

TABLE S1: GAUSSIAN 98 Archive Entries of B3-LYP/6-31G(d) Optimized

Geometries

TS1

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1\1\GINC-RSCQC8\FTS\RB3LYP\6-31G(d)\C2H6\STEFAN\27-Oct-1998\0\#\ RB3LY
P/6-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXD
ISK=1048576000\direct (uncatalyzed) hydrogenation of ethylene\0,1\H,
-1.3527949532,0.,-1.3972441695\H,-1.0072554989,0.,-0.1609879378\C,0.13
57447896,0.,-0.6236545027\C,0.118229775,0.,0.8126813937\H,0.4084578028
,0.9148194897,-1.1395398405\H,0.4084578028,-0.9148194897,-1.1395398405
\H,0.0096437293,0.9326623071,1.3515752213\H,0.0096437293,-0.9326623071
,1.3515752213\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-79.6278633\
RMSD=1.960e-09\RMSF=3.308e-05\Dipole=0.2264144,0.,0.0683402\PG=CS [SG(
C2H2),X(H4)]\@
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TS2(F)

```
1\1\GINC-RSCQC2\FTS\RB3LYP\6-31G(d)\C2H7F1\STEFAN\02-Dec-1998\0\#\ B3L
YP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORAM
AN MAXDISK=786432000 SCF=DIRECT TEST\TS: HF-catalyzed hydrogenation o
f ethene\0,1\H,1.1859488721,-1.0340987666,0.\C,-0.4682516997,-1.24618
45545,0.\C,-1.0760836852,0.0258507849,0.\H,-0.0100226504,0.7827511495,
0.\H,-0.3644757027,-1.8229325299,0.9157497583\H,-0.3644757027,-1.82293
25299,-0.9157497583\H,-1.5863059826,0.315454133,-0.9190839588\H,-1.586
3059826,0.315454133,0.9190839588\H,1.3633215738,-0.1937795278,0.\F,1.1
809253205,1.1980096174,0.\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=
-180.1146568\RMSD=6.352e-09\RMSF=4.439e-05\Dipole=-0.8294334,-1.078248
6,0.\PG=CS [SG(C2H3F1),X(H4)]\@
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TS2(Cl)

```
1\1\GINC-RSCQC8\FTS\RB3LYP\6-31G(d)\C2H7Cl1\STEFAN\02-Dec-1998\0\#\ B3
LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORA
MAN MAXDISK=1048576000 SCF=DIRECT TEST\TS: HCl-catalyzed hydrogenatio
n of ethene\0,1\H,-1.6807348225,0.,-0.4828668917\C,-0.6241218431,0.,-
1.8816988467\C,0.6850881482,0.,-1.3576421175\H,0.5338635069,0.,-0.1365
865864\H,-1.1113928484,0.9210080767,-2.1900124777\H,-1.1113928484,-0.9
210080767,-2.1900124777\H,1.2589434915,-0.9170828683,-1.5012968893\H,1
.2589434915,0.9170828683,-1.5012968893\H,-1.3891535373,0.,0.2668457368
\C1,0.1103015139,0.,1.598310133\Version=IBM-RS6000-G98RevA.6\State=1-
A'\HF=-540.5107078\RMSD=9.563e-09\RMSF=7.751e-06\Dipole=-0.262612,0.,-
2.2346045\PG=CS [SG(C2H3Cl1),X(H4)]\@
```

TS2(Br)

```
1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H7Br1\ROOT\01-Mar-1999\0\#\ B3LY
P/6-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXD
ISK=1048576000\TS: ethylene + H2 + HBr (Bertran-type)\0,1\H,-1.68757
95665,0.,-1.1796145616\C,-0.5546505531,0.,-2.5457352781\C,0.7175187366
,0.,-1.9402709838\H,0.5140487526,0.,-0.7207728987\H,-1.0252528931,0.92
14918419,-2.8768890735\H,-1.0252528931,-0.9214918419,-2.8768890735\H,1
.3010411017,-0.9159187039,-2.0490198897\H,1.3010411017,0.9159187039,-2
.0490198897\H,-1.4813556043,0.,-0.4056779319\Br,0.0321743114,0.,1.1163
977397\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-2652.0267455\RMSD=
4.988e-09\RMSF=1.641e-05\Dipole=-0.1104634,0.,-2.0494204\PG=CS [SG(C2H
3Br1),X(H4)]\@
```

HAIF₄ (1)

```
1\1\GINC-RSCQC9\FOpt\RB3LYP\6-31G(d)\Al1F4H1\ROOT\08-Feb-1999\0\#\ RB3
LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC) FREQ=NORAMAN SCF=DIRECT
TEST MAXDISK=1048576000\aluminiumtrifluoride-hydrogen fluoride AlF3.H
F\0,1\H,-1.551743461,0.,-0.9027602422\F,-1.6735580537,0.,0.0739256911
\Al,0.2785803841,0.,0.0835490539\F,-0.0545636132,0.,-1.5870926928\F,0.
7490718594,1.4290096187,0.7463958643\F,0.7490718594,-1.4290096187,0.74
63958643\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-642.6344434\RMSD
=7.335e-09\RMSF=5.157e-05\Dipole=-0.8520431,0.,-0.4626446\PG=CS [SG(Al
1F2H1),X(F2)]\@
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HAICl₄ (2)

```
1\1\GINC-PC\FOpt\RB3LYP\6-31G(d)\Al1Cl4H1\SXS501\04-Dec-1998\0\#\ B3LY
P/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC) FREQ=NORAMAN SCF=DIRECT TE
ST MAXDISK=5242880000\AlCl3 . HCl complex\0,1\H,0.,-0.9347053916,2.4
942435375\Cl,0.,-1.695446226,1.4459151697\Al,0.,0.2927385548,-0.298280
2912\Cl,0.,1.7865200024,1.2013810605\Cl,1.8080565724,-0.1299750006,-1.
2829598725\Cl,-1.8080565724,-0.1299750006,-1.2829598725\Version=SGI-G
94RevE.2\State=1-A'\HF=-2084.0385119\RMSD=2.946e-09\RMSF=5.924e-06\Dip
ole=0.,-0.66876,1.2513633\PG=CS [SG(Al1Cl2H1),X(Cl2)]\@
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HAIBr₄ (3)

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1\1\GINC-RSCQC9\FOpt\RB3LYP\6-31G(d)\Al1Br4H1\ROOT\01-Mar-1999\0\#\ B3
LYP/6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=104857600
0\AlBr3.HBr complex\0,1\Br,0.,1.5180773785,1.7505026732\Al,0.,0.4014
796677,-0.2079438569\Br,-1.9312346193,0.204585021,-1.3522532716\Br,1.9
312346193,0.204585021,-1.3522532716\Br,0.,-1.9953202588,1.0351469919\H
,0.,-2.8366863396,-0.1367391268\Version=IBM-RS6000-G98RevA.6\State=1-
A'\HF=-10530.103492\RMSD=2.597e-09\RMSF=4.708e-06\Dipole=0.,-1.4438857
,0.2636727\PG=CS [SG(Al1Br2H1),X(Br2)]\@
```

ethene (4)

```
1\1\GINC-PC\FOpt\RB3LYP\6-31G(d)\C2H4\SXS501\16-Sep-1998\0\#\ B3LYP/6-
31G* OPT FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=5242880000\ethylene\0,
1\H,0.923534299,0.,-1.2394373302\C,0.,0.,-0.6655112598\C,0.,0.,0.66551
12598\H,-0.923534299,0.,-1.2394373302\H,0.923534299,0.,1.2394373302\H,
-0.923534299,0.,1.2394373302\Version=SGI-G94RevE.2\State=1-AG\HF=-78.
5874573\RMSD=5.440e-09\RMSF=7.780e-05\Dipole=0.,0.,0.\PG=D02H [C2"(Cl.
Cl),SG(H4)]\@
```

hydrogen (5)

```
1\1\GINC-PC\FOpt\RB3LYP\6-31G(d)\H2\SXS501\11-Sep-1998\0\#\ B3LYP/6-31
G* OPT FREQ SCF=DIRECT TEST MAXDISK=5242880000\Wasserstoff\0,1\H,0.,
0.,-0.3712178894\H,0.,0.,0.3712178894\Version=SGI-G94RevE.2\State=1-S
GG\HF=-1.1754823\RMSD=2.702e-10\RMSF=1.456e-04\Dipole=0.,0.,0.\PG=D*H
[C*(H1.H1)]\@
```

hydrogen fluoride (6)

```
1\1\GINC-RSCQC8\FOpt\RB3LYP\6-31G(d)\F1H1\STEFAN\01-Dec-1998\0\#\ B3LY
P/6-31G* OPT FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=39321600\hydrogen f
luoride\0,1\H,0.,0.,-0.8404046041\F,0.,0.,0.0933782893\Version=IBM-R
S6000-G98RevA.6\State=1-SG\HF=-100.4201721\RMSD=8.604e-10\RMSF=1.392e-
06\Dipole=0.,0.,-0.7315565\PG=C*V [C*(H1F1)]\@
```

