A Theoretical Investigation of the Effects of Electronegative Substitution on the Strength of C–H•••N Hydrogen Bonds

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SUPPORTING INFORMATION

(Tables S1 – S7; 33 pages)

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TABLE S1: GAUSSIAN 98 Archive Entries for the Optimized Geometries of the Monomers at the B3-LYP/6-311+G(3df,2p) level

Ammonia

```
@52\GINC-PC\SP\RMP2-FC\Gen\H3N1\SDW501\15-Dec-2000\0\\#MP2/GEN SCF=TIG
HT MAXDISK=5242880000\\MP2/G3MP2Large single point calculation on ammo
nia\\0,1\N,0,0.,0.,0.108793\H,0,0.,0.94753,-0.253851\H,0,0.820585,-0.4
73765,-0.253851\H,0,-0.820585,-0.473765,-0.253851\\Version=SGI64-G98Re
vA.9\State=1-A1\HF=-56.2178896\MP2=-56.4481976\RMSD=6.835e-09\PG=C03V
[C3(N1),3SGV(H1)]\\@
```

Acetylene

```
@33\GINC-PC\SP\RMP2-FC\Gen\C2H2\RXS501\24-Feb-2000\0\\#MP2/GEN SCF=TIG
HT MAXDISK=5242880000\\MP2/G3MP2large single point calculation on acet
ylene\\0,1\C,0,0.,0.,0.598105\H,0,0.,0.,1.660313\C,0,0.,0.,-0.598105\H
,0,0.,0.,-1.660313\\Version=SGI-G98RevA.6\State=1-SGG\HF=-76.8486398\M
P2=-77.1541556\RMSD=1.398e-09\PG=D*H [C*(H1C1.C1H1)]\\@
```

Fluoroacetylene

```
@35\GINC-PC\SP\RMP2-FC\Gen\C2H1F1\RXS501\02-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single point calculation on fl
uoroacetylene\\0,1\C,0,0.,0.,0.\H,0,0.,0.,1.060742\C,0,0.,0.,-1.191281
\F,0,0.,0.,-2.466504\\Version=SGI-G98RevA.6\State=1-SG\HF=-175.7091162
\MP2=-176.2543398\RMSD=6.496e-09\PG=C*V [C*(H1C1C1F1)]\\@
```

Ethylene

```
@36\GINC-PC\SP\RMP2-FC\Gen\C2H4\RXS501\02-Mar-2000\0\\#MP2/GEN SCF=TIG
HT MAXDISK=5242880000\\MP2/G3MP2large single point calculation on ethy
lene\\0,1\C,0,0.,0.,0.6624514226\C,0,0.,0.,-0.6624514226\H,0,0.,0.9202
867691,1.2323977126\H,0,0.,-0.9202867691,1.2323977126\H,0,0.,-0.920286
7691,-1.2323977126\H,0,0.,0.9202867691,-1.2323977126\\Version=SGI-G98R
evA.6\State=1-AG\HF=-78.0623834\MP2=-78.3909163\RMSD=2.787e-09\PG=D02H
 [C2"(C1.C1),SG(H4)]\\@
```

Fluoroethylene

```
@37\GINC-PC\SP\RMP2-FC\Gen\C2H3F1\RXS501\03-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single point calculation on fl
uorethylene\GINC-PC\SP\RMP2-FC\Gen\C2H4\RXS501\02-Mar-2000\0\\#MP2/GEN
 SCF=TIG\\0,1\C,0,0.,0.433565,0.\C,0,1.184856,-0.141845,0.\F,0,-1.1425
11,-0.27841,0.\H,0,-0.193112,1.497546,0.\H,0,2.070843,0.474124,0.\H,0,
1.295727,-1.216297,0.\\Version=SGI-G98RevA.6\State=1-A'\HF=-176.949036
9\MP2=-177.5170758\RMSD=9.598e-09\PG=CS [SG(C2H3F1)]\\@
```

Difluoroethylene ($X_{\beta1}$, $X_{\beta2}$ = F)

```
@38\GINC-PC\SP\RMP2-FC\Gen\C2H2F2\RXS501\03-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single-point calculation on Di
fluoroethylene (with 2 beta fluorines)\\0,1\C,0,0.,0.,-0.066333841\C,0
,0.,0.,-1.3813707892\F,0,0.,1.0785001036,0.6957228972\F,0,0.,-1.078500
1036,0.6957228972\H,0,0.,-0.9333003853,-1.9183921845\H,0,0.,0.93330038
53,-1.9183921845\\Version=SGI-G98RevA.6\State=1-A1\HF=-275.8407187\MP2
=-276.6486205\RMSD=7.891e-09\PG=C02V [C2(C1C1),SGV(H2F2)]\\@
```

