

Understanding Metal-Free Catalytic Hydrogenation: A Systematic Theoretical Study of the Hydrogenation of Ethene

Bun Chan^A and Leo Radom^{A,B,C}

^A School of Chemistry, University of Sydney, University of Sydney, NSW 2006,
Australia.

^B Research School of Chemistry, Australian National University, Canberra, ACT 0200,
Australia.

^C Author to whom correspondence should be addressed
(email: radom@chem.usyd.edu.au).

ACCESSORY MATERIAL

(Tables A1–A2, Total 21 pages)

**Table A1. GAUSSIAN Archive Entries for the B3-LYP/6-31G(d)
Optimized Geometries**

H₂

1\1\GINC-SC32\FOpt\RB3LYP\6-31G(d)\H2\BUC562\03-Nov-2003\0\#\ G3MP2B3
OPT=(TIGHT,CALCF) SCF=TIGHT MAXDISK=6553600\H2\0,1\H,0.,0.,0.37139\
H,0.,0.,-0.37139\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-SG\HF=-1.1
754824\RMSD=4.911e-15\RMSF=3.360e-06\Dipole=0.,0.,0.\Polar=0.,0.,0.,0.
,0.,6.3774049\PG=D*H [C*(H1.H1)]\@\

CH₂CH₂

1\1\GINC-SC6\FOpt\RB3LYP\6-31G(d)\C2H4\BUC562\25-Nov-2003\0\#\ G3MP2B3
OPT=TIGHT SCF=TIGHT MAXDISK=65536000\CH2CH2\0,1\C,-0.6654719556,0.,
0.\C,0.6654719556,0.,0.\H,1.2395819049,0.9235924413,0.\H,1.2395819049,
-0.9235924413,0.\H,-1.2395819049,-0.9235924413,0.\H,-1.2395819049,0.92
35924413,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-AG\HF=-78.587458
3\RMSD=7.056e-10\RMSF=7.980e-07\Dipole=0.,0.,0.\PG=D02H [C2"(C1.C1),SG
(H4)]\@\

CH₃CH₃

1\1\GINC-SC6\FOpt\RB3LYP\6-31G(d)\C2H6\BUC562\25-Nov-2003\0\#\ G3MP2B3
OPT=TIGHT SCF=TIGHT MAXDISK=65536000\CH3CH3 stagger\0,1\C,-0.765272
6693,-0.0000237693,0.\C,0.7652726693,0.0000237693,0.\H,1.1643654125,1.
0209528767,0.\H,1.1643435687,-0.5104697007,0.884144379\H,-1.1643654125
, -1.0209528767,0.\H,-1.1643435687,0.5104697007,0.884144379\H,1.1643435
687,-0.5104697007,-0.884144379\H,-1.1643435687,0.5104697007,-0.8841443
79\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-AG\HF=-79.8304178\RMSD=9.
586e-10\RMSF=7.928e-07\Dipole=0.,0.,0.\PG=C02H [SGH(C2H2),X(H4)]\@\

TS(uncatalysed)

1\1\GINC-LC84\FTS\RB3LYP\6-31G(d)\C2H6\BUC562\25-Nov-2003\0\#\ G3MP2B3
OPT=(TS,TIGHT,CALCF,NOEIGENTEST) SCF=TIGHT MAXDISK=65536000\CH3CH3
-> CH2CH2 + H2 TS\0,1\H,-1.6373900121,-1.0496033256,0.\H,-0.357494109
6,-0.9554544119,0.\C,-0.5843669635,0.2566836731,0.\C,0.8199509229,-0.0
452702918,0.\H,-1.0361177621,0.6259960123,0.9148524047\H,-1.0361177621
,0.6259960123,-0.9148524047\H,1.3268079445,-0.2577072876,0.9327485726\
H,1.3268079445,-0.2577072876,-0.9327485726\Version=x86-Linux-G03RevB.
03\State=1-A'\HF=-79.627864\RMSD=1.930e-09\RMSF=1.786e-06\Dipole=0.112
1492,0.20947,0.\PG=CS [SG(C2H2),X(H4)]\@\

ZOH

HOH

1\1\GINC-SC118\FOpt\RB3LYP\6-31G(d)\H2O1\BUC562\15-Nov-2003\0\#\ G3MP2
B3 OPT=TIGHT SCF=TIGHT MAXDISK=13107200\H2O\0,1\O,-0.0691363394,-0.0
977734322,0.\H,0.8983592803,-0.0485956373,0.\H,-0.3452685649,0.8307830
947,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A1\HF=-76.4089533\RMS
D=9.476e-09\RMSF=7.346e-09\Dipole=0.4759584,0.673106,0.\PG=C02V [C2(O1
) ,SGV(H2)]\@\

HO⁻

1\1\GINC-SC101\FOpt\RB3LYP\6-31G(d)\H1O1(1-)\BUC562\15-Dec-2003\0\#\ G
3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=39321600\OH-\0,1\O,0.,0.08624374
35,0.06780447\H,0.,-0.6899499481,-0.5424357599\Version=DEC-AXP-OSF/1-
G03RevB.03\State=1-SG\HF=-75.7207738\RMSD=8.970e-10\RMSF=8.832e-07\Dip
ole=0.,-0.3626836,-0.2851403\PG=C*V [C*(H1O1)]\@\

HOH₂⁺

1\1\GINC-SC96\FOpt\RB3LYP\6-31G(d)\H3O1(1+)\BUC562\15-Dec-2003\0\#\ G3
MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\H3O+\0,1\O,-0.0642906624,
-0.0001466124,0.0444580911\H,-0.1036524093,0.8144074971,-0.513718544\
H,-0.0913214061,-0.823595765,-0.5012414513\H,0.7092991147,0.0103611672,
0.6592952663\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-76.689085
7\RMSD=4.414e-09\RMSF=5.688e-06\Dipole=0.5424887,0.0012372,-0.3751435\
PG=C01 [X(H3O1)]\@\

TS(HOH)

1\1\GINC-SC16\FOpt\RB3LYP\6-31G(d)\C2H8O1\BUC562\04-Dec-2003\0\#\ G3MP2
B3 OPT=(TS,TIGHT,CALCF,NOEIGENTEST) SCF=TIGHT NOSYMM MAXDISK=65536000
\(H2O) CH3CH3 -> CH2CH2 + H2 TS\0,1\H,1.175357224,-0.9013306223,0.02
37397088\C,-0.3586065448,-1.2482147991,-0.0473494704\C,-1.1047607672,-
0.0543572665,0.0114322304\H,-0.0120348579,0.8727283373,0.1873702823\H,
-0.2745057542,-1.8912804624,0.8263350556\H,-0.2116691643,-1.768086645,
-0.9923043139\H,-1.5854630031,0.2809527438,-0.9075012647\H,-1.67068762
58,0.1360256415,0.9228150684\H,1.3719676434,-0.0084988681,0.1594686365
\O,1.103031339,1.3180399301,0.3420310793\H,1.3293175109,1.6942290107,-
0.5260370124\Version=DEC-AXP-OSF/1-G03RevB.03\HF=-156.0902977\RMSE=4.
872e-09\RMSE=4.299e-06\Dipole=-0.1201048,-0.2889389,-0.6277962\PG=C01
[X(C2H8O1)]\@\@

(CH₃)₃COH

1\1\GINC-SC12\FOpt\RB3LYP\6-31G(d)\C4H10O1\BUC562\20-Dec-2003\0\#\ G3M
P2B3 OPT=TIGHT SCF=TIGHT MAXDISK=134217728\@t-BuOH\0,1\C,-0.005422000
1,-0.0000039171,0.013743\C,0.6907436488,-1.2653705637,-0.510094\C,0.69
01573564,1.2656964456,-0.510072\C,-1.4905120053,-0.0003342056,-0.35682
2\O,0.0141009998,-0.0000122156,1.452344\H,0.9449700031,0.0001975486,1.
727845\H,0.210268975,-2.1594852159,-0.099426\H,0.6541117907,-1.3214780
035,-1.604342\H,1.7480194364,-1.2792677326,-0.213191\H,1.7474225766,1.
2800862768,-0.213159\H,0.6535012144,1.3217990062,-1.60432\H,0.20925702
65,2.1595778001,-0.099396\H,-1.9838774509,0.8859833396,0.055398\H,-1.6
228050055,-0.0003461824,-1.444055\H,-1.9834795634,-0.8868886667,0.0553
66\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-233.6709581\RMSE=6.
045e-09\RMSE=4.490e-06\Dipole=0.4738681,0.0001179,-0.3592379\PG=C01 [X
(C4H10O1)]\@\@

(CH₃)₃CO⁻

1\1\GINC-SC21\FOpt\RB3LYP\6-31G(d)\C4H9O1(1-)\BUC562\22-Dec-2003\0\#\
G3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\@t-BuO-\-1,1\C,0.0001052526,0.
0000330781,0.1595446317\C,1.4286319813,-0.3163102684,-0.4368717554\C,-
0.4409653998,1.3945712251,-0.4376336764\C,-0.988211233,-1.0795521836,-
0.4356199563\O,0.0005496362,0.0015384079,1.4838000444\H,1.7575022612,-
1.2930232504,-0.054106702\H,1.4956864355,-0.3352033115,-1.5410734422\H
,2.1377257361,0.4350496111,-0.0609310971\H,0.2407050673,2.1680327026,-
0.0560781075\H,-0.4589295882,1.4610901078,-1.5418784789\H,-1.445917922
4,1.6328845732,-0.0610786913\H,-1.9996482598,-0.8728935599,-0.05750720
78\H,-1.0341706722,-1.1326750896,-1.5397843258\H,-0.6947137531,-2.0680
201542,-0.0544777642\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-2
33.0392888\RMSE=7.465e-09\RMSE=4.683e-05\Dipole=-0.0005886,-0.0014922,
-1.3736527\PG=C01 [X(C4H9O1)]\@\@

(CH₃)₃COH₂⁺

1\1\GINC-SC91\FOpt\RB3LYP\6-31G(d)\C4H11O1(1+)\BUC562\25-Jan-2004\0\#\
G3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\@t-BuOH2+\1,1\C,-0.006626177
7,0.1198429257,0.1311360748\O,0.055390081,-0.9429008663,-1.1711944485\
H,0.8627949864,-1.4990050235,-1.1538018182\C,1.2610052746,0.9154682181
,-0.0748082655\C,-1.2875722927,0.866997472,-0.1573418624\C,-0.02974589
52,-0.7629903793,1.3583692966\H,-0.7195342319,-1.5432898702,-1.1934172
61\H,-2.1697395634,0.2204490555,-0.099957913\H,-1.4041851051,1.6353786
258,0.6159464272\H,-1.2558280355,1.3695347358,-1.1272452722\H,1.280091
1438,1.4038528395,-1.052323176\H,1.2887419495,1.6986201902,0.691915985
8\H,2.1621232224,0.3071631399,0.0573773825\H,0.8734881392,-1.374617850
4,1.4506456829\H,-0.0652657732,-0.1093458343,2.2384199801\H,-0.9181728
343,-1.4014424964,1.3978641085\Version=DEC-AXP-OSF/1-G03RevB.03\State
=1-A\HF=-233.9959209\RMSE=7.712e-09\RMSE=1.647e-04\Dipole=0.0395024,-1
.0570792,-0.3791012\PG=C01 [X(C4H11O1)]\@\@

TS((CH₃)₃COH)

1\1\GINC-SC115\FTS\RB3LYP\6-31G(d)\C6H16O1\BUC562\23-Dec-2003\0\#\# G3M
P2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCFC,NOEIGENTEST) MAXDISK=805306368\CH
3CH3 -> CH2CH2 + H2 TS (t-BuOH)\0,1\H,1.698852813,-1.5206756817,-0.32
26584676\C,2.8523740632,-0.5444935096,0.0069325221\C,2.383263646,0.784
556443,-0.0353224334\H,0.9948498374,0.4875947507,-0.4735401754\H,3.459
0563623,-0.9390689914,-0.8061629998\H,3.0262744095,-1.0391632012,0.961
2650902\H,2.2608313386,1.3049780351,0.9138203241\H,2.7152065043,1.4086
05405,-0.8643272311\H,0.8806607975,-1.13666598,-0.5748298574\O,0.06200
86057,-0.119582834,-0.8730734274\C,-1.0758431752,-0.007232941,0.010845
79\C,-0.7431254862,-0.519574742,1.4209842329\C,-1.4736269131,1.4754727
571,0.051487169\C,-2.1839269069,-0.8554745426,-0.6238025939\H,-1.68267
62555,1.8391873105,-0.9597408672\H,-2.368024963,1.625533763,0.66724372
45\H,-0.6650316919,2.0830727129,0.4738364328\H,0.071137107,0.059889628
9,1.8696938847\H,-1.616886921,-0.4334937169,2.0768222427\H,-0.44507617
69,-1.5734922328,1.3943313226\H,-1.8798136825,-1.9067056884,-0.6788195
062\H,-3.1089304841,-0.7955353127,-0.0385343275\H,-2.3911892073,-0.506
9189183,-1.6405602905\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-
313.348368\RMSD=9.076e-09\RMSF=3.481e-06\Dipole=-0.1141033,-0.0960626,
0.4531385\PG=C01 [X(C6H16O1)]\@