hydrogen chloride (7)

```
1\1\GINC-RSCQC8\FOpt\RB3LYP\6-31G(d)\Cl1H1\STEFAN\02-Dec-1998\0\#\ B3L
YP/6-31G* OPT FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=1048576000\hydroge
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n chloride\0,1\H,0.,0.,-1.2179563747\Cl,0.,0.,0.0716444926\Version=IBM-RS6000-G98RevA.6\State=1-SG\HF=-460.7957\RMSD=4.772e-09\RMSF=8.135e-08\Dipole=0.,0.,-0.5776337\PG=C*V [C*(H1Cl1)]\@

hydrogen bromide (8)

1\1\GINC-RSCQC9\FOpt\RB3LYP\6-31G(d)\Br1H1\ROOT\28-Feb-1999\0\# B3LYP/6-31G* OPT FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=39321600\hydrogen bromide\0,1\H,0.,0.,-1.3989859108\Br,0.,0.,0.039971026\Version=IBM-RS6000-G98RevA.6\State=1-SG\HF=-2572.3012759\RMSD=8.521e-10\RMSF=5.244e-06\Dipole=0.,0.,-0.3995101\PG=C*V [C*(H1Br1)]\@

[H₂C=CH₂•HF]

1\1\GINC-RSCQC9\FOpt\RB3LYP\6-31G(d)\C2H5F1\ROOT\11-Dec-1998\0\# B3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC,TIGHT) NOSYMM FREQ=NORAMAN MAXDISK=1048576000 SCF=DIRECT TEST\ethylene - HF complex\0,1\F,0.000000007,0.,1.9443432922\H,0.0000000004,0.,1.0028021282\C,0.6678908031,0.,-1.154966112\C,-0.6678908034,0.,-1.1549661108\H,-1.2407038526,0.9243015203,-1.1611132274\H,1.2407038521,0.9243015204,-1.1611132234\H,-1.2407038525,-0.9243015203,-1.161113225\H,1.2407038522,-0.9243015204,-1.1611132258\Version=IBM-RS6000-G98RevA.6\HF=-179.0164333\RMSD=2.255e-09\RMSF=2.654e-09\Dipole=0.,0.,-1.0689565\PG=C02V [C2(H1F1),SGV(C2),X(H4)]\@

[H₂C=CH₂•HCl]

1\1\GINC-RSCQC8\FOpt\RB3LYP\6-31G(d)\C2H5Cl1\STEFAN\08-Feb-1999\0\# B3LYP/6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=1048576000\H2C=CH2 + H-Cl complex\0,1\Cl,0.,0.,-1.7623297057\H,0.,0.,-0.4604129881\C,0.,-0.667565562,1.8996465547\C,0.,0.667565562,1.8996465547\H,-0.9241258042,1.2406439093,1.9060648322\H,0.9241258042,1.2406439093,1.9060648322\H,-0.9241258042,-1.2406439093,1.9060648322\H,0.9241258042,-1.2406439093,1.9060648322\Version=IBM-RS6000-G98RevA.6\State=1-A1\HF=-539.3888961\RMSD=4.405e-09\RMSF=3.910e-06\Dipole=0.,0.,0.9691884\PG=C02V [C2(H1Cl1),SGV(C2),X(H4)]\@

[H₂C=CH₂•HBr]

1\1\GINC-PC\FOpt\RB3LYP\6-31G(d)\C2H5Br1\SXS501\01-Mar-1999\0\# B3LYP/6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=5242880000\ethylene - HBr complex\0,1\Br,0.,0.,-1.2182220865\H,0.,0.,0.2325751173\C,0.6674640586,0.,2.6489643603\C,-0.6674640586,0.,2.6489643603\H,-1.2405719241,-0.9240787869,2.6544063963\H,1.2405719241,-0.9240787869,2.6544063963\H,-1.2405719241,0.9240787869,2.6544063963\H,1.2405719241,0.9240787869,2.6544063963\Version=SGI-G98RevA.6\State=1-A1\HF=-2650.8937439\RMSD=3.467e-09\RMSF=2.485e-06\Dipole=0.,0.,0.808935\PG=C02V [C2(H1Br1),SGV(C2),X(H4)]\@

TS3(F)

1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H5F1\ROOT\11-Dec-1998\0\# B3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORAMAN MAXDISK=1048576000 SCF=DIRECT TEST\TS: addition of HF to ethylene\0,1\F,-0.4632585538,0.,-1.2400501534\H,-0.8647870301,0.,-0.0530894288\C,-0.2310659846,0.,1.1534362362\C,0.7933205146,0.,0.1933504189\H,1.2828746642,0.9180492636,-0.1148067183\H,1.2828746642,-0.9180492636,-0.1148067183\H,-0.452581247,0.9240703305,1.6812171577\H,-0.452581247,-0.9240703305,1.6812171577\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-178.9501384\RMSD=8.535e-09\RMSF=7.137e-05\Dipole=0.5884536,0.,0.7467487\PG=CS [SG(C2H1F1),X(H4)]\@

TS3(Cl)

1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H5Cl1\ROOT\07-Feb-1999\0\#\ B3LYP/6-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=1048576000\TS: H2C=CH2 + H-Cl\0,1\Cl,-0.2175808436,0.,-1.3341059674\H,-0.7400775835,0.,0.4185194731\Cl,-0.3872318057,0.,1.6286396554\Cl,0.9102965185,0.,1.108310814\H,1.431224925,0.9226529506,0.8749181382\H,1.431224925,-0.9226529506,0.8749181382\H,-0.780943101,0.9254816328,2.0448714401\H,-0.780943101,-0.9254816328,2.0448714401\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-539.330357\RMSD=2.094e-09\RMSF=5.693e-05\Dipole=0.6024673,0.,2.1700777\PG=CS [SG(C2H1Cl1),X(H4)]\@

TS3(Br)

1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H5Br1\ROOT\01-Mar-1999\0\#\ B3LYP/6-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=1048576000\TS: ethylene + HBr\0,1\Br,-0.049196237,0.,-0.9311972667\H,-0.784094928,0.,0.875775042\Cl,-0.5394993678,0.,2.1099810186\Cl,0.8262833775,0.,1.8015249225\H,1.3743655353,0.922889208,1.6424661266\H,1.3743655353,-0.922889208,1.6424661266\H,-0.9817359534,0.9236982691,2.4810806964\H,-0.9817359534,-0.9236982691,2.4810806964\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-2650.8416169\RMSD=1.496e-09\RMSF=9.244e-06\Dipole=0.3508862,0.,2.1089835\PG=CS [SG(C2H1Br1),X(H4)]\@

CH₃CH₂F

1\1\GINC-RSCQC8\Fopt\RB3LYP\6-31G(d)\C2H5F1\STEFAN\09-Feb-1999\0\#\ B3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=1048576000\fluoroethane\0,1\H,-0.9375198185,0.8877643562,1.2069159876\H,-0.9375198185,-0.8877643562,1.2069159876\Cl,-0.2974420306,0.,1.1770015159\H,0.3369805421,0.,2.0708801125\Cl,0.5543565808,0.,-0.0774317485\H,1.1953362512,0.8896748327,-0.1249003313\H,1.1953362512,-0.8896748327,-0.1249003313\F,-0.2660111898,0.,-1.2035922255\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-179.0564197\RMSD=2.128e-09\RMSF=2.528e-05\Dipole=0.3349503,0.,0.5866017\PG=CS [SG(C2H1F1),X(H4)]\@

CH₃CH₂Cl

1\1\GINC-RSCQC9\Fopt\RB3LYP\6-31G(d)\C2H5Cl1\ROOT\07-Feb-1999\0\#\ B3LYP/6-31G* OPT FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=39321600\H3C-CH2Cl\0,1\H,0.0986773054,0.,-2.5848495465\Cl,-0.40136892,0.,-1.6081519425\Cl,0.6452549808,0.,-0.5078785402\Cl,-0.1202108739,0.,1.1452709582\H,-1.0383246294,0.8874205368,-1.5475289633\H,-1.0383246294,-0.8874205368,-1.5475289633\H,1.2791202225,0.8879542304,-0.5467579604\H,1.2791202225,-0.8879542304,-0.5467579604\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-539.426267\RMSD=4.939e-09\RMSF=6.946e-05\Dipole=0.3031073,0.,-0.8392715\PG=CS [SG(C2H1Cl1),X(H4)]\@

CH₃CH₂Br

