	5.96412400
S	-3.14423500	7.59858100	4.81232600
O	-4.07647100	6.50067300	5.06670800
O	-2.72615500	7.96150800	3.46033000
C	-3.70086300	9.08317200	5.66021200
H	-3.93183600	8.83554800	6.69593000
H	-2.90943400	9.83234800	5.59456200
H	-4.59046800	9.42853300	5.12757900
C	-3.21895900	6.63944900	8.23655800
C	-2.57910300	7.65468000	8.95906300
C	-4.62143800	6.64191000	8.16156000
C	-3.32303100	8.65244700	9.59178600
H	-1.49589300	7.66188500	9.01428200
C	-5.36299800	7.64615100	8.78346400
H	-5.12736900	5.87113400	7.58909300
C	-4.71689100	8.65554800	9.50297900

H	-2.81130700	9.43002500	10.15210600
H	-6.44653500	7.63877000	8.70637500
H	-5.29489300	9.43354000	9.99321000

TS_{Oy-Qy} $E_{M06(trifluoromethylbenzene)}$ = -1830.581144

C	-2.00408400	5.27103300	7.12565700
C	-1.56587600	5.81758000	5.85022600
C	0.49914600	5.08798300	7.17359300
C	0.55101900	3.96779600	6.31652000
C	1.72665600	3.20520700	6.26367700
C	2.82714300	3.57819100	7.02798200
C	2.77826500	4.72398900	7.83966900
C	1.61935600	5.48969100	7.90918100
C	-0.64622100	3.72910900	5.49818600
H	1.77917700	2.34347000	5.60360100
H	3.73893000	2.99052700	6.98101800
H	3.64760500	5.00912800	8.42399400
H	1.55304600	6.36942500	8.54097900
H	-0.50086300	3.03951200	4.66617400
N	-0.71595100	5.78760500	7.30891300
O	-1.05565900	4.99536100	4.91605500
C	-4.03082500	2.25025600	7.57178600
C	-5.58291900	1.64207400	9.08811000
C	-6.21706900	1.81240500	7.89673600
H	-5.96060200	1.35356900	10.05667300
H	-7.25325200	1.68770800	7.62318500
C	-3.22102000	1.94825600	9.90964600
C	-5.50084800	2.46666800	5.56348100
N	-5.25014600	2.18822700	6.98135000
N	-4.24344100	1.90945000	8.86533300
Au	-2.29735800	3.02392400	6.66818100
H	-4.98892000	3.38517300	5.26749700
H	-5.14692700	1.63454200	4.94970300
H	-6.57451700	2.59305200	5.41588100
H	-3.18394200	2.94637500	10.35482900
H	-3.45958200	1.20744200	10.67516200
H	-2.25228300	1.71009700	9.46820700
N	-1.96715500	7.05930600	5.31780700
C	-1.98063300	8.24334800	6.19933700
H	-0.98066600	8.34832300	6.62075000
H	-2.21375400	9.11778300	5.59339600
H	-2.71569600	8.16030100	7.00652500
S	-3.31043200	6.88557300	4.21735400
O	-4.09188000	8.11460400	4.31708600
O	-3.93389300	5.57372200	4.46361400
C	-2.46698700	6.81667200	2.63378200
H	-1.94278300	7.76244400	2.48750500
H	-1.77197200	5.97685000	2.66091900
H	-3.23448900	6.67383900	1.86912100
C	-3.07762300	5.58149700	8.06982100
C	-2.75217500	5.72558200	9.43174000
C	-4.42048900	5.65462200	7.65322100
C	-3.76073100	5.93423500	10.36731200
H	-1.70988100	5.68704700	9.73369600
C	-5.42123200	5.87387200	8.59507300
H	-4.65869600	5.54053900	6.60186300
C	-5.09599800	6.00644900	9.95020300
H	-3.51133800	6.05395000	11.41747900
H	-6.45615600	5.94649100	8.27485000
H	-5.88135400	6.17730300	10.68083100