H₂COH

1\1\GINC-LC8\FOpt\RB3LYP\6-31G(d)\C1H4O1\BUC562\17-Nov-2003\0\#\# G3MP2
B3 OPT=TIGHT SCF=TIGHT MAXDISK=26214400\CH3OH\0,1\C,-0.6618139094,-0
.0327053666,0.\O,0.7565074653,-0.0631120463,0.\H,1.0699983483,0.853446
0872,0.\H,-1.0764346811,0.4603728438,-0.8931834944\H,-0.9983052523,-1.
0730632052,0.\H,-1.0764346811,0.4603728438,0.8931834944\Version=x86-L
inux-G03RevB.03\State=1-A\HF=-115.7144073\RMSD=9.264e-09\RMSF=2.485e-
06\Dipole=-0.3403939,0.5731458,0.\PG=CS [SG(C1H2O1),X(H2)]\@

H₃CO⁻

1\1\GINC-SC31\FOpt\RB3LYP\6-31G(d)\C1H3O1(1-)\BUC562\15-Dec-2003\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\CH3O-\-1,1\C,0.01912348
57,0.5204062702,0.\O,-0.0289616742,-0.7880497765,0.\H,-0.4755046074,1.
079573809,0.8917239876\H,1.0679616941,1.0228129733,0.\H,-0.4755046074,
1.079573809,-0.8917239876\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A'
\HF=-115.0720904\RMSD=6.985e-09\RMSF=2.862e-06\Dipole=0.0179081,0.4871
969,0.\PG=CS [SG(C1H1O1),X(H2)]\@

H₃COH₂⁺

1\1\GINC-SC31\FOpt\RB3LYP\6-31G(d)\C1H5O1(1+)\BUC562\15-Dec-2003\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\CH3OH2+\1,1\C,0.0395763
984,0.7956473213,0.0462570768\O,0.0010433231,-0.7255569724,0.022080207
6\H,-0.9035443204,-1.1069331744,0.072170953\H,-0.460575037,1.06280326,
0.9746607624\H,1.0998524629,1.037604397,0.0732577785\H,-0.4682136142,1
.1664794902,-0.8431470674\H,0.4866755336,-1.1293821212,-0.7311265487\H
Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-116.0157452\RMSD=4.281e
-09\RMSF=1.049e-06\Dipole=-0.3054813,-0.5236944,-0.514036\PG=C01 [X(C1
H5O1)]\@

TS(H₃COH)

1\1\GINC-SC113\FTS\RB3LYP\6-31G(d)\C3H10O1\BUC562\05-Dec-2003\0\#\# G3M
P2B3 OPT=(TS,TIGHT,CALCFC,NOEIGENTEST) SCF=TIGHT MAXDISK=134217728\CH
3CH3 -> CH2CH2 + H2 TS (CH3OH)\0,1\H,0.7751239763,-1.4290243634,0.117
7813339\C,-0.7922840508,-1.6883772337,0.1415889019\C,-1.4496418834,-0.
4534872139,0.3054882642\H,-0.2979801865,0.3865164247,0.4247455425\H,-0
.6854636164,-2.3751149888,0.9785107688\H,-0.7396660163,-2.1667832735,-
0.8343096438\H,-1.9726366563,-0.0464615947,-0.5596013606\H,-1.93100822
71,-0.2667109043,1.2650256554\H,1.0209600055,-0.5589399019,0.275466436
7\O,0.8468786428,0.7771002009,0.4610222347\C,1.1391785094,1.3957485775
,-0.7821699632\H,0.2234709031,1.6365433179,-1.3431460152\H,1.681536461
9,2.3267391879,-0.5840406407\H,1.7671187616,0.7531297096,-1.4180531722
\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-195.3968613\RMSD=7.12
9e-09\RMSF=5.105e-06\Dipole=-0.228704,-0.288797,-0.4804696\PG=C01 [X(C
3H10O1)]\@

FH

1\1\GINC-LC46\FOpt\RB3LYP\6-31G(d)\F1H1\BUC562\04-Dec-2003\0\#\ G3MP2B
 3 OPT=TIGHT SCF=TIGHT MAXDISK=26214400\HF\0,1\F,0.,0.,0.09338\H,0.,0
 .,-0.840421\Version=x86-Linux-G03RevB.03\State=1-SG\HF=-100.4201718\R
 MSD=4.709e-09\RMSF=6.544e-08\Dipole=0.,0.,-0.7315651\PG=C*V [C*(H1F1)]
 \\\@

F⁻

1\1\GINC-LC141\FOpt\RB3LYP\6-31G(d)\F1(1-)\BUC562\15-Dec-2003\0\#\ G3M
 P2B3 SCF=TIGHT OPT=TIGHT MAXDISK=39321600\F-\-1,1\F,0.,0.,0.\Version
 n=x86-Linux-G03RevB.03\State=1-A1\HF=-99.7540888\RMSD=4.969e-10\RMSF=
 0.000e+00\Dipole=0.,0.,0.\PG=OH [O(F1)]\\\@

FH₂⁺

1\1\GINC-LC125\FOpt\RB3LYP\6-31G(d)\F1H2(1+)\BUC562\15-Dec-2003\0\#\ G
 3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=39321600\H2F+\1,1\F,-0.0578724516
 ,-0.0818437293,0.\H,0.9258278766,-0.1022149651,0.\H,-0.4049758125,0.83
 88085285,0.\Version=x86-Linux-G03RevB.03\State=1-A1\HF=-100.6230862\R
 MSD=8.133e-10\RMSF=2.432e-06\Dipole=0.5593799,0.79108,0.\PG=C02V [C(2F
 1),SGV(H2)]\\\@

TS(FH)

1\1\GINC-LC8\FTS\RB3LYP\6-31G(d)\C2H7F1\BUC562\04-Dec-2003\0\#\ G3MP2B
 3 OPT=(TS,TIGHT,CALCF,NOEIGENTEST) SCF=TIGHT MAXDISK=134217728\HF)
 CH3CH3 -> CH2CH2 + H2 TS\0,1\H,-1.0335334675,-1.1869080389,0.\C,0.634
 6381542,-1.1704640013,0.\C,1.0622477751,0.1728548333,0.\H,-0.097374596
 3,0.7767480044,0.\H,0.6109520435,-1.7559976041,-0.9157765893\H,0.61095
 20435,-1.7559976041,0.9157765893\H,1.5277663563,0.5298925221,0.9191174
 638\H,1.5277663563,0.5298925221,-0.9191174638\H,-1.3242601373,-0.37884
 28917,0.\F,-1.3337315749,1.0252075665,0.\Version=x86-Linux-G03RevB.03
 \State=1-A'\HF=-180.1146568\RMSD=4.865e-09\RMSF=5.007e-06\Dipole=0.969
 9843,-0.9541652,0.\PG=CS [SG(C2H3F1),X(H4)]\\\@

CH₃C(O)OH

1\1\GINC-LC141\FOpt\RB3LYP\6-31G(d)\C2H4O2\BUC562\02-Dec-2003\0\#\ G3M
 P2B3 OPT=TIGHT SCF=TIGHT MAXDISK=134217728\MeCO2H\0,1\C,0.1525107548
 ,0.0331506142,0.\O,1.3606639963,0.1008423702,0.\O,-0.6397561034,1.1371
 318303,0.\H,-0.0327707486,1.9010598298,0.\C,-0.6685208473,-1.231931949
 2,0.\H,-0.0047728115,-2.0966558884,0.\H,-1.316829514,-1.2577547678,0.8
 820351003\H,-1.316829514,-1.2577547678,-0.8820351003\Version=x86-Linu
 x-G03RevB.03\State=1-A'\HF=-229.0817868\RMSD=9.650e-09\RMSF=4.114e-07\
 Dipole=-0.6204888,0.0266907,0.\PG=CS [SG(C2H2O2),X(H2)]\\\@

CH₃C(O)O⁻

1\1\GINC-LC140\FOpt\RB3LYP\6-31G(d)\C2H3O2(1-)\BUC562\15-Dec-2003\0\#\
 G3MP2B3 OPT SCF=TIGHT MAXDISK=65536000\MeCO2-\-1,1\C,0.00000129,0.
 220224,0.\O,1.1148184687,0.7998613468,0.\O,-1.1603825867,0.7053886799,
 0.\C,0.0442242062,-1.3547830259,0.\H,1.0713509795,-1.7417986277,0.\H,-
 0.4860940233,-1.7464217152,0.880573\H,-0.4860940233,-1.7464217152,-0.8
 80573\Version=x86-Linux-G03RevB.03\State=1-A'\HF=-228.4979114\RMSD=5.
 002e-09\RMSF=7.231e-06\Dipole=0.0306284,-1.2527713,0.\PG=CS [SG(C2H1O2
),X(H2)]\\\@

CH₃C(O)OH₂⁺

1\1\GINC-SC96\FOpt\RB3LYP\6-31G(d)\C2H5O2(1+)\BUC562\23-Jan-2004\0\#\
 G3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\MeCOOH2+\1,1\C,-0.489991074,
 0.2893798747,0.000857\O,-0.5100583643,1.4240988695,0.001386\O,1.550909
 0816,-0.3189926033,-0.002664\H,2.0577339957,0.0166495263,-0.765714\C,-
 1.0142257276,-1.0649532594,-0.001165\H,-2.1089107463,-0.9917635394,-0.
 003559\H,-0.6489095931,-1.590864166,-0.89009\H,-0.6537255927,-1.592189
 1672,0.888981\H,2.0523120075,-0.0292434751,0.78245\Version=DEC-AXP-OS
 F/1-G03RevB.03\State=1-A'\HF=-229.3658067\RMSD=6.905e-09\RMSF=7.691e-06
 \Dipole=0.2079466,-0.5362957,0.0148916\PG=C01 [X(C2H5O2)]\\\@

TS(CH₃C(O)OH)

1\1\GINC-SC11\FTS\RB3LYP\6-31G(d)\C4H10O2\BUC562\10-Dec-2003\0\# G3MP
2B3 OPT=(TS,TIGHT,CALCF,NOEIGENTEST) SCF=TIGHT MAXDISK=268435456\CH3
CH3 -> CH2CH2 + H2 TS (MeCO2H, C1)\0,1\C,2.5119580061,0.2653299424,0.
405498\C,1.9966759933,-0.2933800458,-0.785427\H,2.32571703,1.308825946
6,0.642825\H,3.2768909946,-0.2356770752,0.993326\H,1.7023460098,0.4281
509609,-1.548386\H,2.5067469729,-1.1813190575,-1.161412\H,0.8891389844
, -0.6790570204,-0.417381\O,-0.4012610222,-0.9669839908,0.255249\C,-1.1
229849973,0.1179660258,0.027401\O,-0.6582229714,1.2454880151,-0.098215
\H,0.69261199,-0.4346450159,1.364566\H,1.3930539971,-0.128421032,1.642
159\C,-2.6149760041,-0.17722594,-0.066064\H,-2.9658070145,-0.633502931
9,0.865698\H,-3.1629449828,0.7474660726,-0.2561\H,-2.8059220206,-0.895
9889356,-0.870024\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-308.
766572\RMSD=4.851e-09\RMSF=1.261e-06\Dipole=1.2472898,-0.3109203,0.059
6908\PolAr=94.6502343,4.8327807,48.7864624,3.683761,1.1868594,49.76874
62\PG=C01 [X(C4H10O2)]\@

HC(O)OH

1\1\GINC-LC90\FOpt\RB3LYP\6-31G(d)\C1H2O2\BUC562\21-Nov-2003\0\# G3MP
2B3 OPT=TIGHT SCF=TIGHT MAXDISK=65536000\HCO2H\0,1\C,0.0011620011,0.
4217913912,0.\O,-1.0358146609,-0.4383939783,0.\O,1.1641994205,0.107657
2248,0.\H,-0.6531506336,-1.3377477688,0.\H,-0.3808994493,1.4528934502,
0.\Version=x86-Linux-G03RevB.03\State=1-A\HF=-189.7554578\RMSD=2.638
e-09\RMSF=3.616e-06\Dipole=-0.5368574,-0.1646355,0.\PG=CS [SG(C1H2O2)]
\@

HC(O)O⁻

1\1\GINC-SC160\FOpt\RB3LYP\6-31G(d)\C1H1O2(1-)\BUC562\21-Nov-2003\0\#
G3MP2B3 OPT=TIGHT SCF=TIGHT MAXDISK=65536000\HCO2--\1,1\C,0.,0.3108
584526,0.\O,1.1416699889,-0.2080170009,0.\O,-1.1416699889,-0.208017000
9,0.\H,0.,1.4631212993,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A1
\HF=-189.1775629\RMSD=2.442e-09\RMSF=2.817e-06\Dipole=0.,0.3468279,0.
PG=C02V [C2(C1H1),SGV(O2)]\@