1\1\GINC-RSCQC9\Fopt\RB3LYP\6-31G(d)\C2H5Br1\ROOT\01-Mar-1999\0\#\ B3LYP/6-31G* OPT FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=1048576000\CH3CH2Br\0,1\H,0.050751284,0.,-3.0852620715\Cl,-0.4028640267,0.,-2.0852803504\Cl,0.692477417,0.,-1.0353322909\Br,-0.0672445586,0.,0.7989004407\H,-1.0368235059,0.8868141644,-1.9951958848\H,-1.0368235059,-0.8868141644,-1.9951958848\H,1.3193874677,0.8905302574,-1.0810928685\H,1.3193874677,-0.8905302574,-1.0810928685\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-2650.9347583\RMSD=3.078e-09\RMSF=2.215e-05\Dipole=0.2535916,0.,-0.8167726\PG=CS [SG(C2H1Br1),X(H4)]\@

TS4(F)

1\1\GINC-RSCQC8\FTS\RB3LYP\6-31G(d)\C2H7F1\STEFAN\09-Feb-1999\0\#\ B3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORAM

AN MAXDISK=1048576000 SCF=DIRECT TEST\TS: CH3CH2F + H2\0,1\C,-0.1980
895732,-0.1229486461,0.7226735077\C,-1.2384105455,-0.5814689266,-0.236
2545174\H,-2.2202138863,-0.3832393047,0.2247082002\F,1.1918013854,0.84
77975883,-0.4230447777\H,-1.1596460448,-1.6442976441,-0.4701461523\H,-
1.1856317738,0.0017152234,-1.157891824\H,-0.2392331248,0.9195436667,1.
010702007\H,0.0828346328,-0.7813244398,1.535320374\H,1.3953381696,-0.3
225951766,-0.2905829814\H,1.2193402712,-1.193475183,0.0367794338\Vers
ion=IBM-RS6000-G98RevA.6\HF=-180.0973392\RMDS=3.148e-09\RMSF=1.053e-05
\Dipole=-1.191751,-0.3646015,0.6127487\PG=C01 [X(C2H7F1)]\@

TS4(CI)

1\1\GINC-PC\FTS\RB3LYP\6-31G(d)\C2H7C11\SXS501\05-Feb-1999\0\# B3LYP/
6-31G* GEOM=CHECK GUESS=READ NOSYM OPT=(TS,READFC,NOEIGENTEST) MAXDIS
K=5242880000 FREQ=NORAMAN SCF=DIRECT TEST\TS: CH3CH2Cl + H2\0,1\C,-0
.579049897,0.4012260891,1.0264796011\C,-0.1137642575,-0.2138823415,2.2
724959039\H,-1.025725499,-0.380577804,2.8801021408\C1,0.5788767775,-1.
5276239531,-0.8442467404\H,0.5718408674,0.4137641629,2.8444613736\H,0.
3157588015,-1.200087195,2.0772352126\H,-1.1404892414,-0.1877954405,0.3
114813597\H,-0.6124013732,1.4802487358,0.9167364092\H,1.2123261417,0.2
649335645,-0.1290305362\H,1.2114349959,0.949794182,0.2720180046\Versi
on=SGI-G94RevE.2\HF=-540.4822496\RMDS=3.148e-09\RMSF=9.566e-06\Dipole=
-1.0963043,1.7212257,2.2159849\PG=C01 [X(C2H7C11)]\@

TS4(Br)

1\1\GINC-PC\FTS\RB3LYP\6-31G(d)\C2H7Br1\SXS501\05-Mar-1999\0\# B3LYP/
6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,TIGHT,NOEIGENTEST) MAXDISK
=5242880000 FREQ=NORAMAN SCF=DIRECT TEST\TS: Hydrogenolysis of CH3CH2
Br\0,1\Br,-0.0160803571,0.,1.2695346988\H,-1.3298600311,0.,-0.4602794
934\H,-1.5243975245,0.,-1.2236028847\C,0.4451855522,0.,-1.7738270188\C
, -0.0656631815,0.,-3.1523624558\H,0.8451346064,0.,-3.787375639\H,-0.62
94982382,-0.9004593367,-3.4082700381\H,-0.6294982382,0.9004593367,-3.4
082700381\H,0.7768988491,-0.9144849866,-1.2943897583\H,0.7768988491,0.
9144849866,-1.2943897583\Version=SGI-G98RevA.6\State=1-A'\HF=-2651.99
22361\RMDS=6.602e-09\RMSF=3.072e-06\Dipole=0.3928366,0.,-3.0881725\PG=
CS [SG(C2H3Br1),X(H4)]\@

(HF)₂

1\1\GINC-RSCQC9\FOpt\RB3LYP\6-31G(d)\F2H2\ROOT\11-Mar-1999\0\# B3LYP/
6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=39321600\HF
dimer\0,1\H,-0.6202474987,0.0856301788,-0.6531248975\F,-0.6202474987,
-0.8553698212,-0.6531248975\F,0.6202474987,0.8553698212,0.6531248975\H
,0.6202474987,-0.0856301788,0.6531248975\Version=IBM-RS6000-G98RevA.6
\State=1-AG\HF=-200.8556281\RMDS=1.059e-09\RMSF=2.136e-04\Dipole=0.,0.
,0.\Polar=7.1018972,0.,3.8144243,-0.8594193,0.,8.7500678\PG=C02H [SGH(
F2H2)]\@

(HCl)₂

1\1\GINC-RSCQC8\FOpt\RB3LYP\6-31G(d)\Cl2H2\STEFAN\12-Mar-1999\0\# B3L
YP/6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=1048576000
\HCl dimer\0,1\H,0.2382577464,0.,0.668315566\C1,0.2047948705,0.,1.96
23280541\C1,-0.1349524085,0.,-1.8896125769\H,-1.4255796003,0.,-1.90447
86788\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-921.5942421\RMDS=6.
665e-09\RMSF=5.249e-05\Dipole=-0.5968728,0.,-0.7776278\PG=CS [SG(Cl2H2
)]\@

(HBr)₂

1\1\GINC-RSCQC9\FOpt\RB3LYP\6-31G(d)\Br2H2\ROOT\12-Mar-1999\0\# B3LYP/
6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=1048576000\

HBr dimer\\0,1\\H,-0.0824105282,0.,0.6243850117\\Br,-0.000873443,0.,2.06
82580618\\Br,-0.0368132243,0.,-2.0291256106\\H,1.4014438829,0.,-1.994020
8045\\Version=IBM-RS6000-G98RevA.6\\State=1-A'\\HF=-5144.6078722\\RMSD=3.
608e-09\\RMSF=6.104e-06\\Dipole=0.3867509,0.,-0.690638\\PG=CS [SG(Br2H2)]
\\@

[H₂C=CH₂•2HF]

1\\1\\GINC-PC\\FOpt\\RB3LYP\\6-31G(d)\\C2H6F2\\SXS501\\12-Mar-1999\\0\\# B3LYP/
6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=5242880000\\C
H2CH2.2HF complex\\0,1\\F,1.3725242396,0.,1.0122380852\\H,1.1401889122,0
.,0.0841499624\\C,-0.1686214542,-0.6690443386,-1.4681648904\\C,-0.168621
4542,0.6690443386,-1.4681648904\\H,0.3375904414,1.2495970051,-2.2357532
825\\H,0.3375904414,-1.2495970051,-2.2357532825\\H,-0.7023839258,1.21347
18767,-0.6937137323\\H,-0.7023839258,-1.2134718767,-0.6937137323\\H,-0.2
233792905,0.,1.5118480855\\F,-1.168498151,0.,1.4189746555\\Version=SGI-
G98RevA.6\\State=1-A'\\HF=-279.4600084\\RMSD=2.664e-09\\RMSF=2.232e-06\\Dip
ole=0.4926845,0.,-0.9144256\\PG=CS [SG(H2F2),X(C2H4)]\\@

[H₂C=CH₂•2HCl]

1\\1\\GINC-RSCQC9\\FOpt\\RB3LYP\\6-31G(d)\\C2H6Cl2\\ROOT\\11-Mar-1999\\0\\# B3L
YP/6-31G* OPT=(CALCFC) SCF=DIRECT TEST MAXDISK=1048576000\\H2C=CH2.2HC
l complex\\0,1\\Cl,-0.3174221746,1.8481139589,0.1028947328\\H,-1.0909959
76,0.7923670077,0.1022702014\\C,-2.5959564741,-0.969852562,-0.431751735
3\\C,-1.7806649788,-1.4292771798,0.5223014631\\H,-2.044630492,-1.3714497
214,1.5758069887\\H,-0.8244555428,-1.8912465177,0.2873245781\\H,-3.55812
34707,-0.5206554914,-0.1968053496\\H,-2.3406637482,-1.0429948346,-1.486
3851427\\H,1.6386784759,0.303064556,-0.0695681496\\Cl,2.3456527318,-0.78
18966969,-0.1473618794\\Version=IBM-RS6000-G98RevA.6\\HF=-1000.1892476\\
RMSD=4.846e-09\\RMSF=2.705e-06\\Dipole=-1.0442216,-0.2367978,0.0434262\\P
G=C01 [X(C2H6Cl2)]\\@

[H₂C=CH₂•2HBr]

1\\1\\GINC-PC\\FOpt\\RB3LYP\\6-31G(d)\\C2H6Br2\\SXS501\\13-Mar-1999\\0\\# B3LYP/