Difluoroethylene ($X_{\alpha 1}$, $X_{\beta 2}$ = F)

```
@39\GINC-PC\SP\RMP2-FC\Gen\C2H2F2\RXS501\03-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single-point calculation on di
fluoroethylene (Xa1, Xb2 = F)\\0,1\C,0,0.,0.66045,0.577121\C,0,0.,-0.6
6045,0.577121\F,0,0.,1.381602,-0.549539\H,0,0.,1.246791,1.483125\H,0,0
.,-1.246791,1.483125\F,0,0.,-1.381602,-0.549539\\Version=SGI-G98RevA.6
\State=1-A1\HF=-275.8258006\MP2=-276.6321898\RMSD=2.691e-09\PG=C02V [S
GV(C2H2F2)]\\@
```

Difluoroethylene ($X_{\alpha 1}$, $X_{\beta 1}$ = F)

```
@40\GINC-PC\SP\RMP2-FC\Gen\C2H2F2\RXS501\03-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single point calculation on di
fluoroethylene (with Xa1 and Xb1 = F)\\0,1\C,0,0.,0.659827,0.\C,0,0.,-
0.659827,0.\F,0,1.160334,1.336403,0.\H,0,-0.879731,1.286079,0.\F,0,-1.
160334,-1.336403,0.\H,0,0.879731,-1.286079,0.\\Version=SGI-G98RevA.6\S
tate=1-AG\HF=-275.8241586\MP2=-276.6303612\RMSD=9.498e-09\PG=C02H [SGH
(C2H2F2)]\\@
```

Trifluoroethylene

```
@41\GINC-PC\SP\RMP2-FC\Gen\C2H1F3\RXS501\03-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single-point calculation on tr
ifluoroethylene\\0,1\C,0,-0.701385,-0.688159,0.\C,0,0.,0.431178,0.\F,0
,-0.090297,-1.880128,0.\H,0,-1.778346,-0.709715,0.\F,0,-0.556694,1.626
931,0.\F,0,1.312175,0.503374,0.\\Version=SGI-G98RevA.6\State=1-A'\HF=-
374.709522\MP2=-375.7556952\RMSD=5.717e-09\PG=CS [SG(C2H1F3)]\\@
```

Ethane

```
@42\GINC-PC\SP\RMP2-FC\Gen\C2H6\SDW501\04-Mar-2000\0\\#MP2/GEN SCF=TIG
HT MAXDISK=5242880000\\MP2/G3MP2large single point on ethane\\0,1\C,0,
0.,0.,0.76375\C,0,0.,0.,-0.76375\H,0,0.,1.01597,1.161505\H,0,0.,-1.015
97,-1.161505\H,0,-0.879856,-0.507985,1.161505\H,0,0.879856,-0.507985,1
.161505\H,0,-0.879856,0.507985,-1.161505\H,0,0.879856,0.507985,-1.1615
05\\Version=SGI-G98RevA.6\State=1-A1G\HF=-79.2574261\MP2=-79.6176883\R
MSD=6.840e-09\PG=D03D [C3(C1.C1),3SGD(H2)]\\@
```

Fluoroethane

```
@43\GINC-PC\SP\RMP2-FC\Gen\C2H5F1\SDW501\04-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single point on fluoroethane\\
0,1\C,0,0.,0.556925,0.\C,0,1.130086,-0.445095,0.\F,0,-1.230852,-0.1082
83,0.\H,0,2.087619,0.079148,0.\H,0,0.018486,1.19121,0.888152\H,0,0.018
486,1.19121,-0.888152\H,0,1.086283,-1.079001,0.885338\H,0,1.086283,-1.
079001,-0.885338\\Version=SGI-G98RevA.6\State=1-A'\HF=-178.1442444\MP2
=-178.7411401\RMSD=3.666e-09\PG=CS [SG(C2H1F1),X(H4)]\\@
```

Difluoroethane ($X_{\alpha1}$, $X_{\alpha2}$ = F or $X_{\beta2}$, $X_{\beta3}$ = F)