HC(O)OH₂⁺

1\1\GINC-SC100\FOpt\RB3LYP\6-31G(d)\C1H3O2(1+)\BUC562\15-Dec-2003\0\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\HCOOH2+\1,1\C,0.187956
0912,0.5743621261,-0.0067945144\O,-1.0276052011,-0.5440527664,0.079019
4644\O,1.2433469309,0.1549196562,-0.1863961607\H,-0.7128179797,-1.4744
795208,0.1513425372\H,-0.3326379748,1.5280732883,0.0915217456\H,-1.808
2144319,-0.3867016426,0.6569163743\Version=DEC-AXP-OSF/1-G03RevB.03\St
ate=1-A\HF=-190.0141994\RMSD=5.586e-09\RMSF=2.609e-06\Dipole=-1.55268
54,-0.0796879,0.7003935\PG=C01 [X(C1H3O2)]\@

TS(HC(O)OH)

1\1\GINC-SC8\FTS\RB3LYP\6-31G(d)\C3H8O2\BUC562\10-Dec-2003\0\# G3MP2B
3 OPT=(TS,TIGHT,CALCF,NOEIGENTEST) SCF=TIGHT MAXDISK=134217728\CH3CH
3 -> CH2CH2 + H2 TS (HCO2H)\0,1\C,1.9664381163,0.3544181083,0.4519671
05\C,1.5094151415,-0.1753336009,-0.7765773197\H,1.7058554313,1.3689105
833,0.7404610976\H,2.7493153036,-0.1276321609,1.0319401033\H,1.1807700
563,0.5645349904,-1.5074166522\H,2.0899132186,-1.0024359625,-1.1877026
119\H,0.4364899676,-0.6607306405,-0.456667485\O,-0.8639486881,-1.08990
24243,0.1726884961\C,-1.6490369135,-0.0587328039,-0.0248332104\O,-1.31
60665928,1.114958941,-0.0967955388\H,0.1792908052,-0.5179819213,1.3480
011754\H,0.8467285503,-0.1753356396,1.6494496805\H,-2.709139151,-0.371
8916029,-0.1285484153\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-
269.4429937\RMSD=9.164e-09\RMSF=4.685e-06\Dipole=1.6046359,-0.15041,0.
1025655\PG=C01 [X(C3H8O2)]\@

F₃COH

1\1\GINC-SC12\FOpt\RB3LYP\6-31G(d)\C1H1F3O1\BUC562\20-Dec-2003\0\# G3
MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\CF3OH\0,1\C,0.0168144816
, -0.0081230079,0.0136850241\F,1.3400110002,-0.0589574475,-0.1119369236
\F,-0.3795842536,1.2799866501,-0.0796376535\F,-0.5441789531,-0.6593289
214,-1.0285650569\O,-0.3201012239,-0.56026521,1.200532115\H,-1.2863072
402,-0.5244428044,1.2948896411\Version=DEC-AXP-OSF/1-G03RevB.03\State
=1-A\HF=-413.4572411\RMSD=1.598e-09\RMSF=7.947e-06\Dipole=-0.7064322,-
0.0830162,0.2921758\PG=C01 [X(C1H1F3O1)]\@

F₃CO⁻

1\1\GINC-LC147\FOpt\RB3LYP\6-31G(d)\C1F3O1(1-)\BUC562\22-Dec-2003\0\#\#
G3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\CF3O-\-1,1\C,-0.18883404,-0
.0002693039,-0.030262\F,0.2496429988,-0.0000262929,1.332653\F,0.557139
3453,1.1058632463,-0.554423\F,0.5603889442,-1.1038942352,-0.555074\O,-
1.3964432944,-0.00198358,-0.228353\Version=x86-Linux-G03RevB.03\State
=1-A\HF=-412.9055226\RMSD=8.257e-09\RMSF=1.822e-04\Dipole=0.6732704,0.
001048,0.1138909\PG=C01 [X(C1F3O1)]\#@

F₃COH₂⁺

1\1\GINC-SC96\FOpt\RB3LYP\6-31G(d)\C1H2F3O1(1+)\BUC562\23-Jan-2004\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\CF3OH2+\1,1\C,-0.190
782821,-0.0000004443,-0.0035611998\O,1.3922380022,0.0000085463,-0.1030
670453\H,1.8185312008,0.8112642833,0.2644282532\F,-0.5188317553,1.0891
393107,-0.6130506911\F,-0.5188357582,-1.0890175793,-0.6132665582\F,-0.
4768072154,-0.0001253406,1.2615574389\H,1.8185342678,-0.8112975036,0.2
643136015\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-413.7092154\
RMSD=7.640e-09\RMSF=2.739e-06\Dipole=1.9955612,-0.0000359,0.505531\PG=
C01 [X(C1H2F3O1)]\#@

TS(F₃COH)

1\1\GINC-SC4\FTS\RB3LYP\6-31G(d)\C3H7F3O1\BUC562\20-Dec-2003\0\#\# G3MP
2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=671088640\CH3
CH3 -> CH2CH2 + H2 TS (CF3OH)\0,1\H,1.5748947862,-1.6699565451,-0.393
4919953\C,2.821019585,-0.5245361262,-0.1433295095\C,2.2573759607,0.759
4537113,-0.3096100817\H,1.08531984,0.4993701747,-0.5953755899\H,3.3704
44343,-1.0104136771,-0.945785454\H,2.9463112359,-0.9644579928,0.842827
4172\H,2.1456791401,1.3540344688,0.5978121804\H,2.5960735374,1.3153895
212,-1.1856117387\H,0.8533038086,-1.3325835763,-0.5718146935\O,-0.1852
813556,-0.1268656553,-0.9364682038\C,-1.0392901013,-0.000752031,0.0489
36805\F,-0.6680494346,0.9477803795,0.9739930213\F,-2.2652269101,0.3599
086368,-0.3955653148\F,-1.2138801567,-1.1500724003,0.7734836514\Versi
on=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-493.1486556\RMSD=7.014e-09\R
MSF=4.791e-06\Dipole=2.4487263,-0.1724047,0.0264984\PG=C01 [X(C3H7F3O1
)]\#@

FC(O)OH

1\1\GINC-SC90\FOpt\RB3LYP\6-31G(d)\C1H1F1O2\BUC562\02-Dec-2003\0\#\# G3
MP2B3 OPT SCF=TIGHT MAXDISK=65536000\FCO2H\0,1\C,-0.0000001875,0.125
77,0.\O,-0.0944349621,1.3161058592,0.\O,-0.9819938368,-0.780251464,0.\
H,-1.8193625765,-0.2840637123,0.\F,1.158977788,-0.5285992722,0.\Versi
on=DEC-AXP-OSF/1-G03RevB.03\State=1-A'\HF=-289.0022335\RMSD=8.585e-09\
RMSF=2.553e-05\Dipole=-0.7774114,-0.3319845,0.\PG=CS [SG(C1H1F1O2)]\#@

FC(O)O⁻

1\1\GINC-LC139\FOpt\RB3LYP\6-31G(d)\C1F1O2(1-)\BUC562\15-Dec-2003\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\FCOO-\-1,1\C,-0.17330
93576,0.0775712437,0.\O,-0.1279626901,1.3081442126,0.\O,-1.0607270041,
-0.7761732878,0.\F,1.1721526332,-0.5245772067,0.\Version=x86-Linux-G0
3RevB.03\State=1-A'\HF=-288.4541052\RMSD=1.182e-09\RMSF=6.729e-06\Dipo
le=0.3995719,-0.1787819,0.\PG=CS [SG(C1F1O2)]\#@

FC(O)OH₂⁺

1\1\GINC-SC116\FOpt\RB3LYP\6-31G(d)\C1H2F1O2(1+)\BUC562\15-Dec-2003\0\
\# G3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\FCOOH2+\1,1\C,0.278630026
, -0.0778219068,0.001533\O,0.880813357,-1.0670597053,0.010674\O,-1.2564
829516,-0.1446694204,-0.062997\H,-1.6380466546,-1.0322725481,0.141387\
F,0.5298896067,1.1755401773,0.000109\H,-1.7973782052,0.6131813986,0.26
7018\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-289.2397751\RMSD=
4.454e-09\RMSF=4.622e-06\Dipole=-2.1359071,0.0481156,0.4024384\PG=C01
[X(C1H2F1O2)]\#@

TS(FC(O)OH)

1\1\GINC-SC16\FTS\RB3LYP\6-31G(d)\C3H7F1O2\BUC562\10-Dec-2003\0\#\# G3M
P2B3 OPT=(TS,TIGHT,CALCFC,NOEIGENTEST) SCF=TIGHT MAXDISK=268435456\CH
3CH3 -> CH2CH2 + H2 TS (FCO2H, C1)\0,1\C,2.3209949739,0.396498153,0.3
80025\C,1.9434310246,-0.3726198719,-0.749243\H,1.8873919089,1.38212312
44,0.5215\H,3.1504449923,0.1167292076,1.024942\H,1.5977889847,0.232288
1053,-1.592549\H,2.604209079,-1.1988058284,-1.012952\H,0.9020360544,-0
.8251679405,-0.403146\O,-0.5196129313,-1.0430250342,0.292833\C,-1.0985
980049,0.0746879276,0.020322\O,-0.6157320778,1.1805549594,-0.132408\H,
0.6421310324,-0.4915309577,1.454705\H,1.3005330103,-0.1569989143,1.746
542\F,-2.4440829945,-0.0833641611,-0.10323\Version=DEC-AXP-OSF/1-G03R
evB.03\State=1-A\HF=-368.6965512\RMSD=6.714e-09\RMSF=3.437e-06\Dipole=
2.4463465,-0.0553867,0.1137642\Polar=73.5246583,5.3881716,39.4497983,2
.3884641,1.2634958,40.4713228\PG=C01 [X(C3H7F1O2)]\@\

O₂NOH

1\1\GINC-SC123\FOpt\RB3LYP\6-31G(d)\H1N1O3\BUC562\23-Dec-2003\0\#\# G3M
P2B3 OPT SCF=TIGHT MAXDISK=134217728\HNO3\0,1\N,-0.000000125,0.15231
3,0.\O,1.1777556231,0.4592459666,0.\O,-0.985340691,0.8419301914,0.\O,-
0.2706029894,-1.2313752221,0.\H,0.6255093333,-1.6245964867,0.\Version
=DEC-AXP-OSF/1-G03RevB.03\State=1-A'\HF=-280.8785554\RMSD=5.024e-09\RM
SF=1.138e-05\Dipole=0.4541916,-0.8073311,0.\PG=CS [SG(H1N1O3)]\@\

O₂NOH

1\1\GINC-SC113\FOpt\RB3LYP\6-31G(d)\N1O3(1-)\BUC562\23-Dec-2003\0\#\# G
3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\NO3-\-1,1\N,0.,0.,0.\O,
1.2642719316,-0.0000001819,0.\O,-0.6321358082,1.094891701,0.\O,-0.6321
361233,-1.0948915191,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A1'\
HF=-280.3358789\RMSD=1.252e-09\RMSF=1.516e-08\Dipole=0.,0.,0.\PG=D03H
[O(N1),3C2(O1)]\@\

O₂NOH₂⁺

1\1\GINC-SC30\FOpt\RB3LYP\6-31G(d)\H2N1O3(1+)\BUC562\23-Jan-2004\0\#\#
G3MP2B3 OPT=TIGHT SCF=TIGHT MAXDISK=134217728\H2ONO2+\1,1\N,0.618714
7147,-0.0000201791,0.0120977136\O,0.7772030513,-1.1251511555,0.0007260
427\O,0.7771640497,1.1251169329,0.000789408\O,-1.571809801,0.000055366
2,-0.0619269792\H,-2.0958658415,-0.7784913799,0.1988195225\H,-2.095595
5607,0.7784634847,0.1997887098\Version=DEC-AXP-OSF/1-G03RevB.03\State
=1-A\HF=-281.1587373\RMSD=5.999e-09\RMSF=2.731e-06\Dipole=-0.2766772,-
0.0001458,0.4029889\PG=C01 [X(H2N1O3)]\@\

TS(O₂NOH)

1\1\GINC-SC12\FTS\RB3LYP\6-31G(d)\C2H7N1O3\BUC562\24-Dec-2003\0\#\# G3M
P2B3 SCF=TIGHT OPT=(TS,CALCFC,NOEIGENTEST) MAXDISK=671088640\CH3CH3 -
> CH2CH2 + H2 TS (HNO3)\0,1\H,1.2758619952,-0.0686600886,1.737174\C,2
.3518510264,0.3803238368,0.371535\C,1.9209499743,-0.3703781333,-0.7512
74\H,0.8595709466,-0.7701090597,-0.399936\H,3.1515570027,0.0389007813,
1.024061\H,2.0104010973,1.4021948605,0.505605\H,1.6123790168,0.2426838
881,-1.602518\H,2.5302489141,-1.2379061756,-1.007682\H,0.6051299731,-0
.387609042,1.457243\O,-0.542323071,-1.0235759624,0.317771\N,-1.2444659
954,0.0657920864,0.005677\O,-2.4513930053,-0.0767978299,-0.117435\O,-0
.6276219214,1.1329100436,-0.134742\Version=DEC-AXP-OSF/1-G03RevB.03\St
ate=1-A\HF=-360.5759909\RMSD=4.184e-09\RMSF=2.055e-05\Dipole=2.812894
1,0.0538723,0.1214882\Polar=91.030859,5.8003848,40.491995,4.0503011,1.
0600325,40.0827112\PG=C01 [X(C2H7N1O3)]\@\