/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC) FREQ=NORAMAN SCF=DIRECT TES
T MAXDISK=5242880000\\H2C=CH2.2HBr complex\\0,1\\Br,-1.1201547235,0.357
9783329,-1.6040670551\\H,0.3371911049,0.3557862841,-1.6323057605\\C,2.72
29967143,0.9090698399,-1.4341543804\\C,2.5201540932,-0.2958408551,-0.89
31184921\\H,2.7403510778,-1.2100203642,-1.4398739156\\H,2.1287070883,-0.
4144964586,0.1148029281\\H,3.1187036659,1.0285513222,-2.4400272641\\H,2.
5173475275,1.8241946075,-0.8835111018\\H,-0.6960082087,-0.2029046421,0.
8843652079\\Br,-0.0685651936,-0.5025636088,2.1572152592\\Version=SGI-G9
8RevA.6\\HF=-5223.2038639\\RMSD=3.428e-09\\RMSF=3.521e-06\\Dipole=0.569039
2,0.1309621,-0.5570109\\PG=C01 [X(C2H6Br2)]\\@

TS5(F)

1\\1\\GINC-PC\\FTS\\RB3LYP\\6-31G(d)\\C2H6F2\\SXS501\\12-Mar-1999\\0\\# B3LYP/6
-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK
=5242880000\\TS: CH2CH2 + H-F catalyzed by HF\\0,1\\H,0.0554941027,1.04
66587593,0.\\C,-1.2186036175,0.7643290828,0.\\C,-1.1593239118,-0.6355186
306,0.\\F,1.3165445064,1.0058512681,0.\\H,-1.5606550402,1.2379909906,0.9
205742101\\H,-1.5606550402,1.2379909906,-0.9205742101\\H,-1.2691293781,-
1.204497321,0.9161921874\\H,-1.2691293781,-1.204497321,-0.9161921874\\H,
1.2044846862,-0.205242053,0.\\F,0.7575838518,-1.1926586857,0.\\Version=
SGI-G98RevA.6\\State=1-A'\\HF=-279.4181818\\RMSD=5.046e-09\\RMSF=3.833e-05
\\Dipole=-1.3144428,-0.1810223,0.\\PG=CS [SG(C2H2F2),X(H4)]\\@

TS5(Cl)]

1\\1\\GINC-PC\\FTS\\RB3LYP\\6-31G(d)\\C2H6Cl2\\SXS501\\12-Mar-1999\\0\\# B3LYP/

6-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXDIS
K=5242880000\TS: H2C=CH2 + HCl catalyzed by HCl\0,1\H,-0.8412378496,
-0.9333495269,0.\C,-0.1578787348,-1.9574041387,0.\C,1.1843592261,-1.54
61155819,0.\Cl,-1.7856668927,0.5965164618,0.\H,-0.5129373532,-2.425480
5059,0.9203432327\H,-0.5129373532,-2.4254805059,-0.9203432327\H,1.7486
591686,-1.4458241353,0.9203340887\H,1.7486591686,-1.4458241353,-0.9203
340887\H,-0.0996819905,1.0479633154,0.\Cl,1.3333488493,1.0887255275,0.
\Version=SGI-G98RevA.6\State=1-A'\HF=-1000.1538547\RMSD=3.827e-09\RMS
F=7.591e-06\Dipole=1.059703,-1.940376,0.\PG=CS [SG(C2H2Cl2),X(H4)]\@

TS5(Br)

1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H6Br2\ROOT\12-Mar-1999\0\# B3LY
P/6-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXD
ISK=1048576000\TS: H2C=CH2 + HBr catalyzed by HBr\0,1\H,-0.751311424
4,-1.3293801685,0.\C,-0.0512187236,-2.3759752792,0.\C,1.2889513396,-1.
9793999778,0.\Br,-1.831163493,0.1981698071,0.\H,-0.4224607379,-2.83075
40796,0.9201968099\H,-0.4224607379,-2.8307540796,-0.9201968099\H,1.849
9320457,-1.8655172712,0.9204321891\H,1.8499320457,-1.8655172712,-0.920
4321891\H,-0.0063380822,0.7637472747,0.\Br,1.5590580986,0.8329852539,0
.\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-5223.1785342\RMSD=4.922
e-09\RMSF=3.330e-05\Dipole=0.8928401,-1.6977018,0.\PG=CS [SG(C2H2Br2),
X(H4)]\@

[CH₃CH₂F·HF]

1\1\GINC-PC\FOpt\RB3LYP\6-31G(d)\C2H6F2\SXS501\12-Mar-1999\0\# B3LYP/
6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=5242880000\C
H3CH2F.HF complex\0,1\H,-1.4671708407,0.250085625,-0.465791989\H,-1.7
555485722,-1.221057125,0.5031976598\C,-1.4318063293,-0.1761040341,0.54
01331062\H,-2.1239336306,0.3793513338,1.1829267137\C,-0.0244107306,-0.
0664866692,1.0806097376\H,0.3308545631,0.9675317203,1.0929553449\H,0.0
867721114,-0.50578072,2.0760255291\F,0.858583022,-0.789522269,0.230581
791\H,0.8391289272,0.1981122809,-1.1567092121\F,0.5666614003,0.9436668
362,-1.6702552476\Version=SGI-G98RevA.6\HF=-279.493889\RMSD=5.120e-09
\RMSF=4.995e-06\Dipole=-0.3641797,-0.2689668,0.9767009\PG=C01 [X(C2H6F
2)]\@

[CH₃CH₂Cl·HCl]

1\1\GINC-RSCQC9\FOpt\RB3LYP\6-31G(d)\C2H6Cl2\ROOT\11-Mar-1999\0\# B3L
YP/6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=1048576000
\CH3CH2Cl.HCl complex\0,1\H,-0.5921115246,1.7044268158,-0.5519361013
\H,-2.1558542494,1.1945087864,-1.2268206058\C,-1.6203553759,1.42739163
91,-0.3020097592\H,-2.1035895251,2.2926817535,0.1684973158\C,-1.658266
1359,0.2587667372,0.6652064927\H,-1.1056514642,0.4615139514,1.58403268
87\H,-2.6767412765,-0.0399626414,0.9180904229\Cl,-0.8856084876,-1.2380
230612,-0.0562423179\H,1.3893771686,-0.3865331855,-0.1629587299\Cl,2.4
689202489,0.3354591943,-0.1148215286\Version=IBM-RS6000-G98RevA.6\HF=
-1000.2269914\RMSD=7.124e-09\RMSF=3.889e-06\Dipole=-1.1348985,0.428626
4,0.2958402\PG=C01 [X(C2H6Cl2)]\@

[CH₃CH₂Br·HBr]

1\1\GINC-PC\FOpt\RB3LYP\6-31G(d)\C2H6Br2\SXS501\13-Mar-1999\0\# B3LYP
/6-31G* OPT=(CALCFC) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK=5242880000\
CH3CH2Br.HBr complex\0,1\H,-0.6302582624,1.8563217524,-0.7027128105\H
, -2.3078619761,1.59308413,-1.2394573508\C,-1.6604561921,1.711378638,-0
.3660088035\H,-1.972036252,2.6141158826,0.1757470963\C,-1.7620052489,0
.5205870598,0.566176456\H,-1.0640422541,0.5784223743,1.4012661239\H,-2
.7723585123,0.3428262043,0.9335112094\Br,-1.2746285607,-1.1720362087,-
0.3744141746\H,1.0536716149,-0.3477974848,-0.0707395403\Br,2.081132968
9,0.5997857217,0.3258821562\Version=SGI-G98RevA.6\HF=-5223.2453971\RM

SD=5.227e-09\RMSF=2.997e-06\Dipole=-0.7933891,0.4288185,0.1954028\PG=C
01 [X(C2H6Br2)]\@

TS6(F)

1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H8F2\ROOT\13-Mar-1999\0\#\ B3LYP
/6-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXDI
SK=1048576000\TS: (H2C=CH2 + H2 + HF) complexed with HF\0,1\H,1.2212
393154,-1.256096664,0.629179872\C,-0.5366999193,-1.4447353631,0.334521
5112\C,-1.1815343093,-0.2693788986,0.7869113895\H,-0.2459448321,0.4860
293146,0.8536176078\H,-0.4369859503,-2.3361844391,0.9487385929\H,-0.29
05800153,-1.5287212724,-0.7196580804\H,-1.7344621501,0.2477024171,-0.0
022141578\H,-1.6771157112,-0.3247102542,1.7554025659\H,1.3190723221,-0
.4546693407,0.6089966483\F,1.0448148766,1.0880469627,0.5631193342\H,0.
655955,0.8981465659,-0.8670139391\F,0.2327659449,0.5289740643,-1.66708