@44\GINC-PC\SP\RMP2-FC\Gen\C2H4F2\SDW501\04-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2Large single point calculation on di
fluoroethylene (with 2 fluorines on same carbon)\\0,1\C,0,0.,0.36194,0
.\C,0,-1.33764,-0.323687,0.\H,0,-0.051639,1.452492,0.\H,0,-1.193584,-1
.403146,0.\F,0,0.726241,-0.011485,1.099897\F,0,0.726241,-0.011485,-1.0
99897\H,0,-1.900639,-0.036067,0.886588\H,0,-1.900639,-0.036067,-0.8865
88\\Version=SGI-G98RevA.6\State=1-A'\HF=-277.0454028\MP2=-277.8809275\
RMSD=2.701e-09\PG=CS [SG(C2H2),X(H2F2)]\\@

Difluoroethane ($X_{\alpha1}$, $X_{\beta1}$ = F)

@45\GINC-PC\SP\RMP2-FC\Gen\C2H4F2\SDW501\04-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2Large single point calculation on di
fluoroethylene with each fluorine on a different carbon atom\\0,1\C,0,
-0.4372452136,0.2613993038,0.7513601043\C,0,-0.4435383227,0.2492409251
,-0.7518431512\H,0,-1.4608010593,0.3540853756,1.1231630937\F,0,0.84685
96973,0.3751845245,-1.2519959372\F,0,0.0941625594,-0.9207750271,1.2525
177307\H,0,0.1674325224,1.0866107379,1.1307946674\H,0,-0.8590111622,-0
.6856098657,-1.13130075\H,0,-1.0321193933,1.0913869024,-1.1244548702\\
Version=SGI-G98RevA.6\HF=-277.0263635\MP2=-277.8598604\RMSD=2.709e-09\
PG=C01 [X(C2H4F2)]\\@

Trifluoroethane ($X_{\beta1}$, $X_{\beta2}$, $X_{\beta3}$ = F)

@46\GINC-PC\SP\RMP2-FC\Gen\C2H3F3\SDW501\04-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2Large single point calculation on tr
ifluoroethylene\\0,1\C,0,0.,0.,-0.024692\C,0,0.,0.,1.478168\F,0,0.,1.2
51498,-0.527287\H,0,0.,-1.02588,1.838632\F,0,1.083829,-0.625749,-0.527
287\F,0,-1.083829,-0.625749,-0.527287\H,0,0.888438,0.51294,1.838632\H,
0,-0.888438,0.51294,1.838632\\Version=SGI-G98RevA.6\State=1-A1\HF=-375
.9529907\MP2=-377.0271729\RMSD=2.056e-09\PG=C03V [C3(C1C1),3SGV(H1F1)]
\\@

Trifluoroethane ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta1}$ = F)

@148\GINC-SC35\SP\ROMP2-FC\GTMP2Large\C2H3F3\SDW501\01-May-2001\0\\#RO
MP2/GTMP2LARGE SCF=TIGHT MAXDISK=65536000\\RMP2/G3MP2Large single-poin
t calculation on a,a,b-trifluoroethane monomer\\0,1\H,0,-1.3490205949,
-0.9210826762,0.1203500885\C,0,-0.2622339818,-0.960199477,0.2011357967
\C,0,0.3047294013,0.4442275491,0.1853550439\H,0,1.3939022051,0.4711942
313,0.1229013958\H,0,0.0320223584,-1.4646024415,1.1218423618\F,0,0.245
3460195,-1.665447379,-0.8746980829\F,0,-0.0863578539,1.0756969936,1.33
12164765\F,0,-0.1958633307,1.1464528802,-0.865856048\\Version=DEC-AXP-
OSF/1-G98RevA.9\HF=-375.9236091\MP2=-376.9952627\RMSD=8.536e-09\PG=C01
[X(C2H3F3)]\\@