C1C(O)OH

1\1\GINC-LC53\FOpt\RB3LYP\6-31G(d)\C1H1C11O2\BUC562\02-Dec-2003\0\#\# G
3MP2B3 OPT=TIGHT SCF=TIGHT MAXDISK=134217728\C1CO2H\0,1\C,0.35436273
52,0.358551895,0.\O,1.5480512561,0.3435852744,0.\O,-0.4399420445,1.436
5389799,0.\H,0.1535250697,2.2127010318,0.\C1,-0.6555632455,-1.09441214
33,0.\Version=x86-Linux-G03RevB.03\State=1-A'\HF=-649.3548993\RMSD=6.
007e-09\RMSF=8.525e-06\Dipole=-0.1723311,0.8079052,0.\PG=CS [SG(C1H1C1
1O2)]\@\

CIC(O)⁻

1\1\GINC-SC101\FOpt\RB3LYP\6-31G(d)\C1C11O2(1-)\BUC562\15-Dec-2003\0\#\# G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\C1COO-\-1,1\C,0.2606130592,1.0269656378,0.\O,-0.813466439,1.5213535102,0.\O,1.4404661721,0.9493209447,0.\C1,-0.3870397776,-1.5251287921,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-648.8475516\RMSD=2.242e-09\RMSF=5.977e-06\Dipole=0.4334995,1.7082503,0.\PG=CS [SG(C1C11O2)]\@\

CIC(O)OH₂⁺

1\1\GINC-SC116\FOpt\RB3LYP\6-31G(d)\C1H2C11O2(1+)\BUC562\15-Dec-2003\0\#\# G3MP2B3 OPT=TIGHT SCF=TIGHT MAXDISK=134217728\C1COOH2+\1,1\C,0.2940322317,0.3618620973,0.007475814\O,0.912407381,1.3410807905,0.0147688518\O,1.2268868679,-1.0057586729,-0.0790371451\H,2.1748149593,-0.8067356232,0.1031162016\C1,-1.2933962086,-0.131512172,-0.0022815469\H,0.9343732056,-1.8113069779,0.4049615585\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-649.6032438\RMSD=4.416e-09\RMSF=7.260e-06\Dipole=1.0773578,-1.5253921,0.4839544\PG=C01 [X(C1H2C11O2)]\@\

TS(CIC(O)OH)

1\1\GINC-SC30\FTS\RB3LYP\6-31G(d)\C3H7C11O2\BUC562\12-Dec-2003\0\#\# G3MP2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=402653184\C3H3CH3 -> CH2CH2 + H2 TS (C1CO2H, C1)\0,1\C,2.835916704,0.4228439833,0.4108743946\C,2.4386975191,-0.3348542683,-0.7215869501\H,2.424574291,1.4169771649,0.561363736\H,3.6599834268,0.1226476953,1.0535223684\H,2.1087547114,0.280429976,-1.5638104761\H,3.087632539,-1.1689230253,-0.990429737\H,1.3999313715,-0.7790355719,-0.3833794575\O,-0.0539911128,-1.0005703076,0.3185143182\C,-0.627174033,0.1077610371,0.0423074895\O,-0.172770931,1.2177915341,-0.1244478549\H,1.1351673193,-0.4413679356,1.5052478829\H,1.7960227789,-0.1094645544,1.7819366277\C1,-2.4519183076,-0.1313845926,-0.1121501326\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-729.0533355\RMSD=2.600e-09\RMSF=2.065e-06\Dipole=3.0027509,0.013043,0.1569364\PG=C01 [X(C3H7C11O2)]\@\

HOS(O)₂OH

1\1\GINC-LC62\FOpt\RB3LYP\6-31G(d)\H2O4S1\BUC562\05-Dec-2003\0\#\# G3MP2B3 OPT=TIGHT SCF=TIGHT MAXDISK=134217728\H2SO4 (C2)\0,1\S,-0.0957882681,-0.1354652549,-0.0000000878\O,1.5283419413,-0.0232770645,-0.0292463469\O,-0.5313934162,1.4331751607,0.0292465193\O,-0.4704217613,-0.6927277605,-1.2809365624\O,-0.4963026286,-0.6744269078,1.2809365425\H,1.8383426049,0.0692186598,0.892169844\H,-0.547523397,1.756277995,-0.89216966\Version=x86-Linux-G03RevB.03\State=1-A\HF=-700.203055\RMSD=3.026e-09\RMSF=2.650e-06\Dipole=0.6899852,0.975788,-0.0000004\PG=C01 [X(H2O4S1)]\@\

HOS(O)₂O⁻

1\1\GINC-SC96\FOpt\RB3LYP\6-31G(d)\H1O4S1(1-)\BUC562\08-Dec-2003\0\#\# G3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\HSO4-\-1,1\S,0.1462029989,-0.0052210301,0.055268\O,0.8140287511,-1.2071011678,-0.485121\O,-1.3276849835,0.0801442737,-0.81137\O,-0.3521360278,-0.1348109274,1.451811\O,0.8196692623,1.272311831,-0.254871\H,-1.9702670002,-0.0008165938,-0.087876\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-699.6869265\RMSD=9.066e-09\RMSF=9.573e-05\Dipole=-0.9246534,-0.0126736,0.0704544\PG=C01 [X(H1O4S1)]\@\

HOS(O)₂OH₂⁺

1\1\GINC-LC36\FOpt\RB3LYP\6-31G(d)\H3O4S1(1+)\BUC562\15-Dec-2003\0\#\# G3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\H2OHSO3+\1,1\S,0.2937529711,0.0637271332,-0.148794\O,-1.6789269389,-0.1347507612,0.242604\O,0.7201831753,-0.3867046735,1.29242\O,0.3976374323,-0.9533518197,-1.152661\O,0.4062533279,1.4823031842,-0.264793\H,-2.0851433062,0.6752720546,0.62373\H,0.8123526193,-1.3658446317,1.375034\H,-2.1884388236,-0.3890219923,-0.558619\Version=x86-Linux-G03RevB.03\State=1-A\HF=-700.4707045\RMSD=5.512e-09\RMSF=2.630e-05\Dipole=-1.519856,-0.6286218,0.5844185\PG=C01 [X(H3O4S1)]\@\

TS(HOS(O),OH)

1\1\GINC-SC118\FTS\RB3LYP\6-31G(d)\C2H8O4S1\BUC562\11-Dec-2003\0\#\ G3
MP2B3 OPT=(TS,TIGHT,CALCFC,NOEIGENTEST) SCF=TIGHT MAXDISK=402653184\C
H3CH3 -> CH2CH2 + H2 TS (H2SO4 , C1)\0,1\C,-2.7130739346,0.6008332955
,0.25501\C,-2.5155350825,-0.757341726,-0.113478\H,-2.1416028902,1.0079
582333,1.084907\H,-3.5110498681,1.2107733825,-0.162065\H,-2.2186071501
,-1.3781907583,0.739822\H,-3.2735791302,-1.1950286434,-0.762993\H,-1.4
932660799,-0.7333048373,-0.670597\O,0.0384379718,-0.2588200042,-1.1895
05\S,0.9042359861,-0.1272780985,0.07075\O,0.0582340107,0.0983339937,1.
252536\H,-1.0636318693,1.2000941159,-1.075779\H,-1.6780438213,1.640333
1828,-0.870833\O,1.9504818752,-1.1457752125,0.122084\O,1.6737881438,1.
3196838177,-0.144367\H,2.5161231215,1.1154727259,-0.58964\Version=DEC
-AXP-OSF/1-G03RevB.03\State=1-A\HF=-779.9079931\RMSE=8.750e-09\RMSE=3.
890e-06\Dipole=-2.5244025,0.7607567,-0.370991\Polar=98.4697365,-7.0924
42,56.8021158,-5.3210916,-1.0254496,44.9678524\PG=C01 [X(C2H8O4S1)]\@

ZNH

H₂NH

1\1\GINC-LC35\FOpt\RB3LYP\6-31G(d)\H3N1\BUC562\14-Nov-2003\0\#\ G3MP2B
3 OPT=TIGHT SCF=TIGHT MAXDISK=65536000\NH3\0,1\N,0.1193533475,-0.000
02394,0.\H,-0.2782915655,0.9386583599,0.\H,-0.2785909334,-0.4692453901
, -0.8128472302\H,-0.2785909334,-0.46924539,0.8128472302\Version=x86-L
inux-G03RevB.03\State=1-A\HF=-56.5479476\RMSE=8.679e-09\RMSE=2.206e-0
6\Dipole=-0.7523038,0.0001557,0.\PG=CS [SG(H1N1),X(H2)]\@

H₂N⁻

1\1\GINC-SC160\FOpt\RB3LYP\6-31G(d)\H2N1(1-)\BUC562\15-Dec-2003\0\#\ G
3MP2B3 NOSYMM OPT=TIGHT SCF=TIGHT MAXDISK=13107200\NH2-\-1,1\N,-0.02
03329009,0.1538270517,-0.035217849\H,0.9281615336,-0.2957172497,0.0295
067779\H,-0.4385266326,-0.2957338021,0.8185580711\Version=DEC-AXP-OSF
/1-G03RevB.03\HF=-55.8408361\RMSE=1.690e-09\RMSE=2.335e-06\Dipole=0.23
20656,-0.393456,0.4019418\PG=CS [SG(H2N1)]\@

H₂NH₂⁺

1\1\GINC-SC101\FOpt\RB3LYP\6-31G(d)\H4N1(1+)\BUC562\20-Nov-2003\0\#\ G
3MP2B3 OPT=TIGHT SCF=TIGHT MAXDISK=65536000\NH4+\1,1\N,-0.000021169
,0.0000004276,0.\H,1.0294428823,-0.0000033612,0.\H,-0.3431428838,0.970
5717261,0.0000000001\H,-0.3431425901,-0.485285679,-0.8405385657\H,-0.3
431425901,-0.4852856792,0.8405385656\Version=DEC-AXP-OSF/1-G03RevB.03
\State=1-A\HF=-56.8938877\RMSE=5.277e-10\RMSE=4.220e-06\Dipole=0.0000
093,-0.0000022,0.\PG=CS [SG(H2N1),X(H2)]\@

TS(H₂NH)

1\1\GINC-LC81\FTS\RB3LYP\6-31G(d)\C2H9N1\BUC562\11-Dec-2003\0\#\ G3MP2
B3 SCF=TIGHT OPT=(TS,TIGHT,CALCFC,NOEIGENTEST) MAXDISK=134217728\C
H3 -> CH2CH2 + H2 TS (NH3)\0,1\H,1.0607484154,-0.9963539097,-0.067178
5214\C,-0.4042758834,-1.294096143,-0.1257060845\C,-1.2246010568,-0.155
4198395,-0.0404732009\H,0.1059945601,1.0247913459,0.094922142\H,-0.349
0417929,-1.9766316935,0.7231806835\H,-0.3101415333,-1.8136195223,-1.08
00376054\H,-1.7003602084,0.2241389192,-0.9428707899\H,-1.7399892979,0.
0580922669,0.8941500749\H,1.4018516254,0.0037951971,0.0306014383\N,1.1
864267418,1.2483489134,0.1384471925\H,1.5176822483,1.7929228436,-0.649
9185962\H,1.4815304315,1.6415180539,1.0250965394\Version=x86-Linux-G0
3RevB.03\State=1-A\HF=-136.2299792\RMSE=1.886e-09\RMSE=1.028e-05\Dipol
e=0.8914885,1.0287738,0.1122341\PG=C01 [X(C2H9N1)]\@

(CH₃)HNH

1\1\GINC-SC160\FOpt\RB3LYP\6-31G(d)\C1H5N1\BUC562\02-Dec-2003\0\#\ G3M
P2B3 OPT=TIGHT SCF=TIGHT MAXDISK=39321600\CH3NH2 stagger\0,1\C,-0.70
52389158,-0.0161682837,-0.0280018345\N,0.7593671583,-0.0363146117,-0.0
629014031\H,1.1152250673,0.9177507266,-0.0349678943\H,1.1152278892,-0.
4891551424,0.7773095208\H,-1.0782940874,0.4810877515,-0.9300831393\H,-
1.078291019,-1.0460227506,-0.0484055256\H,-1.1580044636,0.4875513996,0.
.8444678668\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-95.8532048
\RMSE=3.425e-09\RMSE=2.378e-06\Dipole=-0.1197691,0.2831772,0.4904778\PG
=C01 [X(C1H5N1)]\@

(CH₃)HN⁻

1\1\GINC-SC102\FOpt\RB3LYP\6-31G(d)\C1H4N1(1-)\BUC562\15-Jan-2004\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\CH3NH-\-1,1\C,-0.5912
667523,0.0270379712,0.\N,0.8194753902,0.0876923191,0.\H,-1.0155367231,
1.0600368121,0.\H,-1.150589565,-0.4654319932,-0.885762664\H,-1.1505895
65,-0.4654319932,0.885762664\H,1.1279886359,-0.9052468865,0.\Version=
DEC-AXP-OSF/1-G03RevB.03\State=1-A'\HF=-95.1678935\RMSD=1.448e-09\RMSF
=3.380e-06\Dipole=-0.710119,-0.3244547,0.\PG=CS [SG(C1H2N1),X(H2)]\#@