0058\Version=IBM-RS6000-G98RevA.6\HF=-280.5668893\RMSD=6.172e-09\RMSF
=1.579e-05\Dipole=-0.9174236,-1.4322969,0.7761457\PG=C01 [X(C2H8F2)]\@
@

TS6(Cl)

1\1\GINC-VPP03\FTS\RB3LYP\6-31G(d)\C2H8Cl2\SXS501\13-Mar-1999\0\#\ B3L
YP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORAM
AN MAXDISK=13107200 SCF=DIRECT TEST\TS: (H2C=CH2 + H2 + HCl) complexe
d with HCl\0,1\H,-0.9758905513,-1.7450727231,0.7065054459\C,-2.146631
9382,-0.3931952559,0.7179306885\C,-1.4306650924,0.7450703529,1.1539802
798\H,-0.2875625882,0.37873417,1.2255260358\H,-2.7230013608,-1.0067749
01,1.4054819978\H,-2.2874108006,-0.5863837196,-0.3424427062\H,-1.33405
95449,1.5394509724,0.4100407953\H,-1.6524766686,1.0899452558,2.1651964
303\H,-0.2053493409,-1.5960577022,0.8184563131\Cl,1.426328306,-0.35591
4623,1.135455714\H,0.9754885698,0.0781004544,-0.9908439666\Cl,0.335674
3098,0.3404327177,-2.1136548996\Version=Fujitsu-VP-Unix-G98RevA.6\HF=
-1001.3173802\RMSD=4.164e-09\RMSF=9.138e-07\Dipole=-2.2803639,-0.02400
46,0.6742383\PG=C01 [X(C2H8Cl2)]\@

TS6(Br)

1\1\GINC-VPP03\FTS\RB3LYP\6-31G(d)\C2H8Br2\SXS501\14-Mar-1999\0\#\ B3L
YP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORAM
AN MAXDISK=13107200 SCF=DIRECT TEST\TS: (H2C=CH2 + H2 + HBr) complexe
d with HBr\0,1\H,-1.9111865975,-0.1837750919,1.4496118851\C,-1.725257
8192,1.6060490974,1.1739019157\C,-0.3444303187,1.8636350934,1.31401278
12\H,0.185688112,0.78158901,1.4101669621\H,-2.4216264084,1.7230257367,
1.9998918694\H,-2.1478093072,1.4282928417,0.1884991217\H,0.1453584506,
2.2119483741,0.4007480036\H,-0.0411062471,2.3808929775,2.225626539\H,-
1.2952422261,-0.6775719782,1.4584772319\Br,0.8663357595,-1.0750568688,
1.3180163541\H,0.2680009279,-0.4527345322,-0.8321561073\Br,-0.30530569
88,0.2742062264,-1.9816836023\Version=Fujitsu-VP-Unix-G98RevA.6\HF=-5
224.343882\RMSD=9.438e-09\RMSF=6.859e-06\Dipole=-1.2035178,1.5145621,0
.7247276\PG=C01 [X(C2H8Br2)]\@

TS7(F)

1\1\GINC-PC\FTS\RB3LYP\6-31G(d)\C2H8F2\SXS501\15-Apr-1999\0\#\ B3LYP/6
-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK
=5242880000\TS: H2C=CH2 + H2 + 2 HF, Cs symmetry\0,1\F,1.27672112,0.
,0.8620739362\H,0.8997344356,0.,-0.3565476748\C,0.5363638057,0.,-1.588
5632918\C,-0.8755051741,0.,-1.6353700126\H,-1.5371727309,0.,-0.1953508
906\H,-1.3555094166,0.,0.6247483515\F,-0.7621096024,0.,1.948510153\H,1
.0097854074,-0.9177752608,-1.9420334456\H,1.0097854074,0.9177752608,-1
.9420334456\H,-1.4270698012,-0.9152635683,-1.8383622479\H,-1.427069801
2,0.9152635683,-1.8383622479\H,0.230861052,0.,1.5362846237\Version=SG
I-G98RevA.6\State=1-A'\HF=-280.5667202\RMSD=8.518e-09\RMSF=6.742e-06\D

ipole=-0.6010633,0.,-1.7227587\PG=CS [SG(C2H4F2),X(H4)]\@

TS7(Cl)

1\1\GINC-PC\FTS\RB3LYP\6-31G(d)\C2H8Cl2\SXS501\19-Apr-1999\0\#\ B3LYP/
6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORAMAN
MAXDISK=5242880000 SCF=DIRECT TEST\TS: H2C=CH2 + 2 HCl + H2 (analogue
to the Bertran TS, Cs symmetry)\0,1\Cl,1.5956510056,0.,-0.1931284405
\H,0.7400620542,0.,1.493245273\C,0.1620235224,0.,2.5298120923\C,-1.237
321463,0.,2.245009413\H,-1.3721760226,0.,0.6976180903\H,-1.3170456255,
0.,-0.1093715698\Cl,-0.9643246258,0.,-2.1521177264\H,0.2525444335,0.,-
1.4577421931\H,0.5253210054,-0.9145452087,3.0038188314\H,0.5253210054,
0.9145452087,3.0038188314\H,-1.8173938318,-0.918979285,2.2944342715\H,
-1.8173938318,0.918979285,2.2944342715\Version=SGI-G98RevA.6\State=1-
A'\HF=-1001.3083946\RMSD=4.783e-09\RMSF=7.555e-07\Dipole=-1.4825313,0.,
2.3823036\PG=CS [SG(C2H4Cl2),X(H4)]\@

TS7(Br)

1\1\GINC-PC\FTS\RB3LYP\6-31G(d)\C2H8Br2\SXS501\20-Apr-1999\0\#\ B3LYP/
6-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXDIS
K=5242880000\TS: H2C=CH2 + 2 HBr + H2 (analogue to the Bertran TS, Cs
symmetry)\0,1\Br,1.5980517091,0.,0.323264765\H,0.5940232358,0.,2.044
9159781\C,0.0157476709,0.,3.0938565953\C,-1.3808917454,0.,2.8201351544
\H,-1.5088122585,0.,1.219201354\H,-1.515701519,0.,0.4145830894\Br,-1.2
09013943,0.,-1.7799436894\H,0.1434054136,0.,-1.0063930799\H,0.39021029
9,-0.9143676215,3.5592007502\H,0.390210299,0.9143676215,3.5592007502\H
, -1.9593964195,-0.9198954259,2.854551507\H,-1.9593964195,0.9198954259,
2.854551507\Version=SGI-G98RevA.6\State=1-A'\HF=-5224.3322061\RMSD=7.
382e-09\RMSF=1.327e-05\Dipole=-1.2884301,0.,2.2433649\PG=CS [SG(C2H4Br
2),X(H4)]\@

TS8(F)

1\1\GINC-PC\FTS\RB3LYP\6-31G(d)\C2H8F2\SXS501\12-Mar-1999\0\#\ B3LYP/6
-31G* OPT=(TS,CALCFC,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST MAXDISK
=5242880000\TS: CH3CH2F..H-F..H-H...\0,1\H,1.5305210787,1.9798005813
,0.\C,0.4345904601,2.1322609681,0.\C,-0.0919221359,0.7628339936,0.\F,1
.1420037727,-1.1264137981,0.\F,-1.1258140292,-1.5642990226,0.\H,0.1881
574427,2.6942155369,0.9040260407\H,0.1881574427,2.6942155369,-0.904026
0407\H,-0.1875151366,0.2146026155,0.9177685192\H,-0.1875151366,0.21460
26155,-0.9177685192\H,-1.8597666582,-0.146547313,0.\H,-1.949725379,0.6
706724161,0.\H,0.0759687102,-1.4757163727,0.\Version=SGI-G98RevA.6\St
ate=1-A'\HF=-280.5514142\RMSD=1.781e-09\RMSF=1.191e-05\Dipole=0.133256
2,2.307479,0.\PG=CS [SG(C2H4F2),X(H4)]\@

TS8(Cl)

1\1\GINC-RSCQC8\FTS\RB3LYP\6-31G(d)\C2H8Cl2\STEFAN\12-Mar-1999\0\#\ B3
LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORA
MAN MAXDISK=1048576000 SCF=DIRECT TEST\TS: CH3CH2Cl..H-Cl..H-H...\0,
1\C,0.5692281066,0.,-1.2516772986\Cl,-1.751337352,0.,0.2233337766\H,-0
.5094848397,0.,1.105230752\Cl,1.0198730333,0.,1.7910722345\H,2.1768066
918,0.,-0.0125865031\H,2.2565817852,0.,-0.8147573747\C,0.4866095582,0.
, -2.7223619224\H,-0.5957482124,0.,-2.9415027344\H,0.4793106801,0.92123
72514,-0.6960290106\H,0.4793106801,-0.9212372514,-0.6960290106\H,0.906
5453219,-0.9027472932,-3.1724964901\H,0.9065453219,0.9027472932,-3.172
4964901\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-1001.3062592\RMSD
=6.408e-09\RMSF=1.152e-06\Dipole=0.8882773,0.,-2.8215122\PG=CS [SG(C2H
4Cl2),X(H4)]\@

TS8(Br)