Tetrafluoroethane ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$, $X_{\beta3}$ = F)

```
@149\GINC-SC15\SP\ROMP2-FC\GTMP2Large\C2H2F4\SDW501\01-May-2001\0\\#RO
MP2/GTMP2LARGE SCF=TIGHT MAXDISK=65536000\\RMP2/6-31G(d,p) single-poin
t calculation on a,a,b,b-tetrafluoroethane monomer\\0,1\H,0,1.54870484
79,0.092369147,0.\C,0,0.5494249431,0.5310389527,0.\C,0,-0.5494249431,-
0.5310389527,0.\H,0,-1.5487048479,-0.092369147,0.\F,0,0.4008261482,1.3
123279784,1.098075\F,0,0.4008261482,1.3123279784,-1.098075\F,0,-0.4008
261482,-1.3123279784,1.098075\F,0,-0.4008261482,-1.3123279784,-1.09807
5\\Version=DEC-AXP-OSF/1-G98RevA.9\State=1-AG\HF=-474.8178209\MP2=-476
.1281521\RMSD=7.533e-09\PG=C02H [SGH(C2H2),X(F4)]\\@
```

Pentafluoroethane

```
@47\GINC-PC\SP\ROMP2-FC\Gen\C2H1F5\SDW501\10-May-2000\0\\#ROMP2/GEN SC
F=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single point calculation on
 pentafluoroethylene\\0,1\C,0,0.,0.,0.770776\C,0,0.,0.,-0.770776\H,0,-
1.020223,0.,1.158348\F,0,1.23749,0.,-1.26058\F,0,0.650757,-1.097594,1.
209869\F,0,0.650757,1.097594,1.209869\F,0,-0.641275,-1.084809,-1.22011
6\F,0,-0.641275,1.084809,-1.220116\\Version=SGI-G98RevA.6\State=1-A'\H
F=-573.7180256\MP2=-575.2678408\RMSD=7.775e-09\PG=CS [SG(C2H1F1),X(F4)
]\\@
```

Methane

```
@48\GINC-PC\SP\RMP2-FC\Gen\C1H4\RXS501\23-Feb-2000\0\\#MP2/GEN SCF=TIG
HT MAXDISK=5242880000\\MP2/G3MP2large single point calculation on meth
ane\GINC-PC\SP\ROMP2-FC\Gen\C2H1F5\SDW501\10-May-2000\0\\#ROMP2/GEN SC
\\0,1\C,0,0.,0.,0.\H,0,1.0880520032,-0.0000305531,-0.0000327981\H,0,-0
.3626551957,1.0258354511,-0.0000000009\H,0,-0.3627251835,-0.512911917,
-0.8883743413\H,0,-0.362671624,-0.512892981,0.8884071402\\Version=SGI-
G98RevA.6\HF=-40.2122634\MP2=-40.4042813\RMSD=1.694e-09\PG=TD [O(C1),4
C3(H1)]\\@
```

Fluoromethane

```
@49\GINC-PC\SP\RMP2-FC\Gen\C1H3F1\RXS501\02-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single point calculation on fl
uoromethane\\0,1\C,0,0.,0.,0.\F,0,0.,0.,1.388522\H,0,1.031813,0.,-0.34
994\H,0,-0.515906,-0.893576,-0.34994\H,0,-0.515906,0.893576,-0.34994\\
Version=SGI-G98RevA.6\State=1-A\HF=-139.0905772\MP2=-139.518154\RMSD=2
.599e-09\PG=C03 [C3(C1F1),X(H3)]\\@
```

Difluoromethane

```
@50\GINC-PC\SP\RMP2-FC\Gen\C1H2F2\RXS501\02-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single point calculation on di
fluoromethane\\0,1\H,0,-0.9115939388,1.1019037997,0.\C,0,0.,0.50409263
25,0.\H,0,0.9115939388,1.1019037997,0.\F,0,0.,-0.290464633,1.103943894
4\F,0,0.,-0.290464633,-1.1039438944\\Version=SGI-G98RevA.6\State=1-A1\
HF=-237.986681\MP2=-238.652511\RMSD=5.080e-09\PG=C02V [C2(C1),SGV(F2),
SGV'(H2)]\\@
```

Trifluoromethane

@51\GINC-PC\SP\RMP2-FC\Gen\C1H1F3\RXS501\02-Mar-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2large single point calculation on tr
ifluoromethane\\0,1\C,0,0.,0.,0.\H,0,0.,0.,1.089189\F,0,1.253957,0.,-0
.467404\F,0,-0.626979,-1.085959,-0.467404\F,0,-0.626979,1.085959,-0.46
7404\\Version=SGI-G98RevA.6\State=1-A1\HF=-336.892887\MP2=-337.7976104
\RMSD=7.783e-09\PG=C03V [C3(C1H1),3SGV(F1)]\\@

