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Dual-level direct dynamics studies on the hydrogen abstraction reactions of $CH_2CH_{3-n}X_n$ + HBr (X=Cl, Br and *n* = 1, 2)

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Supplementary Material

Table S1 Cartesian coordinates and electronic energies for MPW1K/6-311+G(d,p) optimized geometries of all stationary points

CH_2CH_2Cl				CH_2CHCl_2			
Energy = -538.7930103				Energy = -998.4161798			
C	-1.460212	0.811216	0.000000	C	-0.009670	0.388943	0.420797
H	-1.999361	0.693785	0.925332	H	0.014887	0.393285	1.500907
H	-1.999361	0.693785	-0.925332	C	0.014977	1.731612	-0.152378
C	0.000000	0.856931	0.000000	H	-0.250741	1.874916	-1.185498
H	0.405572	1.327830	0.886462	H	0.469068	2.533540	0.404786
H	0.405572	1.327830	-0.886462	Cl	1.454319	-0.535435	-0.078398
Cl	0.702873	-0.826595	0.000000	Cl	-1.469911	-0.495452	-0.058703
CH_2CH_2Br				CH_2CHBr_2			
Energy = -2652.8523626				Energy = -5226.5296259			
C	0.595565	-2.035394	0.000000	C	-0.024053	0.695597	0.450494
H	1.091283	-2.279975	0.924819	H	0.004213	0.730304	1.528710
H	1.091283	-2.279975	-0.924819	C	0.002335	2.001762	-0.177921
C	-0.567568	-1.172370	0.000000	H	-0.246285	2.104757	-1.220059
H	-1.175276	-1.252913	0.890796	H	0.446305	2.829693	0.350090
H	-1.175276	-1.252913	-0.890796	Br	1.601487	-0.318353	-0.036323
Br	0.000000	0.751782	0.000000	Br	-1.603599	-0.305902	-0.029225
CH_3CH_2Cl				CH_3CHCl_2			
Energy = -539.4641746				Energy = -999.0895033			
C	-1.49669	0.656295	0.000000	C	0.962626	1.432599	0.000000
H	-1.959844	1.641840	0.000000	H	0.926663	2.062402	0.884601
H	-1.836468	0.119422	0.881063	H	0.926663	2.062402	-0.884601
H	-1.836468	0.119422	-0.881063	H	1.895314	0.877435	0.000000
C	0.000000	0.806158	0.000000	C	-0.209239	0.494873	0.000000
H	0.353415	1.328749	-0.881336	H	-1.154851	1.018725	0.000000
H	0.353415	1.328749	0.881336	Cl	-0.209239	-0.517229	-1.458764
Cl	0.818005	-0.783112	0.000000	Cl	-0.209239	-0.517229	1.458764
CH_3CH_2Br				CH_3CHBr_2			
Energy = -2653.5209294				Energy = -5227.2002623			
C	2.060626	-0.394522	0.000001	C	0.000031	2.011233	-0.161869
H	3.047265	0.067994	-0.000330	H	0.884898	2.555447	0.158562
H	1.980461	-1.025526	-0.880454	H	-0.884612	2.555622	0.158879
H	1.980874	-1.025117	0.880784	H	-0.000170	1.950086	-1.245357
C	1.008363	0.680362	0.000001	C	0.000007	0.641919	0.453746
H	1.060107	1.306581	0.882271	H	0.000026	0.669649	1.533370
H	1.060080	1.306533	-0.882304	Br	-1.595103	-0.337846	-0.033667