```

1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H8Br2\ROOT\12-Mar-1999\0\#\ B3LY
P/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORAMA
N MAXDISK=1048576000 SCF=DIRECT TEST\TS: CH3CH2Br..H-Br..H-H...\0,1\
C,-1.5062804141,-1.0131599487,0.\Br,1.3106724499,-1.1472478206,0.\H,0.
7185683821,0.424879714,0.\Br,-0.2874368172,1.9353565466,0.\H,-2.220114
7397,0.911314498,0.\H,-2.6614493717,0.220038712,0.\C,-2.2148863061,-2.
3125218962,0.\H,-1.4288281447,-3.0840677412,0.\H,-1.1300773384,-0.5909
751914,0.9196913011\H,-1.1300773384,-0.5909751914,-0.9196913011\H,-2.8
171341372,-2.4599645701,-0.9000067968\H,-2.8171341372,-2.4599645701,0.
9000067968\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-5224.3341726\R
MSD=5.396e-09\RMSF=5.375e-06\Dipole=-1.8939671,-1.5839475,0.\PG=CS [SG
(C2H4Br2),X(H4)]\@

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[H₂C=CH₂·HAIF₄]

```

1\1\GINC-RSCQC9\FOpt\RB3LYP\6-31G(d)\C2H5Al1F4\ROOT\08-Feb-1999\0\#\ R
B3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC) FREQ=NORAMAN SCF=DIREC
T TEST MAXDISK=1048576000\F3Al.FH * H2C=CH2 complex (Cs symmetry)\0,
1\F,1.4214433663,-0.1240716428,-1.864132794\F,-1.4214433663,-0.1240716
428,-1.864132794\Al,0.,0.1371912191,-1.0617217051\F,0.,-1.2500990998,0
.2372327851\F,0.,1.379534146,0.0567846288\H,0.,-0.8695047021,1.1684238
786\C,-0.6714295259,0.0067506405,2.7207334701\C,0.6714295259,0.0067506
405,2.7207334701\H,1.2213921802,0.7320454776,2.1267473452\H,-1.2213921
802,0.7320454776,2.1267473452\H,1.246292134,-0.6953528163,3.3199477608
\H,-1.246292134,-0.6953528163,3.3199477608\Version=IBM-RS6000-G94RevE
.1\State=1-A'\HF=-721.2425777\RMSD=2.884e-09\RMSF=1.530e-05\Dipole=0.,
-0.4934878,2.2901028\PG=CS [SG(H1Al1F2),X(C2H4F2)]\@

```

[H₂C=CH₂·HAICl₄]

```

1\1\GINC-PC\FOpt\RB3LYP\6-31G(d)\C2H5Al1Cl4\SXS501\05-Dec-1998\0\#\ B3
LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC) FREQ=NORAMAN SCF=DIRECT
TEST MAXDISK=5242880000\H2C=CH2 * HALCl4\0,1\Cl,-1.049070662,-0.6088
988283,1.7892511618\Cl,-1.049070662,-0.6088988283,-1.7892511618\Al,0.0
416291806,-0.9322839271,0.\Cl,1.4837029839,1.0992926093,0.\H,0.5107480
777,2.0286287703,0.\Cl,1.5519131434,-2.4018131073,0.\C,-1.0597800706,3
.3071900105,-0.6703285731\C,-1.0597800706,3.3071900105,0.6703285731\H,
-1.6104086522,2.562407193,-1.2403183399\H,-1.6104086522,2.562407193,1.
2403183399\H,-0.5254104646,4.0626881994,-1.2420494869\H,-0.5254104646,
4.0626881994,1.2420494869\Version=SGI-G94RevE.2\State=1-A'\HF=-2162.6
393238\RMSD=3.526e-09\RMSF=1.684e-06\Dipole=0.0212978,2.2533951,0.\PG=
CS [SG(H1Al1Cl2),X(C2H4Cl2)]\@

```

[H₂C=CH₂·HAIBr₄]

```

1\1\GINC-RSCQC9\FOpt\RB3LYP\6-31G(d)\C2H5Al1Br4\ROOT\05-Mar-1999\0\#\
B3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(CALCFC) FREQ=NORAMAN SCF=DIREC
T TEST MAXDISK=1048576000\ethylene - HALBr4 complex\0,1\Br,2.6551430
967,-0.5375589965,-0.1773883419\Al,0.5599223809,0.156292953,0.28272887
16\Br,-0.552574086,-0.7941842555,2.0170068426\Br,0.0334676274,2.329564
6673,-0.0755930369\Br,-0.6094790013,-0.9928118753,-1.7304549101\H,-1.9
899915257,-0.6760744566,-1.2511870894\C,-3.8006687911,-0.7221564115,-0
.0236975721\C,-3.5375592424,0.5281699491,-0.4289906153\H,-4.0436094861
,0.9722433167,-1.2832366273\H,-4.5301711227,-1.348763767,-0.5316733389
\H,-2.8176169063,1.1563923597,0.0904279887\H,-3.2977509999,-1.14702096
52,0.8413534828\Version=IBM-RS6000-G98RevA.6\HF=-10608.7064345\RMSD=3
.376e-09\RMSF=7.789e-06\Dipole=-1.7575955,-0.5013456,-0.9024428\PG=C01

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TS9(F)

```

1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H5Al1F4\ROOT\08-Feb-1999\0\#\ RB
3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NOR
AMAN MAXDISK=1048576000 SCF=DIRECT TEST\TS: F3AlF....H....H2C=CH2\0,

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```

1\F,-1.2568679768,-0.1926741657,0.\Al,0.0118869757,0.9663340983,0.\F,1
.3623782173,-0.1800670396,0.\H,0.8807381532,-1.4018924675,0.\F,0.05386
6238,1.8207197383,1.4214543336\F,0.0538606238,1.8207197383,-1.4214543
336\C,0.5098519818,-2.6279858308,0.\C,-0.850890054,-2.3745778069,0.\H,
0.9656714158,-2.9802092093,0.9257220798\H,0.9656714158,-2.9802092093,-
0.9257220798\H,-1.4197333139,-2.3014675036,-0.9201403691\H,-1.41973331
39,-2.3014675036,0.9201403691\Version=IBM-RS6000-G98RevA.6\State=1-A'
\HF=-721.229202\RMSD=3.342e-09\RMSF=1.403e-05\Dipole=-0.2621591,-3.148
3205,0.\PG=CS [SG(C2H1A11F2),X(H4F2)]\@

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TS9(Cl)

```

1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H5A11C14\ROOT\07-Feb-1999\0\# B
3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST,MAXCYC=10
0) MAXDISK=1048576000 NOSYMM FREQ=NORAMAN SCF=DIRECT TEST\TS H2C=CH2.
..H...ClAlC13\0,1\Cl,-1.0333636334,1.8078220043,-0.4811271539\Al,-0.2
388798931,0.1022408092,0.587391194\Cl,-1.0111705986,-1.6085352322,-0.7
459626398\H,-0.350252511,-0.8919382041,-2.1144716005\Cl,1.8846853191,0
.0169821466,0.3250029551\Cl,-1.0001517298,-0.2143921683,2.5308585051\C
,0.2412670283,-0.5699951629,-3.2658967853\C,0.2787846062,0.7901852058,
-3.0743696695\H,-0.4921596259,-0.988828207,-3.9551950525\H,1.155744299
9,-1.1447001896,-3.1156773309\H,1.0994862008,1.263303059,-2.5426461022
\H,-0.5339894625,1.4361696189,-3.3925600192\Version=IBM-RS6000-G94Rev
E.1\HF=-2162.6312304\RMSD=3.820e-09\RMSF=3.178e-06\Dipole=0.2402347,-0
.110481,-3.1656378\PG=C01 [X(C2H5A11C14)]\@

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TS9(Br)

```

1\1\GINC-RSCQC2\FTS\RB3LYP\6-31G(d)\C2H5A11Br4\ROOT\04-Mar-1999\0\# B
3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NOR
AMAN MAXDISK=786432000 SCF=DIRECT TEST\TS: H2C=CH2...H...AlBr4\0,1\
Br,-2.130362724,-0.4417271226,-0.3484006234\Al,0.1670110911,-0.4453172
896,-0.2685763088\Br,0.6182799102,1.9689243438,-0.4347477979\H,-0.3865
223482,2.1601635261,0.9666141796\Br,0.8787809672,-0.9442999667,1.84511
34853\Br,1.2489611198,-1.388454951,-2.0079476269\C,-0.9534541361,2.457
3003608,2.2071545971\C,-1.9453640823,1.5145092061,2.2060945316\H,-1.20
14679496,3.5004697179,2.0130893514\H,-0.0466056692,2.2663804824,2.7809
084779\H,-1.7590304076,0.5041785482,2.5565304683\H,-2.93268306,1.72159
4465,1.8042444655\Version=IBM-RS6000-G98RevA.6\HF=-10608.7015178\RMSD
=5.131e-09\RMSF=4.258e-06\Dipole=-1.0289768,1.9642072,1.4736136\PG=C01
[X(C2H5A11Br4)]\@

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[CH₃CH₂F·AlF₃]