TABLE S2: GAUSSIAN 98 Archive Entries for the Optimized Geometries of the Ammonia Complexes at the B3-LYP/6-311+G(3df,2p) level

Acetylene-Ammonia Complex


```
1\GINC-PC\SP\RMP2-FC\Gen\C2H5N1\RXS501\24-Feb-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculation on ac
etlyene-ammonia complex\\0,1\N,0,0.,0.,2.273549\H,0,0.,0.94184,2.64881
9\H,0,-0.815657,-0.47092,2.648819\H,0,0.815657,-0.47092,2.648819\H,0,0
.,0.,-0.034021\C,0,0.,0.,-1.106021\C,0,0.,0.,-2.304171\H,0,0.,0.,-3.36
6131\\Version=SGI-G98RevA.6\State=1-A1\HF=-133.0707609\MP2=-133.608609
1\RMSD=5.071e-09\PG=C03V [C3(H1C1C1H1N1),3SGV(H1)]\\@
```


Fluoroacetylene-Ammonia Complex


```
1\GINC-PC\SP\RMP2-FC\Gen\C2H4F1N1\RXS501\02-Mar-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single point on fluo
roacetylene-ammonia complex\\0,1\N,0,0.,0.,0.\H,0,0.,0.,2.284183\H,0,0
.941898,0.,-0.375075\H,0,-0.470949,-0.815707,-0.375075\H,0,-0.470949,0
.815707,-0.375075\C,0,0.,0.,3.35543\C,0,0.,0.,4.54857\F,0,0.,0.,5.8281
65\\Version=SGI-G98RevA.6\State=1-A\HF=-231.9314874\MP2=-232.7093318\R
MSD=3.082e-09\PG=C03 [C3(N1H1C1C1F1),X(H3)]\\@
```


Ethylene-Ammonia Complex


```
1\GINC-PC\SP\RMP2-FC\Gen\C2H7N1\SDW501\08-Aug-2000\0\\#MP2/GEN GFINPU
T SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculatio
n on ethylene-ammonia complex\\0,1\C,0,-2.11065,0.35902,0.\H,0,-2.1903
2,-0.72105,0.\H,0,-3.04299,0.90996,0.\C,0,-0.93388,0.96945,0.\H,0,-0.8
6322,2.05062,0.\H,0,0.,0.42,0.\N,0,2.34292,-1.00134,0.\H,0,2.39458,-1.
59997,0.81642\H,0,2.39458,-1.59997,-0.81642\H,0,3.17412,-0.42105,0.\\V
ersion=SGI-G98RevA.7\State=1-A'\HF=-134.2813326\MP2=-134.8414089\RMSD=
6.041e-09\PG=CS [SG(C2H5N1),X(H2)]\\@
```


Fluoroethylene-Ammonia Complex ($X_{\beta 2}$ = F)


```
1\GINC-PC\SP\RMP2-FC\Gen\C2H6F1N1\SDW501\08-Aug-2000\0\\#MP2/GEN GFIN
PUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculat
ion on fluoroethylene-ammonia complex with Xb2 = F\\0,1\H,0,0.,0.,0.\N
,0,2.61082,0.,0.\H,0,2.986318,-0.145812,0.93023\H,0,2.986318,-0.73316,
-0.590817\H,0,2.986318,0.878612,-0.338569\C,0,-1.081424,0.001177,-0.02
1719\H,0,-1.628715,0.001773,0.910536\C,0,-1.708888,0.00186,-1.179321\H
,0,-1.246403,0.001357,-2.156789\F,0,-3.056331,0.003327,-1.271464\\Vers
ion=SGI-G98RevA.7\HF=-233.1688322\MP2=-233.9687555\RMSD=8.918e-09\PG=C
01 [X(C2H6F1N1)]\\@
```

Fluoroethylene-Ammonia Complex ($X_{\beta 1}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H6F1N1\SDW501\09-Aug-2000\0\\#MP2/GEN GFIN
PUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculat
ion on fluoroethylene-ammonia complex with Xb1 = F\\0,1\H,0,0.19440131
93,0.765608955,0.0027266704\N,0,2.7842269301,0.8612001867,0.0028306163
\C,0,-0.8877525151,0.8001578351,0.0026990864\H,0,-1.377286582,1.762828
8194,0.0058308306\C,0,-1.6346761833,-0.284430431,-0.0010581913\F,0,-1.
1018573696,-1.5253576255,-0.0050290879\H,0,-2.7155801793,-0.3202588192
,-0.0014196438\H,0,3.2509475755,1.3811572545,0.7370990906\H,0,2.999366
3896,-0.1189453611,0.1467246158\H,0,3.2098514827,1.1350620495,-0.87535
94569\\Version=SGI-G98RevA.7\HF=-233.1687292\MP2=-233.9686884\RMSD=8.8
72e-09\PG=C01 [X(C2H6F1N1)]\\@