Qy $E_{M06(trifluoromethylbenzene)}$ = -1830.630745

C	-1.59396900	5.86334300	7.31606800
C	-1.70284100	6.27823500	5.87657500
C	0.30133100	4.44488900	6.96549200
C	-0.06519000	3.80638400	5.74714600
C	0.88219800	3.00386600	5.10126200
C	2.16060000	2.83294600	5.62973400
C	2.51774400	3.46690800	6.82716100
C	1.58863200	4.24816400	7.50096900
C	-1.45533500	3.93578100	5.22222500
H	0.60777700	2.50496300	4.17527400
H	2.87850200	2.20392400	5.11208900
H	3.51353100	3.33396800	7.23867900
H	1.83132700	4.72675200	8.44431100
H	-1.50511900	3.54445200	4.20587100
N	-0.60792900	5.14777600	7.73973600
O	-1.62145000	5.43564500	4.91356500
C	-4.55776900	2.35371500	7.51633200
C	-5.88726900	1.84389500	9.26959300
C	-6.39748100	1.21955600	8.17649200
H	-6.22050200	1.86047800	10.29568800
H	-7.25676600	0.57673500	8.06356000
C	-3.95200300	3.37889300	9.72235900
C	-5.75730300	1.02575800	5.75931500
N	-5.57256000	1.54474600	7.11287400
N	-4.76060300	2.52866300	8.84806400
Au	-3.03030800	3.16246100	6.38031800
H	-5.10353600	1.57220300	5.07961600
H	-5.50657000	-0.03834200	5.72673700
H	-6.79706600	1.16625100	5.45343200
H	-4.42765300	4.35402500	9.84866900
H	-3.84323500	2.89058800	10.69348100
H	-2.96710800	3.51774800	9.27767300
N	-1.87975100	7.55668600	5.49989000
C	-2.29108600	7.86041400	4.11324800
H	-2.97832900	7.08417800	3.77512200
H	-2.81346600	8.81851600	4.11752800
H	-1.42907000	7.89053000	3.44145800
S	-1.49697800	8.98739000	6.52617800
O	-0.79004100	8.49650400	7.69669900
O	-2.72795100	9.75702700	6.58808400
C	-0.30214100	9.81200600	5.45789700
H	0.52595000	9.12682000	5.26787400
H	-0.77835800	10.14762300	4.53666400
H	0.04376200	10.67320800	6.03646100
C	-2.62533800	6.35460600	8.25678200
C	-2.31366200	6.50890100	9.61719300
C	-3.93160300	6.61056800	7.81341400
C	-3.29298600	6.92395600	10.51324600
H	-1.29877800	6.31792600	9.94745200
C	-4.91410000	7.01711200	8.71711300
H	-4.19272900	6.47104700	6.76790100
C	-4.59594800	7.17982600	10.06690800
H	-3.04084600	7.06082700	11.56067800
H	-5.92295700	7.21007400	8.36516800
H	-5.35617600	7.51051600	10.76854500

TS_{Qy-Ay} $E_{M06(trifluoromethylbenzene)}$ = -1830.611328

C	-1.20188200	6.39246300	7.41634400
C	-1.53733900	5.82490700	6.04120000
C	0.49398500	4.77935900	7.85315600
C	0.39104400	4.06544100	6.63435700
C	1.15983000	2.91186400	6.42099900
C	2.05263700	2.48198300	7.39947200
C	2.17887700	3.19930200	8.59819300
C	1.40849700	4.33531200	8.82415300
C	-0.58731700	4.52886200	5.64211700
H	1.06314900	2.36970200	5.48377000
H	2.66164500	1.60033000	7.22530000

H	2.88484200	2.86785100	9.35360700
H	1.49055700	4.90317200	9.74510800
H	-0.81416400	3.89206500	4.78615300
N	-0.27245300	5.89459400	8.16206500
O	-0.46897100	5.89396400	5.16199100
C	-3.84680000	1.88207100	6.96337300
C	-5.19257500	0.36637200	7.92802300
C	-5.74687800	0.70967700	6.73533700
H	-5.51686100	-0.32924600	8.68640500
H	-6.65461100	0.37827300	6.25536400
C	-3.10727500	0.98073500	9.18887000
C	-5.17751400	2.30305700	4.86834800
N	-4.90589600	1.64038200	6.15115400
N	-4.02396900	1.09828100	8.05355700
Au	-2.37031500	3.17447300	6.56313900
H	-4.24150100	2.61297800	4.40262900
H	-5.68988600	1.59653800	4.21305900
H	-5.80855200	3.18229000	5.02336600
H	-3.66953400	1.08458700	10.11965600
H	-2.60906900	0.00803000	9.16440600
H	-2.36091400	1.77273400	9.12641800
N	-2.81965700	6.12341400	5.48746200
C	-4.02406400	6.03597200	6.35041900
H	-3.70895900	6.02608400	7.39134700
H	-4.65296800	6.90953600	6.17994600
H	-4.59994900	5.12892200	6.14922700
S	-3.15677100	5.69319500	3.84152300
O	-4.59366800	5.91374500	3.69173500
O	-2.60327500	4.35817100	3.55160400
C	-2.25593600	6.92535000	2.89640300
H	-2.62961700	7.90865900	3.18668400
H	-1.19140400	6.81888900	3.10191300
H	-2.47922300	6.72236100	1.84579600
C	-1.88442300	7.61717300	7.90200100
C	-2.27179900	8.64531000	7.02440700
C	-2.08122800	7.78682100	9.28359700
C	-2.84620300	9.81386700	7.52069500
H	-2.10803400	8.53948700	5.95756400
C	-2.67073500	8.94904500	9.77319500
H	-1.76090500	7.00074600	9.95923600
C	-3.05534000	9.96556900	8.89372600
H	-3.12638400	10.60862700	6.83566500
H	-2.82685200	9.06541400	10.84161600
H	-3.51188400	10.87337400	9.27703900