Br	-0.786935	-0.067014	0.000001	Br	1.595093	-0.337860	-0.033668

HBr				Br			
Energy = -2574.8918725				Energy = -2574.2448174			
Br	0.000000	0.000000	0.039249				
H	0.000000	0.000000	-1.373727				
TS1				TS2			
Energy = -3113.6865625				Energy = -3573.3074846			
C	0.896528	0.911192	0.000014	C	-0.510273	-0.915250	0.674757
H	-0.775434	0.425142	0.000025	H	1.054827	-0.430454	0.334526
H	0.848314	1.474030	-0.920425	H	-0.333703	-1.951897	0.427181
H	0.848316	1.474081	0.920421	H	-0.529423	-0.642153	1.719145
C	1.585298	-0.389573	0.000042	C	-1.351469	-0.144986	-0.257199
H	1.372501	-0.973624	-0.886295	H	-1.050615	-0.266691	-1.288698
H	1.372544	-0.973566	0.886428	Cl	-3.024744	-0.781246	-0.161191
Cl	3.369475	-0.112266	-0.000019	Br	2.451851	-0.112213	-0.077519
Br	-2.166808	-0.075636	-0.000005	Cl	-1.315574	1.580073	0.103290
TS3				TS4			
Energy = -5227.7456698				Energy = -7801.4204353			
C	-0.120732	0.896557	0.000025	C	-0.145742	-1.025336	0.672528
H	1.511254	0.413432	0.000008	H	-1.702476	-0.626788	0.316951
H	-0.073374	1.461207	0.919482	H	-0.147876	-0.735764	1.712777
H	-0.073378	1.461255	-0.919403	H	-0.280075	-2.074415	0.448669
C	-0.814912	-0.391975	-0.000007	C	0.682531	-0.255694	-0.259694
H	-0.633588	-0.979951	0.889469	H	0.439214	-0.430310	-1.297369
H	-0.633592	-0.979906	-0.889513	Br	-3.133398	-0.414467	-0.076635
Br	2.916525	-0.075856	-0.000010	Br	2.529650	-0.891642	-0.068440
Br	-2.758910	-0.049959	0.000006	Br	0.560048	1.636207	0.040560
CR1				CR2			
Energy = -3113.6869597				Energy = -3573.3110042			
C	1.103365	0.947791	0.000164	C	-1.341228	-1.119917	1.238675
H	-0.989261	0.394810	0.000103	H	1.542497	0.805621	0.085321
H	1.002519	1.495387	-0.923972	H	-0.402766	-1.609312	1.438034
H	1.002704	1.495503	0.924251	H	-2.099291	-1.066413	2.000914
C	1.763975	-0.360942	0.000187	C	-1.489631	-0.341724	0.014414
H	1.543914	-0.942073	-0.886443	H	-0.834191	-0.673511	-0.778205
H	1.544110	-0.941931	0.886960	Cl	-3.142936	-0.399200	-0.609710
Cl	3.564303	-0.138553	-0.000032	Br	2.558440	-0.156733	-0.146748
Br	-2.340034	-0.076211	-0.000070	Cl	-1.019799	1.387385	0.308039

CP2				CR3			
Energy = -3573.3378844				Energy = -5227.7462763			
C	1.372962	1.595192	0.638929	C	0.305932	1.000456	0.000026
H	0.353217	1.924951	0.816449	H	-1.797283	0.440339	0.001069
H	1.904374	2.369130	0.091970	H	0.212090	1.549480	-0.923917
H	1.867715	1.432839	1.591142	H	0.213078	1.550412	0.923517
C	1.360103	0.335084	-0.173562	C	0.934285	-0.311679	0.000370
H	0.861453	0.457872	-1.124767	H	0.735751	-0.892881	-0.889862
Cl	3.000149	-0.227075	-0.525809	H	0.736093	-0.892235	0.891103
Br	-2.288329	0.065181	-0.191155	Br	-3.126494	-0.087531	-0.000048
Cl	0.453166	-0.952207	0.674247	Br	2.911036	-0.080692	-0.000074
CR4				CP4			
Energy = -7801.424033				Energy = -7801.4523396			
C	0.549900	-1.545562	0.635207	C	0.670027	1.497349	1.215889
H	-2.285112	0.292530	0.048261	H	-0.378768	1.728390	1.382289
H	0.509921	-1.368240	1.696147	H	1.205326	2.421258	1.011662
H	0.355715	-2.531987	0.248196	H	1.083830	1.042901	2.110067
C	1.062988	-0.522896	-0.255765	C	0.799253	0.584952	0.033911
H	0.880764	-0.722247	-1.300470	H	0.383678	1.000020	-0.872562
Br	-3.550087	-0.337203	-0.083487	Br	-2.743458	0.365743	-0.281604
Br	3.020274	-0.396978	-0.109268	Br	2.637993	0.158825	-0.350970
Br	0.268710	1.212487	0.107933	Br	-0.211956	-1.058464	0.314567