(CH₃)HNH₂⁺

1\1\GINC-SC32\FOpt\RB3LYP\6-31G(d)\C1H6N1(1+)\BUC562\14-Oct-2003\0\#\#
B3LYP/6-31G(D) OPT FREQ MAXDISK=13107200\CH3NH3+ staggered\1,1\C,0.,
0.,-0.804367636\N,0.,0.,0.7124306364\H,0.9559969512,0.,1.090824\H,-0.4
779984756,0.8279176457,1.090824\H,-0.4779984756,-0.8279176457,1.090824
\H,-1.035388275,0.,-1.1444268794\H,0.5176941375,0.8966725489,-1.144426
8794\H,0.5176941375,-0.8966725489,-1.1444268794\Version=DEC-AXP-OSF/1
-G98RevA.11.3\HF=-96.2148648\RMSD=7.710e-10\RMSF=6.925e-05\Dipole=0.,0
,0.8999528\PG=C03V [C3(C1N1),3SGV(H2)]\#@

TS((CH₃)HNH)

1\1\GINC-SC110\FTS\RB3LYP\6-31G(d)\C3H11N1\BUC562\23-Dec-2003\0\#\# G3M
P2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=65536000\CH3
CH3 -> CH2CH2 + H2 TS (MeNH2)\0,1\H,0.5711284152,-1.4959518408,-0.326
4747292\C,1.8102291411,-0.6260135169,-0.3054307715\C,1.5503790989,0.75
37934987,-0.2962502883\H,-0.2603590458,0.6029518866,-0.3370858663\H,2.
2031912445,-1.0886106981,-1.2113162675\H,2.1853889887,-1.1049250667,0.
5996382851\H,1.652027428,1.3112300778,0.6330486258\H,1.6745305756,1.32
73465077,-1.2127748851\H,-0.3961000088,-1.0295978982,-0.3370384516\N,-
1.1520893075,-0.0277581832,-0.3144438775\C,-1.9402108318,0.0868503135,
0.9103039025\H,-1.6893508823,0.0451742247,-1.172939039\H,-2.6326011403
, -0.7565673037,1.0106513271\H,-1.255835133,0.0720599649,1.7623203392\H
, -2.509779738,1.0234156569,0.9413407475\Version=DEC-AXP-OSF/1-G03RevB
.03\State=1-A'\HF=-175.5385768\RMSD=2.104e-09\RMSF=1.524e-06\Dipole=-1.
449947,0.0921529,0.0507737\PG=C01 [X(C3H11N1)]\#@

(CH₃)₂NH

1\1\GINC-LC147\FOpt\RB3LYP\6-31G(d)\C2H7N1\BUC562\23-Dec-2003\0\#\# G3M
P2B3 NOSYMM SCF=TIGHT OPT=TIGHT MAXDISK=65536000\Me2NH\0,1\N,0.02934
5902,0.0004123001,0.047658239\C,1.4850632891,0.0206636184,-0.013439607
3\H,1.9303742541,1.0344372593,0.007859307\H,1.890757277,-0.5331828486,
0.8421195298\H,1.8223348001,-0.4831309688,-0.9255535339\C,-0.496212346
3,0.7208184378,1.2001129185\H,-0.3452284835,0.4149442641,-0.8031707857
\H,-0.1478893968,1.7688070871,1.2829100034\H,-1.5908186447,0.724766959
6,1.1638548603\H,-0.1955706509,0.202259891,2.1188340689\Version=x86-L
inux-G03RevB.03\HF=-135.1628532\RMSD=9.408e-09\RMSF=4.131e-06\Dipole=0
.0693614,0.3836354,-0.1079618\PG=C01 [X(C2H7N1)]\#@

(CH₃)₂NH⁻

1\1\GINC-SC106\FOpt\RB3LYP\6-31G(d)\C2H6N1(1-)\BUC562\15-Jan-2004\0\#\#
G3MP2B3 NOSYMM SCF=TIGHT OPT=TIGHT MAXDISK=134217728\Me2N-\-1,1\C,0
.1018267374,-0.0099386758,0.000006595\N,1.5094136012,0.0038618235,-0.
0000039178\H,-0.3166551759,1.0187195593,-0.000006041\H,-0.4014335426,
-0.5320482242,-0.8866754419\H,-0.4014282018,-0.5320437248,0.8866824809
\C,1.9656805758,-1.3278712406,-0.000009676\H,1.6413276193,-1.97652724
09,-0.8866972554\H,3.0749988636,-1.3796690009,0.0000053904\H,1.6413175
23,-1.9765272756,0.886691656\Version=DEC-AXP-OSF/1-G03RevB.03\HF=-134
.4979237\RMSD=7.985e-09\RMSF=4.904e-06\Dipole=-0.2605914,-0.3684294,0.
0000038\PG=C01 [X(C2H6N1)]\#@

(CH₃)₂NH₂⁺

```
1\1\GINC-SC123\FOpt\RB3LYP\6-31G(d)\C2H8N1(1+)\BUC562\23-Dec-2003\0\#\#
G3MP2B3 OPT=TIGHT SCF=TIGHT NOSYMM MAXDISK=134217728\Me2NH2+\1,1\N,
0.0279786828,0.0215941101,0.0332280888\C,1.5367323068,-0.0109343024,-0.
.0224648837\H,1.9018088512,1.0165370235,-0.0338256923\H,1.9014479633,-
0.5339833332,0.8621552293\H,1.8427123641,-0.5348569759,-0.9289779303\C
,-0.5357329186,0.721239752,1.2469529217\H,-0.3301333066,0.4775974421,-
0.8144868163\H,-0.180032035,1.7520844564,1.2447835659\H,-1.6248666698,
0.6931204841,1.1933528082\H,-0.1839040811,0.1999410762,2.1377991705\H,
-0.3305181572,-0.9403517328,0.0026665381\Version=DEC-AXP-OSF/1-G03Rev
B.03\HF=-135.5340156\RMSD=7.568e-09\RMSF=1.192e-06\Dipole=-0.3568897,-
0.2519885,-0.4374014\PG=C01 [X(C2H8N1)]\#@
```

TS((CH₃)₂NH)

```
1\1\GINC-SC121\FOpt\RB3LYP\6-31G(d)\C4H13N1\BUC562\24-Dec-2003\0\#\# G3
MP2B3 OPT=TIGHT SCF=TIGHT MAXDISK=134217728\CH3CH3 -> CH2CH2 + H2 TS
(Me2NH)\0,1\H,-0.964226,-0.0000000717,-1.478889\C,-2.188733,-0.000000
134,-0.579467\C,-1.905321,-0.0000001196,0.794606\H,-0.072679,-0.000000
0264,0.608387\H,-2.581979977,-0.9056000656,-1.042407\H,-2.581980023,0.
9055989344,-1.042407\H,-1.9993530235,0.9232349492,1.363044\H,-1.999352
9765,-0.9232350508,1.363045\H,0.009983,-0.0000000222,-1.020986\N,0.793
125,0.0000000176,-0.04744\C,1.5582399685,1.2392570396,0.012091\C,1.558
2400315,-1.2392569604,0.012092\H,2.2064699661,1.3333830561,-0.868342\H
,0.8641459471,2.083580022,0.025684\H,2.1809599675,1.2792510554,0.91583
7\H,2.1809590325,-1.2792509446,0.915838\H,0.8641470529,-2.083579978,0.
025683\H,2.2064720339,-1.3333819439,-0.868341\Version=DEC-AXP-OSF/1-G
03RevB.03\State=1-A\HF=-214.8502396\RMSD=3.871e-09\RMSF=9.263e-06\Dipo
le=1.4419608,0.0000002,0.0541688\PG=C01 [X(C4H13N1)]\#@
```

ZSH

HSH

```
1\1\GINC-SC17\FOpt\RB3LYP\6-31G(d)\H2S1\BUC562\04-Dec-2003\0\#\# G3MP2B
3 OPT=TIGHT SCF=TIGHT MAXDISK=39321600\H2S\0,1\S,-0.0597189134,-0.08
44549262,0.\H,1.2755844307,0.1114837207,0.\H,-0.3200818157,1.239795098
8,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A'\HF=-399.3854355\RMSD
=5.214e-10\RMSF=6.817e-07\Dipole=0.324071,0.4583036,0.\PG=CS [SG(H2S1)
]\#@
```

HS⁻

```
1\1\GINC-SC96\FOpt\RB3LYP\6-31G(d)\H1S1(1-)\BUC562\15-Dec-2003\0\#\# G3
MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\SH-\-1,1\S,-0.0801660871,
0.,0.\H,1.2826573934,0.,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-S
G\HF=-398.8062523\RMSD=7.108e-10\RMSF=3.985e-09\Dipole=0.3605665,0.,0.
\PG=C*V [C*(H1S1)]\#@
```

HSH₂⁺

```
1\1\GINC-LC130\FOpt\RB3LYP\6-31G(d)\H3S1(1+)\BUC562\15-Dec-2003\0\#\# G
3MP2B3 OPT SCF=TIGHT MAXDISK=65536000\H3S+\1,1\S,0.0000030012,-0.000
0029988,0.112257\H,1.1362255016,-0.2171552215,-0.598728\H,-0.380050846
4,1.0925476214,-0.598681\H,-0.7562256733,-0.8753484208,-0.598705\Vers
ion=x86-Linux-G03RevB.03\State=1-A\HF=-399.6615887\RMSD=3.480e-09\RMSF
=1.317e-05\Dipole=0.0000029,0.0000112,0.7238222\PG=C01 [X(H3S1)]\#@
```

TS(HSH)

```
1\1\GINC-LC23\FTS\RB3LYP\6-31G(d)\C2H8S1\BUC562\04-Dec-2003\0\#\# G3MP2
B3 OPT=(TS,TIGHT,CALCFC,NOEIGENTEST) SCF=TIGHT MAXDISK=134217728\CH3C
H3 -> CH2CH2 + H2 TS(H2S)\0,1\H,-0.6306697226,1.5926890476,-0.0016028
769\C,-1.9670585671,0.4999934339,0.0141250383\C,-1.3390883824,-0.75999
96454,0.0065305964\H,-0.0856163536,-0.5248064609,-0.0204559772\H,-2.33
63039241,0.9529025041,-0.9016893198\H,-2.3157012467,0.9530998211,0.938
1046917\H,-1.4113430938,-1.3497728835,0.9218972379\H,-1.4366527694,-1.
3511392454,-0.9054797392\H,0.1653843295,1.4000640157,-0.0465312014\S,1.
6349711699,-0.0141922707,-0.0854188316\H,1.7282457587,0.1140768019,1.
2585246832\Version=x86-Linux-G03RevB.03\State=1-A\HF=-479.0879371\RMS
D=4.289e-09\RMSF=2.394e-06\Dipole=-1.4675913,0.0490318,0.3975005\PG=CO
1 [X(C2H8S1)]\#@
```

(CH₃)₃CSH

1\1\GINC-SC16\FOpt\RB3LYP\6-31G(d)\C4H10S1\BUC562\23-Jan-2004\0\#\# G3M
P2B3 SCF=TIGHT OPT=TIGHT MAXDISK=268435456\\t-BuSH\0,1\C,-0.010043763
2,0.3558473671,0.\S,-0.0104661668,-1.5173525794,0.\H,1.3318157627,-1.6
762496539,0.\C,-1.4929896865,0.7587071776,0.\C,0.6878800406,0.87859759
2,1.2631526048\C,0.6878800406,0.878597592,-1.2631526048\H,-2.009891169
,0.3797691924,0.888153564\H,-1.5769487208,1.8523759127,0.\H,-2.0098911
69,0.3797691924,-0.888153564\H,0.2024915073,0.5014378243,-2.1682584416
\H,0.6540650384,1.976311281,-1.2838974325\H,1.7414505424,0.5779900215,
-1.2908907095\H,1.7414505424,0.5779900215,1.2908907095\H,0.6540650384,
1.976311281,1.2838974325\H,0.2024915073,0.5014378243,2.1682584416\\Ver
sion=DEC-AXP-OSF/1-G03RevB.03\State=1-A'\HF=-556.643017\RMSD=6.591e-09
\RMSF=3.704e-07\Dipole=0.2908972,0.663138,0.\PG=CS [SG(C2H2S1),X(C2H8)
]\#@

(CH₃)₃CS⁻

1\1\GINC-SC96\FOpt\RB3LYP\6-31G(d)\C4H9S1(1-)\BUC562\23-Jan-2004\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=268435456\\t-BuS-1,1\C,-0.01280
051,0.2878388265,0.\S,0.0695754697,-1.568356714,0.\C,-1.4804063183,0.7
589212644,0.\C,0.6854612189,0.8549910076,1.2516572904\C,0.6854612189,0
.8549910076,-1.2516572904\H,-2.0022677615,0.3732698556,0.8833785159\H,
-1.5670172267,1.8630146922,0.\H,-2.0022677615,0.3732698556,-0.88337851
59\H,0.2051952482,0.4722689815,-2.1595096377\H,0.6564548111,1.96162183
57,-1.2836626172\H,1.734375729,0.5379593749,-1.2768120768\H,1.73437572
9,0.5379593749,1.2768120768\H,0.6564548111,1.9616218357,1.2836626172\H
,0.2051952482,0.4722689815,2.1595096377\\Version=DEC-AXP-OSF/1-G03RevB
.03\State=1-A'\HF=-556.0607262\RMSD=2.932e-09\RMSF=3.751e-06\Dipole=-0
.0955349,2.1519182,0.\PG=CS [SG(C2H1S1),X(C2H8)]\#@