PQy $E_{M06(trifluoromethylbenzene)}$ = -1390.291061

C	-1.10821800	6.46808500	7.36073700
C	-1.44883700	5.81568500	6.03232800
C	0.50409400	4.81640300	7.83552000
C	0.27767200	4.05598400	6.66753400
C	0.93916900	2.84013100	6.48569400
C	1.85558600	2.38999700	7.43702000
C	2.10812000	3.15645300	8.58083300
C	1.43479200	4.35869400	8.78139400
C	-0.69353100	4.57310200	5.69329500
H	0.74393200	2.25529100	5.59007100
H	2.37743500	1.44967600	7.28413700
H	2.82601600	2.80943300	9.31873000
H	1.59973900	4.96138600	9.66900400
H	-1.14927500	3.88595600	4.98609800
N	-0.18994700	5.99146300	8.13400100
O	-0.39725900	5.87155700	5.08497900
N	-2.79588200	6.05646200	5.54485100
C	-3.83135400	5.45843000	6.41064700
H	-3.71874700	5.87777800	7.41306600
H	-4.81311100	5.73235900	6.02661100
H	-3.74474800	4.36470800	6.46052900
S	-3.11907600	5.87570500	3.86231700
O	-4.56049200	6.10303400	3.72725700
O	-2.53057000	4.64504400	3.31629000
C	-2.25502900	7.28960100	3.16183000
H	-2.68539200	8.19811600	3.58501300
H	-1.19153000	7.19800200	3.37895900
H	-2.43926900	7.24397500	2.08566300
C	-1.81442700	7.69344100	7.80900700
C	-2.25830400	8.66937800	6.90148900
C	-2.00179500	7.91201400	9.18512800
C	-2.87596200	9.83209400	7.35893600
H	-2.10490200	8.52386800	5.83975200
C	-2.63148500	9.06799100	9.63909500
H	-1.64335300	7.16315700	9.88354500
C	-3.07231000	10.03162100	8.72727700
H	-3.20472100	10.58284900	6.64561100
H	-2.77890300	9.21864300	10.70506100
H	-3.56446600	10.93333800	9.08147700

$TS_{My1\text{-}Fy3}$ $E_{M06(trifluoromethylbenzene)}$ = -1830.609140

C	-3.11901400	5.15743800	10.87243000
C	-2.47418700	5.90287500	9.78365900
C	0.06218300	5.60663300	9.96411800
C	0.54415600	4.48886100	9.20830000
C	1.91056500	4.15499300	9.28610800
C	2.80482600	4.89035600	10.04905100
C	2.32956900	5.99703500	10.76966400
C	0.98795900	6.34678400	10.73723800
C	-0.29194200	3.68086300	8.32794800
H	2.26228000	3.29679900	8.71754900
H	3.85360300	4.61591900	10.08801100
H	3.01561500	6.58538000	11.37233500
H	0.61826700	7.19252900	11.30762100
H	0.24781400	2.84800700	7.83222300
N	-1.22754800	5.99236200	9.98430100
O	-1.48524500	3.85253900	8.08852600
C	-4.14020200	1.39699400	9.59966900
C	-4.82854700	-0.74162300	9.39503900
C	-4.75476100	-0.21010500	8.14501100
H	-5.10863700	-1.72793500	9.73081600
H	-4.95903800	-0.64573100	7.17940700
C	-4.42692600	0.10115400	11.72445200
C	-4.13083700	2.04426800	7.18592200
N	-4.32990200	1.09637700	8.28979800
N	-4.44647200	0.25759400	10.27230600
Au	-3.57003600	3.24255300	10.31080000
H	-4.22470300	1.50083700	6.24423500
H	-4.88052400	2.83630100	7.23377300
H	-3.13765400	2.49017300	7.26382300
H	-3.86258800	0.92600800	12.15973700
H	-5.44721800	0.10872900	12.11855100
H	-3.94194700	-0.84336600	11.98264800
N	-3.12692200	6.40889600	8.67325800
C	-2.37593900	6.65195700	7.42859500
H	-1.33464400	6.82590800	7.69945100
H	-2.44260300	5.78356100	6.77211300
H	-2.75866600	7.54518400	6.93136300
S	-4.83901300	6.22776900	8.53234600
O	-5.33289900	5.98412700	9.88983000
O	-5.10849700	5.29552400	7.43972800
C	-5.35994000	7.87813100	8.03502700
H	-6.45198200	7.84220900	8.00290200
H	-5.02221300	8.59076700	8.78904500