Table S2 Cartesian coordinates and electronic energies for BMK/6-311+G(d,p) optimized geometries of all stationary points

CH_2CH_2Cl				CH_2CHCl_2			
Energy = -538.6005366				Energy = -998.0844585			
C	-1.470441	0.825345	0.000000	C	-0.010584	0.405565	0.433827
H	-2.010988	0.701646	0.931943	H	0.015437	0.400912	1.520252
H	-2.010988	0.701646	-0.931943	C	0.019172	1.749799	-0.159154
C	0.000000	0.882710	0.000000	H	-0.246110	1.878978	-1.201727
H	0.414487	1.340482	0.897006	H	0.469304	2.563563	0.398118
H	0.414487	1.340482	-0.897006	Cl	1.475269	-0.544103	-0.079072
Cl	0.706803	-0.843093	0.000000	Cl	-1.492337	-0.501523	-0.060027
CH_2CH_2Br				CH_2CHBr_2			
Energy = -2651.3327064				Energy = -5223.5439471			
C	0.603613	-2.049861	0.000000	C	-0.027195	0.707540	0.459054
H	1.104493	-2.289899	0.931403	H	0.004497	0.739846	1.544138
H	1.104493	-2.289899	-0.931403	C	0.005136	2.019882	-0.182328
C	-0.577022	-1.194084	0.000000	H	-0.245099	2.114815	-1.232295
H	-1.184265	-1.266955	0.899717	H	0.449316	2.856140	0.347164
H	-1.184265	-1.266955	-0.899717	Br	1.616787	-0.321889	-0.036551
Br	0.000000	0.759354	0.000000	Br	-1.618968	-0.308835	-0.029717
CH_3CH_2Cl				CH_3CHCl_2			
Energy = -539.2707907				Energy = -998.7570585			
C	-1.515023	0.666275	0.000000	C	0.980588	1.449113	0.000000
H	-1.982893	1.657518	0.000000	H	0.945881	2.081194	0.891906
H	-1.848794	0.123292	0.887955	H	0.945881	2.081194	-0.891906
H	-1.848794	0.123292	-0.887955	H	1.911558	0.877487	0.000000
C	0.000000	0.826422	0.000000	C	-0.212990	0.510609	0.000000
H	0.359002	1.342910	-0.890690	H	-1.167248	1.032108	0.000000
H	0.359002	1.342910	0.890690	Cl	-0.212990	-0.524421	-1.480695
Cl	0.826624	-0.796830	0.000000	Cl	-0.212990	-0.524421	1.480695
CH_3CH_2Br				CH_3CHBr_2			
Energy = -2652.0003384				Energy = -5224.2139573			
C	-2.080387	-0.401062	0.000107	C	-0.000003	2.033235	-0.164359
H	-3.074643	0.061538	0.000272	H	0.891356	2.579957	0.157853
H	-1.992474	-1.033264	0.887375	H	-0.891326	2.579978	0.157914
H	-1.992663	-1.033035	-0.887344	H	-0.000040	1.964234	-1.254566
C	-1.017999	0.692074	0.000136	C	0.000000	0.647053	0.462131
H	-1.068816	1.318720	-0.890051	H	-0.000002	0.673419	1.548777
H	-1.068695	1.318556	0.890444	Br	-1.610510	-0.341134	-0.034237
Br	0.793932	-0.067960	-0.000061	Br	1.610511	-0.341133	-0.034237