(CH₃)₃CSH₂⁺

1\1\GINC-SC18\FOpt\RB3LYP\6-31G(d)\C4H11S1(1+)\BUC562\23-Jan-2004\0\#\#
G3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\\t-BuSH2+1,1\C,0.472307,-0.
0000000792,0.009409\S,-1.499947,-0.0000237497,-0.115489\H,-1.786814165
5,-0.9919877019,0.759683\C,0.8791042129,1.2757198533,-0.727582\C,0.856
1189999,-0.0003511428,1.484813\C,0.8791597872,-1.2753401467,-0.728212\
H,0.5375693641,2.1821549103,-0.217686\H,1.974769218,1.3065656705,-0.74
6344\H,0.5328652149,1.2878299111,-1.765429\H,0.5331987853,-1.286793089
, -1.766157\H,1.974827782,-1.3063123295,-0.746678\H,0.5373786359,-2.182
0400897,-0.218952\H,0.5053728508,-0.8941450843,2.010228\H,1.951555,-0.
0001953256,1.538349\H,0.505101149,0.8930369157,2.010734\H,-1.786809834
5,0.9920992981,0.759505\\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A'\HF
=-556.9632282\RMSD=8.303e-09\RMSF=1.261e-06\Dipole=-0.7295845,0.000041
6,0.497422\PG=C01 [X(C4H11S1)]\#@

TS((CH₃)₃CSH)

1\1\GINC-LC23\FTS\RB3LYP\6-31G(d)\C2H8S1\BUC562\04-Dec-2003\0\#\# G3MP2
B3 OPT=(TS,TIGHT,CALCF,NOEIGENTEST) SCF=TIGHT MAXDISK=134217728\\CH3C
H3 -> CH2CH2 + H2 TS(H2S)\0,1\H,-0.6306697226,1.5926890476,-0.0016028
769\C,-1.9670585671,0.4999934339,0.0141250383\C,-1.3390883824,-0.75999
96454,0.0065305964\H,-0.0856163536,-0.5248064609,-0.0204559772\H,-2.33
63039241,0.9529025041,-0.9016893198\H,-2.3157012467,0.9530998211,0.938
1046917\H,-1.4113430938,-1.3497728835,0.9218972379\H,-1.4366527694,-1.
3511392454,-0.9054797392\H,0.1653843295,1.4000640157,-0.0465312014\S,1
.6349711699,-0.0141922707,-0.0854188316\H,1.7282457587,0.1140768019,1.
2585246832\\Version=x86-Linux-G03RevB.03\State=1-A'\HF=-479.0879371\RMS
D=4.289e-09\RMSF=2.394e-06\Dipole=-1.4675913,0.0490318,0.3975005\PG=C0
1 [X(C2H8S1)]\#@

H₂CSH

1\1\GINC-SC17\FOpt\RB3LYP\6-31G(d)\C1H4S1\BUC562\05-Dec-2003\0\#\# G3MP
2B3 OPT=TIGHT SCF=TIGHT MAXDISK=65536000\\CH3SH\0,1\C,-1.1650931809,0
.0157822358,0.\S,0.6680287714,-0.0850028367,0.\H,0.904757834,1.2448147
682,0.\H,-1.5272147752,-1.014969398,0.\H,-1.5377221583,0.5177533007,0.
8957856283\H,-1.5377221583,0.5177533007,-0.8957856283\\Version=DEC-AXP
-OSF/1-G03RevB.03\State=1-A'\HF=-438.6983472\RMSD=5.434e-09\RMSF=3.962
e-06\Dipole=-0.5643441,0.3846557,0.\PG=CS [SG(C1H2S1),X(H2)]\#@

H₃CS⁻

```
1\1\GINC-SC116\FOpt\RB3LYP\6-31G(d)\C1H3S1(1-)\BUC562\15-Dec-2003\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\CH3S-\-1,1\C,-0.030368
4485,1.128111861,0.\S,0.0192248909,-0.7141862104,0.\H,-1.0606004356,1.
5254069945,0.\H,0.4676064364,1.5664506032,0.8826223985\H,0.4676064364,
1.5664506032,-0.8826223985\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A
'\HF=-438.1096317\RMSD=7.383e-09\RMSF=2.481e-06\Dipole=-0.0332209,1.23
43658,0.\PG=CS [SG(C1H1S1),X(H2)]\#@
```

H₃CSH₂⁺

```
1\1\GINC-SC31\FOpt\RB3LYP\6-31G(d)\C1H5S1(1+)\BUC562\15-Dec-2003\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\CH3SH2+\1,1\C,-0.052929
434,1.2116219405,-0.055464729\S,-0.0204482421,-0.6278636418,0.11165967
49\H,1.2908869213,-0.8651924537,-0.1338081322\H,-1.1067156822,1.498083
9852,-0.0574706471\H,0.4397198162,1.6065337846,0.8355304144\H,0.452990
2371,1.5226645229,-0.9693431437\H,-0.4321328154,-0.9860032139,-1.12867
49162\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A'\HF=-439.0000926\RMSD
=9.627e-09\RMSF=8.337e-07\Dipole=0.2913642,-0.0922848,-0.493409\PG=C01
[X(C1H5S1)]\#@
```

TS(H₃CSH)

```
1\1\GINC-LC124\FTS\RB3LYP\6-31G(d)\C3H10S1\BUC562\05-Dec-2003\0\#\# G3M
P2B3 OPT=(TS,CALCF, TIGHT,NOEIGENTEST) SCF=TIGHT MAXDISK=134217728\CH
3CH3 -> CH2 CH2 + H2 TS (CH3SH)\0,1\H,-1.0511373609,1.4980454197,-0.4
032015194\C,-2.3172556239,0.3308621336,-0.3408690292\C,-1.6026558778,-
0.8817909532,-0.3607390409\H,-0.3592174378,-0.5580125652,-0.4199619986
\H,-2.7466885574,0.7474100218,-1.2475468814\H,-2.6754274232,0.76112617
45,0.5902858108\H,-1.6096619126,-1.4725447807,0.5572127537\H,-1.677712
0348,-1.4829145602,-1.2683456851\H,-0.2398821474,1.3535724849,-0.46546
9132\S,1.2963897719,0.0684624487,-0.4276309073\C,1.4426400618,0.147485
6452,1.3982221127\H,0.8760179445,-0.6547016085,1.8814968085\H,2.499566
763,0.0206602619,1.650019707\H,1.1055344549,1.1126190185,1.7879203979\
\Version=x86-Linux-G03RevB.03\State=1-A'\HF=-518.3994505\RMSD=8.384e-09
\RMSF=4.256e-06\Dipole=-1.1426165,-0.0775278,0.5277546\PG=C01 [X(C3H10
S1)]\#@
```

ClH

```
1\1\GINC-LC10\FOpt\RB3LYP\6-31G(d)\Cl1H1\BUC562\11-Dec-2003\0\#\# G3MP2
B3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\HCl\0,1\C1,-0.0716385263,0.,
0.\H,1.2178549476,0.,0.\Version=x86-Linux-G03RevB.03\State=1-SG\HF=-4
60.7956941\RMSD=3.886e-09\RMSF=3.351e-07\Dipole=0.5776138,0.,0.\PG=C*V
[C*(H1Cl1)]\#@
```

Cl⁻

```
1\1\GINC-LC147\FOpt\RB3LYP\6-31G(d)\Cl1(1-)\BUC562\15-Dec-2003\0\#\# G3
MP2B3 SCF=TIGHT MAXDISK=39321600\Cl-\-1,1\C1,0.,0.,0.\Version=x86-L
inux-G03RevB.03\State=1-AlG\HF=-460.2522333\RMSD=6.493e-09\RMSF=0.000e
+00\Dipole=0.,0.,0.\PG=OH [O(C11)]\#@
```

ClH₂⁺

```
1\1\GINC-LC139\FOpt\RB3LYP\6-31G(d)\Cl1H2(1+)\BUC562\15-Dec-2003\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\H2Cl+\1,1\C1,-0.0534372
447,-0.0755712563,0.\H,1.2516508632,0.0784813494,0.\H,-0.3432177037,1.
2062300072,0.\Version=x86-Linux-G03RevB.03\State=1-A'\HF=-461.0087158
\RMSD=6.726e-09\RMSF=1.708e-06\Dipole=0.5265153,0.7446009,0.\PG=CS [SG
(C11H2)]\#@
```

TS(C1H)

N-N= 1.014177267217D+02 E-N=-1.481878014919D+03 KE= 5.382423339437D+02
1\1\GINC-LC64\FTS\RB3LYP\6-31G(d)\C2H7Cl1\BUC562\11-Dec-2003\0\#\# G3MP
2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=134217728\CH3
CH3 -> CH2CH2 + H2 TS (HCl)\0,1\H,-0.628195528,1.6322716614,-0.012308
4955\C,-1.9291384004,0.4567815899,0.0303850488\C,-1.292063565,-0.80133
50861,0.0369179801\H,-0.089541203,-0.5436103861,0.0098513872\H,-2.2966
885979,0.901452617,-0.8904607882\H,-2.2611532105,0.9290104102,0.951009
0687\H,-1.3672751645,-1.371781758,0.9642250175\H,-1.4026622785,-1.3992
208262,-0.8693189108\H,0.1440174366,1.4074015884,-0.0238377117\C1,1.60
16888434,0.0301057453,-0.0313516318\Version=x86-Linux-G03RevB.03\Stat
e=1-A\HF=-540.5107075\RMSD=3.153e-09\RMSF=5.068e-06\Dipole=-2.2499742,
0.0656184,0.0424263\PG=C01 [X(C2H7Cl1)]\@

F₃CSH

1\1\GINC-SC14\FOpt\RB3LYP\6-31G(d)\C1H1F3S1\BUC562\23-Jan-2004\0\#\# G3
MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=268435456\CF3SH\0,1\C,-0.016229679
3,0.3640114074,0.\S,-0.0218410518,-1.4608409321,0.\H,1.323623693,-1.55
99259992,0.\F,-1.2909692969,0.7776225097,0.\F,0.5967741603,0.875039437
9,1.0800596918\F,0.5967741603,0.8750394379,-1.0800596918\Version=DEC-
AXP-OSF/1-G03RevB.03\State=1-A\HF=-736.4069574\RMSD=6.050e-09\RMSF=2.
379e-06\Dipole=0.3998767,-0.3179876,0.\PG=CS [SG(C1H1F1S1),X(F2)]\@

F₃CS⁻

1\1\GINC-SC16\FOpt\RB3LYP\6-31G(d)\C1F3S1(1-)\BUC562\23-Jan-2004\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=268435456\CF3S-\-1,1\C,-0.244452
2678,-0.000137649,0.\S,1.5059025016,0.0002018147,0.\F,-0.8378823471,1.
2533038974,0.\F,-0.8381547386,-0.6267854565,-1.085657007\F,-0.83815473
86,-0.6267854565,1.085657007\Version=DEC-AXP-OSF/1-G03RevB.03\State=1
-A\HF=-735.8661899\RMSD=7.337e-09\RMSF=1.440e-05\Dipole=-1.3352699,-0
.0000424,0.\PG=CS [SG(C1F1S1),X(F2)]\@

F₃CSH₂⁺

1\1\GINC-SC16\FOpt\RB3LYP\6-31G(d)\C1H2F3S1(1+)\BUC562\23-Jan-2004\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=268435456\CF3SH2+\1,1\C,-0.512
5192348,-0.0000002796,0.006321084\S,1.4588836742,0.0000037191,-0.13683
73385\H,1.6771391518,-1.0008732701,0.7523310018\F,-0.8989337648,1.0894
000061,-0.6024546375\F,-0.8989376776,-1.0893395279,-0.6025612595\F,-0.
8267176106,-0.0000618247,1.276876896\H,1.6771389467,1.0008275643,0.752
39092\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-736.6769732\RMSD
=2.408e-09\RMSF=2.789e-06\Dipole=1.8821951,-0.0000174,0.5346499\PG=C01
[X(C1H2F3S1)]\@

TS(F₃CSH)

1\1\GINC-SC101\FTS\RB3LYP\6-31G(d)\C3H7F3S1\BUC562\22-Jan-2004\0\#\# G3
MP2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=805306368\C
H3CH3 -> CH2CH2 + H2 TS (CF3SH)\0,1\H,1.7420640878,-0.7705519428,1.78
12331665\C,2.8983621508,-0.2062377815,0.6073196094\C,2.2272442455,-0.3
894890197,-0.6210794202\H,1.1171864618,-0.8431831562,-0.3248063108\H,3
.6060132099,-0.9401329846,0.9831704338\H,2.8960267711,0.7566603243,1.1
102301402\H,1.9317176078,0.5168991446,-1.151304859\H,2.6151890509,-1.1
769654186,-1.2697234225\H,0.9720286861,-0.9639324247,1.6353003446\S,-0
.589349445,-1.2753753178,0.2823772805\C,-1.0050672006,0.4343450755,-0.
1245722789\F,-0.7677128358,0.7437102836,-1.4240338575\F,-2.3049760116,
0.6862867732,0.1061702418\F,-0.279963367,1.3250587094,0.6009587888\Ve
rsion=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-816.1156727\RMSD=2.689e-0
9\RMSF=4.836e-06\Dipole=1.8966444,0.0340511,0.1099288\PG=C01 [X(C3H7F3
S1)]\@