H	-4.96638500	8.11427800	7.04564000
C	-3.25550400	5.77582600	12.15404400
C	-3.65511900	4.99859900	13.27118700
C	-3.05565100	7.17138000	12.34019400
C	-3.84614600	5.58578000	14.51432200
H	-3.81236800	3.93344400	13.13495400
C	-3.24841900	7.75361500	13.58160900
H	-2.74783200	7.78301000	11.49845400
C	-3.64338600	6.96176400	14.67076400
H	-4.15194100	4.98108200	15.36223300
H	-3.09773200	8.82057400	13.71357000
H	-3.79392000	7.42192300	15.64319200
C	-4.64471100	6.60374300	12.43422100
H	-3.94361100	8.34849200	11.36910500
H	-5.29206100	4.71605000	13.26189000
H	-4.90711000	7.16658500	13.32574000

Fy3 $E_{M06(trifluoromethylbenzene)}$ = -1830.621956

C	-3.63712500	4.39824300	8.97829500
C	-2.71571000	4.96848700	7.96405900
C	-0.79887300	5.01472100	9.41229500
C	-0.27542400	3.76224100	9.83384200
C	0.47314300	3.69862900	11.02439000
C	0.72092100	4.83007000	11.79034700
C	0.22917700	6.06357700	11.35082600
C	-0.51119200	6.15727800	10.17429900
C	-0.43953900	2.51617400	9.07686000
H	0.86656400	2.73448600	11.33894100
H	1.29983800	4.76088600	12.70538000
H	0.42663300	6.96353800	11.92634900
H	-0.86928400	7.11982600	9.82550000
H	0.07649800	1.64667900	9.53702000
N	-1.47379700	5.16221900	8.20236800
O	-1.06335700	2.36304600	8.03315000
C	-4.66567700	0.61065900	7.80767500
C	-4.66157300	-1.54435700	7.15223600
C	-5.85289800	-1.00412600	6.77950100
H	-4.26590600	-2.54017700	7.02797200
H	-6.69392800	-1.43594500	6.26004800
C	-2.60068500	-0.68951800	8.33457200
C	-6.89805500	1.29520100	6.93689000
N	-5.83646600	0.31626600	7.19082000
N	-3.94587700	-0.53735000	7.77617200
Au	-4.11407800	2.46434700	8.51114800
H	-6.51528000	2.09532500	6.29933100
H	-7.72932600	0.78984400	6.44301600
H	-7.24093100	1.71798600	7.88377100
H	-2.65760100	-0.82594900	9.41827300
H	-2.13233300	-1.56651800	7.88415400
H	-2.01035000	0.19901000	8.10080900
N	-3.12901900	5.03486900	6.62961800
C	-2.14654300	4.80178600	5.55515500
H	-1.45178200	4.03207500	5.89596800
H	-2.67506700	4.43924200	4.67107400
H	-1.59631200	5.71709400	5.32252500
S	-4.78090300	5.11109300	6.24584600
O	-5.46151600	5.36023600	7.52595900
O	-5.14656300	3.96293700	5.41506200
C	-4.87791400	6.59614000	5.23390900
H	-4.56373100	7.44800900	5.83885500
H	-4.23994700	6.47357800	4.35649800
H	-5.92224400	6.69842900	4.92878400
C	-3.96703100	5.15315900	10.13310400
C	-3.75555400	6.55976400	10.19539000
C	-4.54160800	4.50242900	11.25984000
C	-4.09648000	7.27466000	11.33042600
H	-3.34319600	7.06900000	9.33121000
C	-4.86500500	5.21968100	12.40072100
H	-4.70881600	3.43103400	11.21173700