HBr				Br			
Energy = -2573.414869				Energy = -2572.773766			
Br	0.000000	0.000000	0.039584				
H	0.000000	0.000000	-1.385451				
TS1				TS2			
Energy = -3112.0169738				Energy = -3571.4989579			
C	-0.917982	0.973803	0.000020	C	-0.549810	-0.962608	0.720767
H	0.800931	0.494004	0.000002	H	1.080024	-0.461037	0.387944
H	-0.893874	1.540022	0.927425	H	-0.378753	-2.007049	0.470906
H	-0.893881	1.540069	-0.927357	H	-0.598749	-0.684650	1.770142
C	-1.554477	-0.367373	-0.000011	C	-1.340649	-0.164298	-0.248793
H	-1.333268	-0.946103	0.895886	H	-1.026068	-0.295133	-1.282067
H	-1.333280	-0.946057	-0.895941	Cl	-3.071225	-0.745036	-0.186342
Cl	-3.384087	-0.141106	0.000007	Br	2.454328	-0.119550	-0.085554
Br	2.171932	-0.083478	-0.000005	Cl	-1.260257	1.591716	0.116673
TS3				TS4			
Energy = -5224.7489067				Energy = -7796.9582534			
C	-0.138131	0.959692	0.000019	C	-0.099805	-1.078756	0.726248
H	1.543294	0.470402	0.000002	H	-1.718854	-0.674384	0.362504
H	-0.106022	1.527463	0.926321	H	-0.083624	-0.780294	1.771218
H	-0.106028	1.527512	-0.926253	H	-0.220005	-2.137032	0.503487
C	-0.797796	-0.361820	-0.000013	C	0.683620	-0.281090	-0.241914
H	-0.606285	-0.947281	0.897482	H	0.426055	-0.476869	-1.279734
H	-0.606296	-0.947233	-0.897541	Br	-3.130704	-0.431187	-0.086300
Br	2.931763	-0.084946	-0.000009	Br	2.580270	-0.846885	-0.082047
Br	-2.774709	-0.064142	0.000007	Br	0.495963	1.627434	0.046533

Table S3 Frequencies (in cm^{-1}) of the reactants, products, complexes, and transition-states calculated at the MPW1K/6-311+G(d,p) and BMK/6-311+G(d,p) levels along with the available experimental values

Species	MPW1K/6-311+G(d,p) (BMK/6-311+G(d,p))
HBr	2652(2625)[2649][a]
CH_2CH_2Cl	198,305,590,676,774,1066,1093,1253,1267,1445,1483,3081,3129,3145,3241 (247,301,603,683,771,1051,1073,1239,1241,1444,1481,3067,3106,3136,3220)
CH_2CHCl_2	144,274,296,399,580,647,718,1003,1128,1242,1301,1440,3135,3136,3256 (165,267,294,397,588,651,728,1001,1112,1230,1296,1436,3109,3135,3235)
CH_2CH_2Br	260,264,464,673,766,1019,1097,1194,1240,1443,1485,3093,3129,3164,3241 (259,301,455,679,771,1012,1071,1183,1240,1446,1493,3075,3105,3147,3219)
CH_2CHBr_2	153,180,251,337,504,577,655,984,1122,1177,1272,1440,3131,3152,3250 (148,179,250,338,500,580,651,983,1100,1176,1270,1437,3105,3138,3229)
CH_3CH_2Cl	262,332,689,780,990,1080,1092,1271,1322,1404,1469,1476,1484,3017,3068,3094,3103,3133 (283,329,691,779,978,1073,1079,1264,1315,1399,1477,1481,1490,2996,3054,3073,3083,3122) [251,336,677,786,974,974,1081,1251,1289,1385,1448,1448,1463,2881,2946,2967,2986,3014][b]
CH_3CHCl_2	271,281,320,405,661,724,995,1071,1109,1271,1305,1407,1465,1469,3028,3112,3116,3135 (266,273,322,400,669,749,988,1075,1096,1258,1289,1405,1474,1476,2999,3078,3092,3130)