HC(S)SH

1\1\GINC-SC6\FOpt\RB3LYP\6-31G(d)\C1H2S2\BUC562\10-Dec-2003\0\#\# G3MP2
B3 SCF=TIGHT OPT=TIGHT MAXDISK=6553600\HCS2H\0,1\C,-0.382622529,-0.
4743176152,0.\S,1.3550997903,-0.6705313002,0.\S,-1.2618874501,0.899200
7682,0.\H,1.6624664685,0.6458048309,0.\H,-0.8581287391,-1.4586106274,0
.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-835.666456\RMSD=4.5
46e-09\RMSF=7.244e-06\Dipole=0.5693264,-0.3841217,0.\PG=CS [SG(C1H2S2)
]\@

HC(S)⁻

1\1\GINC-LC69\FOpt\RB3LYP\6-31G(d)\C1H1S2(1-)\BUC562\15-Dec-2003\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\HCS2-\-1,1\C,-0.077561
2111,0.5368774912,0.\S,-1.5072687787,-0.372322222,0.\S,1.5510159552,0.
0695063002,0.\H,-0.2345875569,1.623789801,0.\Version=x86-Linux-G03Rev
B.03\State=1-A'\HF=-835.1343397\RMSD=2.337e-09\RMSF=4.701e-07\Dipole=-
0.0808425,0.5596206,0.\PG=CS [SG(C1H1S2)]\#@

HC(S)SH₂⁺

1\1\GINC-SC21\FOpt\RB3LYP\6-31G(d)\C1H3S2(1+)\BUC562\15-Dec-2003\0\#\#
G3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\HCSSH2+\1,1\C,0.2948890412,0
.6700839819,-0.003649\S,-1.5295550061,-0.0990519059,-0.09423\S,1.60708
09881,-0.1933870989,0.009781\H,-1.2006210838,-1.3622599261,0.264336\H,
0.1476041076,1.7494649909,-0.03052\H,-1.9567329833,0.2713011204,1.1392
64\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A'\HF=-835.938065\RMSD=8.9
82e-09\RMSF=6.011e-06\Dipole=-1.2822742,0.0484577,0.5126985\PG=C01 [X(
C1H3S2)]\#@

TS(HC(S)SH)

1\1\GINC-SC115\FTS\RB3LYP\6-31G(d)\C3H8S2\BUC562\10-Dec-2003\0\#\# G3MP
2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=134217728\CH3
CH3 -> CH2CH2 + H2 TS (HCS2H, C1)\0,1\C,2.509970716,0.2629975968,0.44
84260422\C,2.0236273816,-0.2942955473,-0.7536922816\H,2.2599183898,1.2
840591229,0.7209691555\H,3.2798874326,-0.229786198,1.0360730588\H,1.67
97588899,0.4222797704,-1.5011209685\H,2.5860192457,-1.1367135775,-1.16
04560581\H,0.9468428198,-0.8045057998,-0.4520830705\S,-0.7111490294,-1
.4675015566,0.1045294679\C,-1.5759489637,0.012517428,-0.0784970012\S,-
1.0281089797,1.5705883505,-0.0578607712\H,0.6470434006,-0.6456663157,1
.4922636458\H,1.3274533244,-0.254364693,1.6449233207\H,-2.6446901605,-
0.1720078755,-0.2246887878\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A
\HF=-915.3785585\RMSD=5.606e-09\RMSF=2.072e-06\Dipole=1.5889389,-0.415
286,0.0180098\PG=C01 [X(C3H8S2)]\#@

FC(S)SH

1\1\GINC-SC32\FOpt\RB3LYP\6-31G(d)\C1H1F1S2\BUC562\19-Jan-2004\0\#\# G3
MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\FCS2H\0,1\C,0.2573557429
,0.1126812003,0.\F,1.5920426322,-0.0230998128,0.\S,-0.4704857012,1.559
3953227,0.\S,-0.4150203068,-1.518091572,0.\H,-1.7044220193,-1.12904889
84,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A'\HF=-934.9004186\RMS
D=5.649e-09\RMSF=5.299e-06\Dipole=-0.4791029,-0.6501559,0.\PG=CS [SG(
C1H1F1S2)]\#@

FC(S)⁻

1\1\GINC-SC96\FOpt\RB3LYP\6-31G(d)\C1F1S2(1-)\BUC562\19-Jan-2004\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\FCS2H-\-1,1\C,0.197801
3678,0.,0.\F,1.5816680189,0.,0.\S,-0.4819318868,1.539749704,0.\S,-0.48
19318868,-1.539749704,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A1\
HF=-934.3822809\RMSD=3.780e-09\RMSF=4.620e-06\Dipole=0.5127313,0.,0.\P
G=C02V [C2(C1F1),SGV(S2)]\#@

FC(S)SH₂⁺

1\1\GINC-SC91\FOpt\RB3LYP\6-31G(d)\C1H2F1S2(1+)\BUC562\23-Jan-2004\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\FCSSH2+\1,1\C,0.2708
521798,0.3265706129,0.0337489423\S,-1.5206776034,-0.4561926487,-0.1015
936739\S,1.6218360356,-0.4642786351,-0.0991273512\H,-1.2247397138,-1.6
656712149,0.4274891158\F,0.0035872158,1.5972361598,0.1716247931\H,-2.0
511932239,0.0586626403,1.0369304938\Version=DEC-AXP-OSF/1-G03RevB.03\
State=1-A'\HF=-935.1641932\RMSD=6.221e-09\RMSF=8.636e-06\Dipole=-1.4835
797,-0.9065421,0.5230109\PG=C01 [X(C1H2F1S2)]\#@

TS(FC(S)SH)

1\1\GINC-SC30\FTS\RB3LYP\6-31G(d)\C3H7F1S2\BUC562\19-Jan-2004\0\#\# G3M
P2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=402653184\CH
3CH3 -> CH2CH2 + H2 TS (FCS2H)\0,1\C,-2.7303677127,-0.7679860263,0.45
87687158\C,-2.3715375423,-0.1288632464,-0.7514762605\H,-2.2758412624,-
1.7133055624,0.738500654\H,-3.5747782798,-0.4314681216,1.0542236182\H,
-1.908045842,-0.7806941715,-1.4959383765\H,-3.1025549499,0.5735459756,
-1.156770659\H,-1.4250909215,0.567202513,-0.4752474864\S,0.1501949631,
1.5119913517,0.0946068937\C,1.1986856555,0.1455590549,-0.0295737526\S,
0.8637854415,-1.4630821154,0.0118021132\H,-1.1092626359,0.5397587575,1
.5014983332\H,-1.692648051,0.0313671554,1.681496036\F,2.475983674,0.54
87541087,-0.1796242718\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=
-1014.6156216\RMSD=5.042e-09\RMSF=1.757e-06\Dipole=-2.2307971,-0.09103
85,0.07121\PG=C01 [X(C3H7F1S2)]\#@

CIC(S)SH

1\1\GINC-LC19\FOpt\RB3LYP\6-31G(d)\C1H1C11S2\BUC562\22-Jan-2004\0\#\# G
3MP2B3 OPT SCF=TIGHT MAXDISK=134217728\C1CS2H\0,1\C,0.0000000179,0.1
48298,0.\C1,-1.3755031171,-0.9720728344,0.\S,-0.167885788,1.7608550202
,0.\S,1.4844969037,-0.8000151788,0.\H,2.3177740315,0.2620107209,0.\Ve
rsion=x86-Linux-G03RevB.03\State=1-A'\HF=-1295.2598444\RMSD=2.268e-09\
RMSF=1.298e-04\Dipole=0.711279,-0.2056127,0.\PG=CS [SG(C1H1C11S2)]\#@

CIC(S)S-

1\1\GINC-SC96\FOpt\RB3LYP\6-31G(d)\C1C11S2(1-)\BUC562\19-Jan-2004\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=268435456\C1CS2H-\-1,1\C,-0.265
5189039,0.,0.\C1,1.7580519831,0.,0.\S,-0.8841803216,1.5318873762,0.\S,
-0.8841803216,-1.5318873762,0.\Version=DEC-AXP-OSF/1-G03RevB.03\State
=1-A1\HF=-1294.7485059\RMSD=4.258e-09\RMSF=9.557e-08\Dipole=0.0459938,
0.,0.\PG=C02V [C2(C1C11),SGV(S2)]\#@

CIC(S)SH₂⁺

1\1\GINC-SC91\FOpt\RB3LYP\6-31G(d)\C1H2C11S2(1+)\BUC562\23-Jan-2004\0\
\# G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\C1CSSH2+\1,1\C,0.28
66188974,0.0257641826,0.0048185288\S,-1.5364154355,-0.8035962975,-0.09
71819615\S,1.5867066382,-0.8682552505,-0.0468035396\H,-1.196376949,-2.
0265269851,0.3722733992\C1,0.0414977884,1.7045772969,0.0482137257\H,-2
.0334580801,-0.3562473882,1.0829501087\Version=DEC-AXP-OSF/1-G03RevB.
03\State=1-A\HF=-1295.52846\RMSD=7.415e-09\RMSF=4.099e-06\Dipole=-1.37
80916,-1.0485416,0.529762\PG=C01 [X(C1H2C11S2)]\#@

TS(CIC(S)SH)

1\1\GINC-SC30\FTS\RB3LYP\6-31G(d)\C3H7C11S2\BUC562\19-Jan-2004\0\#\# G3
MP2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=402653184\C
H3CH3 -> CH2CH2 + H2 TS (C1CS2H)\0,1\C,-3.1220929259,-0.8589997165,0.
494864245\C,-2.7435440757,-0.2317490721,-0.7151336455\H,-2.6919073298,
-1.8140125246,0.7805375904\H,-3.9622277081,-0.5022003955,1.0844875489\
H,-2.288619735,-0.8920051393,-1.4569080608\H,-3.4572605159,0.484667407
6,-1.1266783807\H,-1.7852481877,0.4522521168,-0.4341020941\S,-0.221762
9785,1.4035968362,0.1310600852\C,0.8482067219,0.0601933499,-0.00051253
04\S,0.5071368731,-1.5446976375,0.0501965303\H,-1.4718839139,0.4192813
137,1.5403954193\H,-2.0627216239,-0.0842303024,1.7111970763\C1,2.54461
57871,0.6104231163,-0.2161378448\Version=DEC-AXP-OSF/1-G03RevB.03\Sta
te=1-A\HF=-1374.9750662\RMSD=4.875e-09\RMSF=1.031e-05\Dipole=-2.321976
, -0.159897,0.0806411\PG=C01 [X(C3H7C11S2)]\#@

ZPH

H₂PH

1\1\GINC-SC17\FOpt\RB3LYP\6-31G(d)\H3P1\BUC562\12-Dec-2003\0\#\# G3MP2B
3 SCF=TIGHT OPT=TIGHT MAXDISK=65536000\PH3\0,1\P,-0.0436204301,-0.06
0565424,0.1049023966\H,1.3438695749,0.1001030738,-0.1733835336\H,-0.34
47815977,1.3015597596,-0.1819790765\H,-0.3447815253,-0.4931814623,-1.2
181733322\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-343.1402804\
RMSD=1.452e-09\RMSF=7.478e-06\Dipole=0.1282931,0.1780791,-0.3084422\PG
=C01 [X(H3P1)]\#@

H₂P⁻

1\1\GINC-SC160\FOpt\RB3LYP\6-31G(d)\H2P1(1-)\BUC562\15-Dec-2003\0\#\# G
 3MP2B3 NOSYMM OPT=TIGHT SCF=TIGHT MAXDISK=65536000\PH2-\-1,1\,P,-0.00
 72269442,0.0126454492,-0.1475646593\H,1.1999623434,-0.0064332008,0.653
 2220058\H,-0.5946453992,-1.0424312484,0.6531036535\Version=DEC-AXP-OS
 F/1-G03RevB.03\HF=-342.5286046\RMSD=3.295e-09\RMSF=3.702e-06\Dipole=0.
 1043672,-0.1806103,0.2693748\PG=CS [SG(H2P1)]\#@

H₂PH₂⁺

1\1\GINC-SC160\FOpt\RB3LYP\6-31G(d)\H4P1(1+)\BUC562\15-Dec-2003\0\#\# G
 3MP2B3 OPT SCF=TIGHT MAXDISK=65536000\PH4+\-1,1\,P,-0.0000140047,0.000
 0069906,0.000014\H,0.9387489615,-0.2492171816,1.008031\H,-1.1374006185
 ,-0.7868617662,0.216444\H,-0.357995876,1.3531283384,0.019822\H,0.55685
 0607,-0.317159254,-1.244513\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-
 A\HF=-343.4467574\RMSD=8.257e-09\RMSF=1.771e-05\Dipole=0.0000539,0.000
 0121,-0.0000415\PG=C01 [X(H4P1)]\#@

TS(H₂PH)