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1\1\GINC-RSCQC9\Fopt\RB3LYP\6-31G(d)\C2H5A11F4\ROOT\10-Feb-1999\0\# B
3LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC) NOSYMM FREQ=NORAMAN MAX
DISK=1048576000 SCF=DIRECT TEST\H3C-CH2-F...AlF3 complex\0,1\H,-1.35
75883691,0.8928355785,3.0577012868\H,-1.3587110029,-0.8919863268,3.057
3681008\C,-0.726844901,0.0000330199,3.0306783953\H,-0.0925511119,-0.00
05364695,3.9249215057\C,0.1620477573,-0.0003125699,1.8210474114\H,0.76
43917196,0.8987499644,1.69443628\H,0.7633830819,-0.8999944325,1.694128
0154\F,-0.7199022782,0.0003879856,0.6249641264\Al,0.1780867703,0.00024
56416,-1.0678149845\F,-1.0936754404,-0.0009020235,-2.1201237215\F,1.04
04614172,-1.4007293938,-0.8465897612\F,1.0391475262,1.402209026,-0.847
9658569\Version=IBM-RS6000-G98RevA.6\HF=-721.2713858\RMSD=6.300e-09\R
MSF=7.699e-06\Dipole=-0.1544809,-0.0003826,2.3112517\PG=C01 [X(C2H5A11
F4)]\@

```

[CH₃CH₂Cl·AlCl₃]

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1\1\GINC-PC\Fopt\RB3LYP\6-31G(d)\C2H5A11C14\SXS501\04-Dec-1998\0\# B3
LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC) FREQ=NORAMAN SCF=DIRECT

```

TEST MAXDISK=5242880000\H3C-CH2-Cl...AlCl3 complex\0,1\H,0.,0.584017
8014,-4.5669889406\C,0.,-0.2550766487,-3.860504918\C,0.,0.3204597753,-
2.4616909465\Cl,0.,-1.0644259938,-1.2110759013\H,-0.891204603,-0.85970
2048,-4.0496229458\H,0.891204603,-0.859702048,-4.0496229458\H,-0.89569
65766,0.8937023235,-2.2219430609\H,0.8956965766,0.8937023235,-2.221943
0609\Al,0.,0.1150442266,0.9397033288\Cl,0.,-1.5593642156,2.2238414832\
Cl,-1.7909622428,1.2371923971,0.7532393522\Cl,1.7909622428,1.237192397
1,0.7532393522\Version=SGI-G94RevE.2\State=1-A'\HF=-2162.6798457\RMSD
=2.467e-09\RMSF=1.847e-05\Dipole=0.,-0.0850416,-2.4950446\PG=CS [SG(C2
H1Al1Cl2),X(H4Cl2)]\@

[CH₃CH₂Br•AlBr₃]

1\1\GINC-PC\FOpt\RB3LYP\6-31G(d)\C2H5Al1Br4\SXS501\07-Mar-1999\0\# B3
LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(READFC) FREQ=NORAMAN SCF=DIRECT
TEST MAXDISK=5242880000\CH3CH2Br.AlBr3 complex\0,1\H,-1.6026109398,-
4.237407803,-0.2810276172\C,-0.6877563292,-3.6304699272,-0.3066162218\
C,-0.7475883256,-2.6516021787,0.8421937783\Br,0.928364127,-1.509839493
2,0.8921757329\H,0.1706009813,-4.3032035151,-0.227504451\H,-0.65388158
81,-3.1050007335,-1.2638449048\H,-0.7495993218,-3.1116622705,1.8295147
866\H,-1.5472148976,-1.9154753855,0.7599159756\Al,-0.008238652,0.63118
9502,-0.1527435384\Br,1.9334388975,1.7759838497,-0.2526171528\Br,-1.57
26535777,1.2358711455,1.37250256\Br,-0.9148101277,-0.1831663929,-2.070
4855152\Version=SGI-G98RevA.6\HF=-10608.7509817\RMSD=8.582e-09\RMSF=4
.546e-06\Dipole=-0.1667479,-2.2014696,0.5999644\PG=C01 [X(C2H5Al1Br4)]
\@

TS10(F)

1\1\GINC-RSCQC9\FTS\RB3LYP\6-31G(d)\C2H7Al1F4\ROOT\08-Feb-1999\0\# B3
LYP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORA
MAN MAXDISK=1048576000 SCF=DIRECT TEST\TS: H3C-CH2-F...AlF3 + H2\0,1
\H,0.,-1.37331838,-3.2929733225\C,0.,-0.2760161052,-3.4510633298\C,0.,
0.2115014241,-2.0690668789\F,0.,-1.2130652673,-0.1710669941\Al,0.,-0.0
672843968,1.1317925886\F,0.,1.4230739374,0.2400146095\H,0.9063110439,-
0.0324267582,-4.0093394748\H,-0.9063110439,-0.0324267582,-4.0093394748
\H,0.9144118322,0.2445972828,-1.4998860428\H,-0.9144118322,0.244597282
8,-1.4998860428\F,1.4184359916,-0.2006392472,1.9958673977\F,-1.4184359
916,-0.2006392472,1.9958673977\H,0.,1.9882909343,-1.5225191026\H,0.,1.
9439000601,-2.3047206379\Version=IBM-RS6000-G98RevA.6\State=1-A'\HF=-
722.3808272\RMSD=8.063e-09\RMSF=1.398e-05\Dipole=0.,0.4569525,-4.40222
\PG=CS [SG(C2H3Al1F2),X(H4F2)]\@

TS10(Cl)

1\1\GINC-PC\FTS\RB3LYP\6-31G(d)\C2H7Al1Cl4\SXS501\05-Dec-1998\0\# B3L
YP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NORAM
AN MAXDISK=5242880000 SCF=DIRECT TEST\TS: H3C-CH2-Cl...AlCl3 + H2\0,
1\H,-1.6934668293,-3.671209995,0.4787767746\C,-0.6169666482,-3.8630036
836,0.6517610524\C,-0.0066362229,-2.5710901935,0.3002966276\Cl,-1.6512
075402,-0.4075043841,-0.8165362825\Al,0.0247706801,0.8615450373,-0.116
09241\Cl,1.8587062708,-0.1693967135,-0.8198682651\H,-0.5064435177,-4.1
241948258,1.706461967\H,-0.3246964673,-4.6835022397,-0.0069313501\H,-0
.0388575672,-1.7508601701,1.0147698888\H,0.1641565913,-2.3081231958,-0
.7359990558\Cl,0.0392204172,0.620096578,2.0361769001\Cl,-0.1076667053,
2.8433127927,-0.8471679742\H,1.8531625769,-2.2246692838,0.3196044545\H
,1.6018520766,-2.9036031555,0.6258981401\Version=SGI-G94RevE.2\HF=-21
63.7953495\RMSD=8.591e-09\RMSF=5.935e-06\Dipole=0.0525015,-4.3712094,0
.5617363\PG=C01 [X(C2H7Al1Cl4)]\@

TS10(Br)

1\1\GINC-RSCQC2\FTS\RB3LYP\6-31G(d)\C2H7Al1Br4\ROOT\07-Mar-1999\0\# B

3LYP/6-31G* OPT=(TS,CALCF,NOEIGENTEST) FREQ=NORAMAN SCF=DIRECT TEST M
 AXDISK=786432000\TS: H3C-CH2-Br...AlBr3 + H2\0,1\H,4.1054451875,-1.5
 704551152,-0.1925793177\C,4.2661957436,-0.4847196545,-0.0743350128\C,2
 .9154603711,0.096126382,-0.2076101418\Br,0.7251775332,-1.7762050284,-0
 .9059225873\Al,-0.5594481185,-0.0267780403,0.0441887757\Br,0.265838001
 4,2.0094800036,-0.8795150091\H,4.6979538734,-0.3314313058,0.9174577528
 \H,4.9523021574,-0.1685682773,-0.8634266366\H,2.2360334343,0.074245221
 2,0.6400130014\H,2.47967624,0.2603890188,-1.1833742618\Br,0.0558149491
 ,0.0526210606,2.2617224925\Br,-2.7583988172,-0.2662773364,-0.420544369
 8\H,2.4509908977,2.0204889476,-0.1704145568\H,3.1653787349,1.708351189
 4,0.01862244\Version=IBM-RS6000-G98RevA.6\HF=-10609.8677179\RMSD=3.71
 1e-09\RMSF=9.283e-06\Dipole=3.7122915,0.1627124,-0.3085583\PG=C01 [X(C
 2H7Al1Br4)]\@

TS11(F)

1\1\GINC-RSCQC9\SP\RB3LYP\6-31G(d)\C2H7Al1F4\ROOT\25-Mar-1999\0\#\ B3L
 YP/6-31G* SCF=(TIGHT,DIRECT) TEST MAXDISK=1048576000\TS: H2C=CH2 + HA
 1F4 + H2\0,1\F,0,-0.5918071455,1.7158019033,0.1298149699\H,0,1.134971
 2027,1.7464817423,0.5766944607\H,0,1.8965567309,1.6796126308,0.7037862
 275\C,0,2.5070996074,0.2705404209,-0.4517881864\C,0,2.3366802487,-0.96
 37153953,0.2206650114\H,0,1.3603463196,-0.8707239025,0.8343838522\F,0,
 -0.1613343579,-0.6721671635,1.3248534201\Al,0,-0.9809585888,0.06366837
 88,-0.0094021093\H,0,3.4023546157,0.8815308825,-0.3583824256\H,0,1.772
 7441541,0.5383271194,-1.2087702937\H,0,3.1659871868,-1.3100789264,0.83
 44697805\H,0,1.9253119557,-1.7025953292,-0.486182905\F,0,-2.6005605723
 , -0.288739502,-0.0405091383\F,0,-0.0872412184,-0.4916944929,-1.3460517
 212\Version=IBM-RS6000-G98RevA.6\HF=-722.3873317\RMSD=2.798e-09\Dipol
 e=3.595271,-0.0866133,-0.1942077\PG=C01 [X(C2H7Al1F4)]\@