CH_3CH_2Br	261,286,582,765,978,1036,1084,1258,1282,1401,1469,1472,1482,3013,3075,3090,3105,3143 (283,287,587,776,968,1031,1070,1256,1271,1401,1482,1482,1497,2994,3050,3069,3083,3118) [247,290,583,770,964,964,1061,1247,1258,1386,1451,1451,1451,2880,2937,2988,2988,3018][b]
CH_3CHBr_2	172,260,289,341,556,633,974,1059,1096,1207,1281,1404,1464,1469,3023,3103,3117,3146 (171,270,297,341,558,644,971,1066,1081,1213,1279,1405,1473,1482,3000,3078,3093,3131)
TS1	113i,51,55,320,335,559,603,681,777,799,1068,1085,1265,1280,1446,1481,1714,3084,3109,3149,3217 (167i,50,66,301,364,545,615,681,779,796,1061,1068,1253,1259,1449,1487,1707,3064,3084,3132,3194)
TS2	194i,44,48,270,296,359,400,576,647,681,723,792,1015,1115,1241,1297,1436,1531,3108,3128,3222 (177i,45,50,264,289,349,398,559,633,679,727,795,1010,1099,1228,1282,1433,1626,3084,3127,3201)
TS3	127i,48,52,268,366,528,609,644,769,801,1026,1090,1218,1252,1443,1480,1613,3095,3109,3165,3216 (135i,44,58,261,392,518,593,652,771,795,1023,1069,1209,1248,1448,1488,1660,3075,3083,3146,3192)
TS4	207i,37,46,165,241,332,385,528,597,642,689,797,998,1106,1175,1268,1436,1475,3103,3144,3215 (174i,36,53,165,241,338,376,526,590,633,692,798,994,1086,1159,1257,1435,1556,3078,3125,3192)
CR1	24,37,53,237,302,338,361,640,744,775,1067,1089,1260,1275,1445,1482,2393,3082,3117,3146,3227
CR2	18,29,55,167,203,239,275,298,400,575,645,715,1007,1130,1247,1304,1440,2608,3134,3136,3257
CP2	21,43,76,271,281,318,403,655,718,993,1070,1110,1268,1303,1407,1465,1467,3029,3114,3119,3139
CR3	22,32,48,260,269,318,380,504,746,766,1022,1093,1207,1247,1442,1484,2389,3094,3118,3164,3228

CR4	11,16,39,120,171,211,252,261,337,517,563,655,981,1124,1178,1274,1440,2583,3133,3154,3253
CP4	28,53,95,174,262,290,339,552,627,975,1057,1098,1202,1282,1405,1464,1468,3025,3108,3120,3150

[a]From ref.[20] [b]From ref.[21]

Table S4 Cartesian coordinates and electronic energies for MPW1K/6-311+G(2df,2p) optimized geometries of all stationary points

CH_2CH_2Cl				CH_2CHCl_2			
Energy = -538.8016635				Energy = -998.4294125			
C	-1.456656	0.804349	0.000000	C	-0.010018	0.388034	0.422258
H	-1.993981	0.683992	0.923372	H	0.015129	0.388912	1.500725
H	-1.993981	0.683992	-0.923372	C	0.021326	1.727486	-0.151005
C	0.000000	0.855788	0.000000	H	-0.261331	1.873259	-1.177090
H	0.405654	1.325146	0.884717	H	0.501539	2.520475	0.392983
H	0.405654	1.325146	-0.884717	Cl	1.446019	-0.537116	-0.079150
Cl	0.700976	-0.822300	0.000000	Cl	-1.465030	-0.490870	-0.058741
CH_2CH_2Br				CH_2CHBr_2			
Energy = -2652.853998				Energy = -5226.5287684			
C	0.595098	-2.027151	0.000000	C	-0.023575	0.695696	0.450687
H	1.090258	-2.270473	0.922846	H	0.004997	0.728222	1.526642
H	1.090258	-2.270473	-0.922846	C	0.005167	1.997713	-0.178075
C	-0.567102	-1.168491	0.000000	H	-0.244745	2.099213	-1.217817
H	-1.174247	-1.247663	0.888541	H	0.447396	2.825239	0.347591
H	-1.174247	-1.247663	-0.888541	Br	1.593271	-0.318314	-0.036284
Br	0.000000	0.748861	0.000000	Br	-1.596049	-0.304918	-0.029205
CH_3CH_2Cl				CH_3CHCl_2			
Energy = -539.4729612				Energy = -999.1027489			
C	-1.493497	0.651788	0.000000	C	0.962299	1.429754	0.000000
H	-1.958881	1.633883	0.000000	H	0.928684	2.057555	0.883474
H	-1.830276	0.114323	0.878931	H	0.928684	2.057555	-0.883474
H	-1.830276	0.114323	-0.878931	H	1.890415	0.871575	0.000000
C	0.000000	0.804651	0.000000	C	-0.209200	0.495487	0.000000
H	0.353359	1.325822	-0.879560	H	-1.153569	1.017827	0.000000
H	0.353359	1.325822	0.879560	Cl	-0.209200	-0.516352	-1.451712
Cl	0.816100	-0.779577	0.000000	Cl	-0.209200	-0.516352	1.451712
CH_3CH_2Br				CH_3CHBr_2			
Energy = -2653.5226159				Energy = -5227.1993616			
C	-2.053541	-0.393819	0.000083	C	-0.000004	2.007780	-0.161548
H	-3.039850	0.063968	0.000287	H	0.883285	2.551684	0.156387
H	-1.971273	-1.023510	0.878336	H	-0.883247	2.551711	0.156472
H	-1.971509	-1.023239	-0.878386	H	-0.000057	1.943959	-1.242610
C	-1.004926	0.679954	0.000108	C	0.000000	0.641892	0.453621
H	-1.055617	1.305050	-0.879959	H	-0.000003	0.667781	1.530972
H	-1.055525	1.304922	0.880271	Br	-1.587516	-0.337332	-0.033624
Br	0.784131	-0.066971	-0.000048	Br	1.587517	-0.337330	-0.033624