1\1\GINC-SC16\FTS\RB3LYP\6-31G(d)\C2H9P1\BUC562\12-Dec-2003\0\#\# G3MP2
 B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=134217728\CH3C
 H3 -> CH2CH2 + H2 TS (PH3)\-0,1\,H,-0.7294736189,1.4772509612,0.1946650
 739\C,-2.0221733759,0.4615240772,0.1300496754\C,-1.3347973743,-0.76023
 31211,-0.0307664877\H,-0.0861727675,-0.4457977714,-0.0561960165\H,-2.4
 579094944,0.9723776665,-0.7238971691\H,-2.3852363654,0.7716358481,1.10
 59713201\H,-1.3443923498,-1.4525436023,0.8122852802\H,-1.4262545276,-1
 .2604600486,-0.9960432782\H,0.0931924443,1.4072136289,0.12631407\,P,1.6
 536304201,0.0734726356,-0.1633299153\H,1.9217408642,0.5205619548,1.165
 0545018\H,1.7518740152,-1.3000739071,0.2260958217\Version=DEC-AXP-OSF
 /1-G03RevB.03\State=1-A\HF=-422.8377827\RMSD=8.190e-09\RMSF=3.682e-06\
 Dipole=-0.8683061,-0.2101496,0.3180468\PG=C01 [X(C2H9P1)]\#@

(CH₃)HPH

1\1\GINC-SC90\FOpt\RB3LYP\6-31G(d)\C1H5P1\BUC562\22-Jan-2004\0\#\# G3MP
 2B3 OPT=TIGHT SCF=TIGHT NOSYMM MAXDISK=134217728\MePH2\-0,1\,P,-0.0643
 258059,0.0987608277,0.1701297264\C,1.8007446585,-0.0028058617,-0.00511
 46971\H,2.2104282314,1.0120591386,-0.0120264403\H,2.2099746487,-0.5177
 866964,0.8696272455\H,2.1298432223,-0.5232811265,-0.9079999018\H,-0.35
 25362777,0.5270993101,-1.1587614408\H,-0.3526656773,-1.2667405918,-0.1
 209984918\Version=DEC-AXP-OSF/1-G03RevB.03\HF=-382.4577789\RMSD=5.239
 e-09\RMSF=2.229e-06\Dipole=0.3987741,-0.1672222,-0.2889888\PG=C01 [X(C
 1H5P1)]\#@

(CH₃)HP⁻

1\1\GINC-SC96\FOpt\RB3LYP\6-31G(d)\C1H4P1(1-)\BUC562\19-Jan-2004\0\#\#
 G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\MePH-\-1,1\,P,-0.730702
 9718,-0.0517185512,0.0895789673\C,1.183769655,0.0137878404,-0.02388092
 72\H,1.6125481797,1.0305543993,-0.0128850773\H,1.585323813,-0.49881423
 41,0.863972109\H,1.6125484178,-0.504118102,-0.8989285694\H,-0.95249376
 33,0.6654291645,-1.1525574068\Version=DEC-AXP-OSF/1-G03RevB.03\State=
 1-A\HF=-381.836312\RMSD=2.673e-09\RMSF=6.725e-06\Dipole=1.2310842,0.12
 16805,-0.2107565\PG=C01 [X(C1H4P1)]\#@

(CH₃)HPH₂⁺

1\1\GINC-SC64\FOpt\RB3LYP\6-31G(d)\C1H6P1(1+)\BUC562\19-Jan-2004\0\#\#
 G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\MePH3+\-1,1\,P,-0.586206
 9017,-0.0000000431,0.0000000431\C,1.2277473548,0.0000000902,-0.0000000
 902\H,1.5895712181,1.0326264287,0.000000039\H,1.5895713976,-0.5163131
 437,0.8942804417\H,1.5895712662,-0.5163129347,-0.8942807959\H,-1.11403
 16254,0.6486810521,-1.1235482969\H,-1.1140313999,-1.2973620871,-0.0000
 000698\H,-1.1140314603,0.6486807895,1.1235486121\Version=DEC-AXP-OSF/
 1-G03RevB.03\State=1-A\HF=-382.7913515\RMSD=3.454e-09\RMSF=4.928e-07\
 Dipole=-0.3786942,0.,0.\PG=C03V [C3(C1P1),3SGV(H2)]\#@

TS((CH₃)₂HPH)

1\1\GINC-SC31\FOpt\RB3LYP\6-31G(d)\C3H11P1\BUC562\19-Jan-2004\0\#\# G3MP
2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCF,NOEIGENTEST) MAXDISK=402653184\CH3
CH3 -> CH2CH2 + H2 TS (MePH2)\0,1\H,1.1312481515,-1.3066979469,-0.484
8458877\C,2.3944575713,-0.2610032125,-0.3161059405\C,1.6560749863,0.94
16650106,-0.2430503254\H,0.4259378355,0.6010296907,-0.3478950036\H,2.8
625993817,-0.5706420591,-1.2460551022\H,2.764653483,-0.7425680846,0.58
46715305\H,1.6361470176,1.4550458863,0.720156611\H,1.7394063093,1.6289
950366,-1.086635677\H,0.305176476,-1.2431680282,-0.5652782548\H,-1.307
058147,0.0351323309,-0.4549106794\C,-1.5520623238,-0.6036928839,1.2944
346624\H,-1.4029716206,1.4221939719,-0.1064393062\H,-2.5240614706,-0.2
709746326,1.6740770417\H,-1.5451588404,-1.6977651598,1.2795895997\H,-0
.7779259213,-0.2642471226,1.9906442602\Version=DEC-AXP-OSF/1-G03RevB.
03\State=1-A\HF=-462.1543202\RMSD=2.817e-09\RMSF=2.521e-06\Dipole=0.63
41425,0.1499639,0.4942079\PG=C01 [X(C3H11P1)]\@

(CH₃)₂PH

1\1\GINC-SC93\FOpt\RB3LYP\6-31G(d)\C2H7P1\BUC562\22-Jan-2004\0\#\# G3MP
2B3 OPT SCF=TIGHT MAXDISK=134217728\Me2PH\0,1\H,0.0000018603,-0.6611
08,-0.112691\C,1.4349961124,0.5322206968,0.021524\H,1.3247192638,1.248
7097201,0.842367\H,2.3628889935,-0.0308814992,0.165953\H,1.5288312298,
1.087427677,-0.917922\C,-1.4349878875,0.5322323032,0.021513\H,-1.52962
87704,1.0865643232,-0.918366\H,-2.3627050065,-0.0308375008,0.167204\H,
-1.324147736,1.2494802798,0.84162\H,-0.000402283,-1.080562,1.251281\#
Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-421.7772347\RMSD=3.973e
-09\RMSF=3.652e-06\Dipole=0.000002,0.4909419,0.243282\PG=C01 [X(C2H7P
1)]\@

(CH₃)₂P⁻

1\1\GINC-SC32\FOpt\RB3LYP\6-31G(d)\C2H6P1(1-)\BUC562\19-Jan-2004\0\#\#
G3MP2B3 SCF=TIGHT OPT=TIGHT MAXDISK=134217728\Me2P-\-1,1\H,0.430341
2268,-0.3042959738,0.5270561168\C,1.4633263896,-0.1907412162,0.3303735
511\H,1.8525941846,0.8445302249,0.3084281795\H,1.9392579948,-0.6871894
674,1.1902472311\H,1.8525942126,-0.6893717414,-0.5771704609\C,-0.84743
59022,0.6262398018,-1.0846792703\H,-0.4712398441,0.1322308614,-2.00022
8103\H,-1.9421911979,0.685115388,-1.18665482\H,-0.4712398721,1.6661328
276,-1.1146294626\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-421
.1484647\RMSD=4.415e-09\RMSF=3.084e-06\Dipole=0.6623976,0.4683839,-0.8
112648\PG=C02V [C2(P1),SGV(C2H2),X(H4)]\@

(CH₃)₂PH₂⁺

1\1\GINC-SC93\FOpt\RB3LYP\6-31G(d)\C2H8P1(1+)\BUC562\22-Jan-2004\0\#\#
G3MP2B3 NOSYMM OPT=TIGHT SCF=TIGHT MAXDISK=134217728\Me2PH2+\1,1\H,0
.0439336287,0.031034947,-0.0537079023\C,1.8566677418,-0.0065180937,0.0
109920711\H,2.24552841,1.0161813976,0.0252451398\H,2.1795723346,-0.529
0192238,0.916701869\H,2.2455223477,-0.5307608709,-0.8672364342\C,-0.63
08414521,0.8731170713,-1.5121922681\H,-0.2897915234,0.3667150708,-2.42
02581393\H,-1.7242945188,0.8504481518,-1.4743090645\H,-0.290999857,1.9
131431514,-1.5268965851\H,-0.4487762186,0.6454312974,1.1056811574\H,-0
.4493008929,-1.280061899,-0.0058818436\Version=DEC-AXP-OSF/1-G03RevB.
03\HF=-422.1327273\RMSD=3.786e-09\RMSF=2.390e-06\Dipole=-0.1250737,-0.
0884499,0.1532704\PG=C01 [X(C2H8P1)]\@

TS((CH₃)₂PH)

```
1\1\GINC-SC31\FTS\RB3LYP\6-31G(d)\C4H13P1\BUC562\19-Jan-2004\0\#\ G3MP
2B3 SCF=TIGHT OPT=(TS,TIGHT,CALCFC,NOEIGENTEST) MAXDISK=536870912\CH3
CH3 -> CH2CH2 + H2 TS (Me2PH)\0,1\H,1.3078181008,-1.6093865695,-0.669
0232485\C,2.6042285112,-0.6419579143,-0.4362045367\C,1.9008048955,0.57
26942378,-0.2507345216\H,0.6677894541,0.2702062337,-0.3606995973\H,3.0
620935063,-0.876812671,-1.3928711842\H,2.9753483667,-1.2036798306,0.41
65824857\H,1.9148756203,1.0075860916,0.7513737839\H,1.9963625682,1.326
2875708,-1.0347347087\H,0.4761574027,-1.515237276,-0.7177320197\P,-1.0
895788339,-0.2095012945,-0.4271224333\C,-1.2485680729,-0.9787159346,1.
2730470927\C,-1.2812775668,1.593547743,0.0847528909\H,-2.2118108046,-0
.6958921724,1.7138303034\H,-1.2158441456,-2.0694348714,1.1901694498\H,
-0.454737595,-0.6596339725,1.9595745959\H,-0.6525369501,1.8823693999,0
.9357002315\H,-1.0427911321,2.2428529407,-0.7642079758\H,-2.3301684844
,1.7698857529,0.3537088323\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A
\HF=-501.4724247\RMSD=7.289e-09\RMSF=2.665e-06\Dipole=0.4679107,0.3030
037,0.4848038\PG=C01 [X(C4H13P1)]\@
```

Table A2: G3(MP)-RAD Total Energies (0 K, hartrees)

	H ₂	-1.16981				
	CH ₂ CH ₂	-78.43394				
	CH ₃ CH ₃	-79.64937				
	TS(uncatalysed)	-79.46734				
			ZXH	ZX ⁻	ZXH ₂ ⁺	TS
ZOH	HOH	-76.34264	-75.72079	-76.60239	-155.83460	
	(CH ₃) ₃ COH	-233.27135	-232.67410	-233.57804	-312.77106	
	H ₃ COH	-115.55181	-114.94244	-115.83678	-195.05158	
	FH	-100.35921	-99.76649	-100.54158	-179.85915	
	CH ₃ C(O)OH	-228.78239	-228.22923	-229.06144	-308.28662	
	HC(O)OH	-189.53699	-188.98971	-189.78689	-269.04269	
	F ₃ COH	-413.08312	-412.56028	-413.31608	-492.59145	
	FC(O)OH	-288.71319	-288.19410	-288.93803	-368.22567	
	O ₂ NOH	-280.58512	-280.06878	-280.87015	-360.09891	
	ClC(O)OH	-648.70095	-648.20985	-648.94265	-728.21493	
	HOS(O) ₂ OH	-699.53085	-699.03546	-699.77684	-779.05627	
ZNH	H ₂ NH	-56.46974	-55.82791	-56.79256	-135.96703	
	(CH ₃)HNH	-95.68521	-95.04433	-96.02579	-175.19110	
	(CH ₃) ₂ NH	-134.90873	-134.28128	-135.26094	-214.42167	
ZSH	HSH	-398.94461	-398.38645	-399.21190	-478.46726	
	(CH ₃) ₃ CSH	-555.88137	-555.32125	-556.18943	-635.40581	
	H ₃ CSH	-438.16995	-437.60195	-438.46361	-517.69471	
	CIH	-460.35292	-459.82262	-460.56482	-539.88089	
	F ₃ CSH	-735.67106	-735.15123	-735.92577	-815.20254	
	HC(S)SH	-834.72456	-834.20530	-834.99217	-914.26056	
	FC(S)SH	-933.88950	-933.38397	-934.14681	-1013.42741	
	ClC(S)SH	-1293.88757	-1293.38261	-1294.15178	-1373.42575	
ZPH	H ₂ PH	-342.69237	-342.10959	-342.98855	-422.21682	
	(CH ₃)HPH	-381.92723	-381.33386	-382.25051	-461.45298	
	(CH ₃) ₂ PH	-421.16672	-420.56583	-421.51120	-500.69379	