TS11(Cl)

1\1\GINC-VPP05\FTS\RB3LYP\6-31G(d)\C2H7Al1Cl4\SXS501\09-Mar-1999\0\#\ B3L
 YP/6-31G* GEOM=CHECK GUESS=READ OPT=(TS,READFC,NOEIGENTEST) FREQ=NO
 RAMAN MAXDISK=19660800 SCF=DIRECT TEST\TS: H2C=CH2 + HAlCl4 + H2 (one
 -step)\0,1\Cl,-0.4272646214,-1.8859641506,1.20303455\H,1.8176583285,-
 1.4428675116,0.9012189761\H,2.5332971243,-1.1717987172,0.8045195449\C,
 3.2748982411,0.5374532637,0.7985730311\C,3.0810559452,1.0864839486,-0.
 4946928884\H,2.1987299313,0.5053900434,-0.9708159569\Cl,0.5212016815,-
 0.3488751034,-1.7920051374\Al,-0.8192329201,-0.1283899123,-0.020296801
 5\H,4.1558058103,-0.0467560073,1.0570251796\H,2.599983541,0.8095785931
 ,1.6073840427\H,3.9257486434,1.004838861,-1.179284777\H,2.6030729354,2
 .0744377437,-0.4550391089\Cl,-2.8350928816,0.0524007437,-0.6463267443\
 Cl,-0.0423732062,1.6055339563,1.039742606\Version=Fujitsu-VP-Unix-G98
 RevA.6\HF=-2163.7927766\RMSD=2.244e-09\RMSF=9.296e-06\Dipole=4.1858067
 ,0.6776906,0.4046617\PG=C01 [X(C2H7Al1Cl4)]\@

TS11(Br)

1\1\GINC-PC\SP\RB3LYP\6-31G(d)\C2H7Al1Br4\SXS501\25-Mar-1999\0\#\ B3LY
 P/6-31G* SCF=(TIGHT,DIRECT) TEST MAXDISK=5242880000\TS: H2C=CH2 + HAl
 Br4 + H2\0,1\Br,0,0.5330399399,2.2078719549,-0.6888264773\H,0,-1.8335
 901214,1.6812527914,-0.8306076797\H,0,-2.5570763071,1.4214758488,-0.78
 25608118\C,0,-3.7865540444,0.4263063281,0.2115888718\C,0,-3.588821259,
 -0.9304957672,-0.1385337219\H,0,-2.5655156241,-0.9685317373,-0.7112587
 389\Br,0,-0.6526417709,-1.2140843816,-1.5810146726\Al,0,0.5480707327,0
 .0210989315,0.0766216079\H,0,-4.4903584865,1.063896024,-0.31856017\H,0
 ,-3.3035339844,0.8307345866,1.0976315596\H,0,-4.3212240198,-1.35827415
 58,-0.824881419\H,0,-3.320404809,-1.5632275834,0.7148400287\Br,0,2.610
 903917,-0.8804363906,0.3074481872\Br,0,-0.7907582103,-0.0663933327,1.9
 68706832\Version=SGI-G94RevE.2\HF=-10609.8622755\RMSD=8.975e-09\Dipol
 e=-3.7628599,0.0057761,-0.2006586\PG=C01 [X(C2H7Al1Br4)]\@

TABLE S2: Selected B3-LYP/6-31G(d) Total Energies and ZPVEs and MP2/6-311+G(3df,2p) Total Energies (Hartrees) of the B3-LYP/6-31G(d) Optimized Geometries

Molecule	B3-LYP/6-31G(d)	B3-LYP/6-31G(d)	MP2/6-311+G(3df,2p)
	Energy	ZPVE	Energy
TS1	-79.62786	0.06447	-79.41928
TS2(F)	-180.11466	0.07773	-179.79217
TS2(Cl)	-540.51071	0.07639	-539.78671
TS2(Br)	-2652.02675	0.07595	-2652.63349
HAIF ₄	-642.63444	0.02058	-641.77707
HAICl ₄	-2084.03851	0.01325	-2081.63030
HAIBr ₄	-10530.10349	0.01104	-10532.96903
ethene (4)	-78.58746	0.05122	-78.39326
hydrogen (5)	-1.17548	0.01016	-1.16274
HF (6)	-100.42017	0.00906	-100.32917
HCl (6)	-460.79570	0.00670	-460.29859
HBr (6)	-2572.30128	0.00589	-2573.13373
[H ₂ C=CH ₂ •HF]	-179.01643	0.06247	-178.73069
[H ₂ C=CH ₂ •HCl]	-539.38890	0.06004	-538.69805
[H ₂ C=CH ₂ •HBr]	-2650.89374	0.05882	-2651.53221
TS3(F)	-178.95014	0.06050	-178.64739
TS3(Cl)	-539.33036	0.05885	-538.62369
TS3(Br)	-2650.84162	0.05827	-2651.46436
CH ₃ CH ₂ F	-179.05642	0.06851	-178.74912
CH ₃ CH ₂ Cl	-539.42627	0.06713	-538.72986
CH ₃ CH ₂ Br	-2650.93476	0.06644	-2651.56848
TS4(F)	-180.09734	0.07854	-179.77204
TS4(Cl)	-540.48225	0.07656	-539.75345
TS4(Br)	-2651.99224	0.07576	-2652.59060

TABLE S2 (contd): Selected B3-LYP/6-31G(d) Total Energies and ZPVEs and MP2/6-311+G(3df,2p) Total Energies (Hartrees) of the B3-LYP/6-31G(d) Optimized Geometries

Molecule	B3-LYP/6-31G(d)	B3-LYP/6-31G(d)	MP2/6-311+G(3df,2p)
	Energy	ZPVE	Energy
(HF) ₂	-200.85563	0.02168	-200.66271
(HCl) ₂	-921.59424	0.01484	-920.60086
(HBr) ₂	-5144.60787	0.01356	-5146.27040
[H ₂ C=CH ₂ •2HF]	-279.46001	0.07671	-279.06931
[H ₂ C=CH ₂ •2HCl]	-100.18925	0.06835	-999.00254
[H ₂ C=CH ₂ •2HBr]	-5223.20386	0.06706	-5224.67055
TS5(F)	-279.41818	0.07328	-279.00570
TS5(Cl)	-1000.15385	0.06827	-998.94650
TS5(Br)	-5223.17853	0.06665	-5224.62644
[CH ₃ CH ₂ F•HF]	-279.49389	0.08134	-279.08827
[CH ₃ CH ₂ Cl•HCl]	-1000.22699	0.07532	-999.03532
[CH ₃ CH ₂ Br•HBr]	-5223.24540	0.07430	-5224.70845
TS6(F)	-280.56689	0.09229	-280.14061
TS6(Cl)	-1001.31738	0.08542	-1000.09656
TS6(Br)	-5224.34388	0.08473	-5225.77604
TS7(F)	-280.56672	0.08819	-280.13691
TS7(Cl)	-1001.30839	0.08430	-1000.07971
TS7(Br)	-5224.33221	0.082756	-5225.75817
TS8(F)	-280.55141	0.09167	-280.12787
TS8(Cl)	-1001.30626	0.08610	-1000.08583
TS8(Br)	-5224.33417	0.08547	-5225.76616
[H ₂ C=CH ₂ •HAIF ₄]	-721.24258	0.07336	-720.19316
[H ₂ C=CH ₂ •HAICl ₄]	-2162.63932	0.06644	-2160.03839
[H ₂ C=CH ₂ •HAIBr ₄]	-10608.70643	0.06480	-10611.37554

TABLE S2 (contd): Selected B3-LYP/6-31G(d) Total Energies and ZPVEs and MP2/6-311+G(3df,2p) Total Energies (Hartrees) of the B3-LYP/6-31G(d) Optimized Geometries

Molecule	B3-LYP/6-31G(d)	B3-LYP/6-31G(d)	MP2/6-311+G(3df,2p)
	Energy	ZPVE	Energy
TS9(F)	-721.22920	0.07143	-720.16500
TS9(Cl)	-2162.63123	0.06538	-2160.02102
TS9(Br)	-10608.70152	0.06318	-10611.36452
[CH ₃ CH ₂ F•AlF ₃]	-721.27139	0.07819	-720.21071
[CH ₃ CH ₂ Cl•AlCl ₃]	-2162.67985	0.07306	-2160.07489
[CH ₃ CH ₂ Br•AlBr ₃]	-10608.75098	0.07146	-10611.41675
TS10(F)	-722.38082	0.09038	-721.30871
TS10(Cl)	-2163.79535	0.08517	-2161.17009
TS10(Br)	-10609.86772	0.08404	-10612.50972
TS11(F)	-722.38733	0.08858	-721.30816
TS11(Cl)	-2163.79278	0.08265	-2161.15889
TS11(Br)	-10609.86228	0.08063	-10612.49959