HBr				Br			
Energy = -2574.888738				Energy = -2574.2405207			
Br	0.000000	0.000000	0.039175				
H	0.000000	0.000000	-1.371118				
TS1				TS2			
Energy = -3113.6922199				Energy = -3573.3176909			
C	0.893595	0.908420	0.000001	C	-0.508492	-0.915477	0.677904
H	-0.767694	0.424184	0.000000	H	1.047962	-0.441182	0.333528
H	0.845733	1.470486	-0.918136	H	-0.338615	-1.952552	0.437203
H	0.845733	1.470488	0.918136	H	-0.526075	-0.637607	1.718605
C	1.579375	-0.390595	0.000002	C	-1.342662	-0.145009	-0.256079
H	1.366229	-0.974923	-0.883703	H	-1.040227	-0.265205	-1.285519
H	1.366231	-0.974920	0.883710	Cl	-3.011258	-0.777829	-0.163442
Cl	3.356587	-0.111233	-0.000001	Br	2.441910	-0.110785	-0.078013
Br	-2.158744	-0.075180	0.000000	Cl	-1.312446	1.574120	0.104365
TS3				TS4			
Energy = -5227.7441948				Energy = -7801.4165113			
C	-0.117185	0.890392	0.000023	C	-0.144303	-1.026298	0.682834
H	1.497163	0.412201	0.000006	H	-1.689352	-0.638457	0.321836
H	-0.069746	1.454544	0.917061	H	-0.148184	-0.729759	1.718693
H	-0.069752	1.454591	-0.916985	H	-0.273633	-2.075604	0.467858
C	-0.811398	-0.394636	-0.000008	C	0.674535	-0.258657	-0.253985
H	-0.631370	-0.982867	0.886849	H	0.428323	-0.434521	-1.288459
H	-0.631376	-0.982822	-0.886896	Br	-3.116441	-0.412229	-0.078506
Br	2.904342	-0.075062	-0.000011	Br	2.518784	-0.884650	-0.071076
Br	-2.747868	-0.048658	0.000007	Br	0.554841	1.627966	0.041210

Table S5 Cartesian coordinates and electronic energies for MPW1K/ma-TZVP optimized geometries of all stationary points

CH_2CH_2Cl				CH_2CHCl_2			
Energy = -538.8049464				Energy = -998.4328558			
C	-1.456874	0.802473	0.000000	C	-0.009890	0.386198	0.421494
H	-1.994227	0.680854	0.924316	H	0.015159	0.388055	1.501315
H	-1.994227	0.680854	-0.924316	C	0.022085	1.727298	-0.150399
C	0.000000	0.855427	0.000000	H	-0.261033	1.873954	-1.177136
H	0.405595	1.324927	0.886112	H	0.505907	2.518998	0.394121
H	0.405595	1.324927	-0.886112	Cl	1.444926	-0.537206	-0.079227
Cl	0.701089	-0.821115	0.000000	Cl	-1.464526	-0.489969	-0.058707
CH_2CH_2Br				CH_2CHBr_2			
Energy = -2652.901127				Energy = -5226.6199179			
C	0.595346	-2.026901	0.000000	C	-0.023440	0.695355	0.450835
H	1.091184	-2.269426	0.923762	H	0.005188	0.728712	1.528165
H	1.091184	-2.269426	-0.923762	C	0.005333	1.997939	-0.178139
C	-0.567527	-1.168652	0.000000	H	-0.244631	2.099380	-1.218788
H	-1.174641	-1.247956	0.889976	H	0.448960	2.825688	0.347964
H	-1.174641	-1.247956	-0.889976	Br	1.593680	-0.318396	-0.036316
Br	0.000000	0.748802	0.000000	Br	-1.596562	-0.304848	-0.029213
CH_3CH_2Cl				CH_3CHCl_2			
Energy = -539.4758813				Energy = -999.105801			
C	-1.493990	0.650247	0.000000	C	0.961504	1.430063	0.000000
H	-1.960133	1.633166	0.000000	H	0.925791	2.058068	0.884542
H	-1.830219	0.111975	0.879931	H	0.925791	2.058068	-0.884542
H	-1.830219	0.111975	-0.879931	H	1.891066	0.872370	0.000000
C	0.000000	0.802831	0.000000	C	-0.208935	0.493767	0.000000
H	0.352251	1.326106	-0.880334	H	-1.154277	1.017131	0.000000
H	0.352251	1.326106	0.880334	Cl	-0.208935	-0.516136	-1.450773
Cl	0.816471	-0.778105	0.000000	Cl	-0.208935	-0.516136	1.450773
CH_3CH_2Br				CH_3CHBr_2			
Energy = -2653.5693391				Energy = -5227.2901459			
C	-2.053567	-0.394112	0.000083	C	-0.000005	2.007989	-0.161874
H	-3.040421	0.065205	0.000288	H	0.884390	2.551632	0.157201
H	-1.970875	-1.023811	0.879586	H	-0.884343	2.551665	0.157301
H	-1.971113	-1.023539	-0.879638	H	-0.000067	1.943571	-1.243929
C	-1.005036	0.679889	0.000108	C	0.000000	0.641851	0.453576
H	-1.056059	1.305081	-0.881401	H	-0.000003	0.668810	1.532310
H	-1.055968	1.304954	0.881712	Br	-1.587895	-0.337354	-0.033616
Br	0.784173	-0.066930	-0.000048	Br	1.587896	-0.337352	-0.033616

HBr				Br			
Energy = -2574.9320231				Energy = -2574.2843997			
Br	0.000000	0.000000	0.039207				
H	0.000000	0.000000	-1.372251				
TS1				TS2			
Energy = -3113.738736				Energy = -3573.3642391			
C	0.890618	0.899131	0.000001	C	-0.504203	-0.910044	0.669344
H	-0.760378	0.409447	0.000001	H	1.045599	-0.429969	0.320799
H	0.843190	1.461808	-0.919001	H	-0.333432	-1.947408	0.425981
H	0.843190	1.461811	0.919001	H	-0.520369	-0.633860	1.711539
C	1.584231	-0.396563	0.000003	C	-1.348479	-0.142131	-0.259087
H	1.373658	-0.982132	-0.884943	H	-1.049542	-0.260403	-1.291159
H	1.373662	-0.982128	0.884952	Cl	-3.010594	-0.785005	-0.158605
Cl	3.357012	-0.106197	-0.000001	Br	2.447966	-0.109810	-0.076348
Br	-2.159761	-0.073682	0.000000	Cl	-1.324992	1.574890	0.102340
TS3				TS4			
Energy = -5227.8345412				Energy = -7801.5508054			
C	-0.114748	0.881055	0.000022	C	-0.145276	-1.026488	0.679369
H	1.490915	0.398392	0.000005	H	-1.687336	-0.638215	0.315372
H	-0.068211	1.445710	0.917986	H	-0.149815	-0.729333	1.716053
H	-0.068217	1.445758	-0.917913	H	-0.271054	-2.077184	0.463907
C	-0.814291	-0.401670	-0.000009	C	0.675499	-0.257914	-0.256110
H	-0.636763	-0.990516	0.888354	H	0.429693	-0.433752	-1.292127
H	-0.636770	-0.990469	-0.888404	Br	-3.117996	-0.412029	-0.077820
Br	2.906059	-0.073357	-0.000010	Br	2.518896	-0.885651	-0.070242
Br	-2.749109	-0.046220	0.000007	Br	0.556162	1.628678	0.041125