Fluoroethylene-Ammonia Complex ($X_{\alpha 1}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H6F1N1\SDW501\08-Aug-2000\0\\#MP2/GEN GFIN
PUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculat
ion on fluoroethylene-ammonia complex with Xa1 = F\\0,1\H,0,0.29245,0.
21447,0.0429\N,0,2.7814,0.0902,0.09283\H,0,2.96296,-0.88416,-0.12071\H
,0,3.27505,0.64389,-0.59802\H,0,3.20882,0.28309,0.99154\C,0,-0.78374,0
.09931,-0.00619\F,0,-1.13919,-1.18705,-0.21987\C,0,-1.68973,1.04881,0.
11796\H,0,-1.3674,2.06469,0.28789\H,0,-2.74818,0.84138,0.05475\\Versio
n=SGI-G98RevA.7\HF=-233.1698528\MP2=-233.9699037\RMSD=6.488e-09\PG=C01
[X(C2H6F1N1)]\\@

Difluoroethylene-Ammonia Complex ($X_{\beta 2}$, $X_{\beta 3}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H5F2N1\SDW501\08-Aug-2000\0\\#MP2/GEN GFIN
PUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculat
ion on difluoroethylene-ammonia complex with Xb1 and Xb2 = F\\0,1\H,0,
-0.7290740021,0.919190392,-0.0123607413\C,0,0.3515143172,0.9155678354,
-0.0176318625\H,0,0.900754939,1.8426763289,-0.0197441613\C,0,1.0136398
513,-0.2195650479,-0.0198546974\F,0,0.4668402318,-1.4254054516,-0.0178
359316\F,0,2.3325827267,-0.3415065393,-0.024417917\N,0,-3.2441252089,0
.9103153223,0.0587180412\H,0,-3.5085203958,-0.059356838,-0.0741353512\
H,0,-3.7214510781,1.4501323495,-0.6542436087\H,0,-3.618564639,1.201341
7043,0.95466157\\Version=SGI-G98RevA.7\HF=-332.0609881\MP2=-333.101109
3\RMSD=6.161e-09\PG=C01 [X(C2H5F2N1)]\\@

Difluoroethylene-Ammonia Complex ($X_{\alpha 1}$, $X_{\beta 2}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H5F2N1\SDW501\08-Aug-2000\0\\#MP2/GEN GFIN
PUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculat
ion on difluoroethylene-ammonia complex wtih Xa1 and Xb2 = F\\0,1\H,0,
-0.8669754638,0.1538114221,0.0002119053\C,0,0.2157800073,0.1503472868,
0.0000640028\F,0,0.7805045074,1.3681194251,-0.0001614167\C,0,0.9387354
867,-0.9552927974,0.000044527\H,0,0.4987414839,-1.9406122948,0.0002278
375\F,0,2.2802251719,-0.9504447474,-0.0001967251\N,0,-3.2988275204,0.2
686819686,0.0001959505\H,0,-3.530297597,1.2541801334,-0.0578569837\H,0
,-3.7493814735,-0.1885358615,-0.7845856478\H,0,-3.7339543843,-0.089016
216,0.8432033322\\Version=SGI-G98RevA.7\HF=-332.0475188\MP2=-333.08607
59\RMSD=2.738e-09\PG=C01 [X(C2H5F2N1)]\\@

Difluoroethylene-Ammonia Complex ($X_{\alpha 1}$, $X_{\beta 1}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H5F2N1\SDW501\09-Aug-2000\0\\#MP2/GEN GFIN
PUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculat
ion on difluoroethylene-ammonia complex with Xa1 and Xb1 = F\\0,1\H,0,
-0.5283240971,0.4088697941,0.0072361499\C,0,0.5554019343,0.4088462391,
0.0105150878\F,0,1.1119965258,1.6370727905,0.0118241772\C,0,1.33814611
53,-0.6539905811,0.0120398922\F,0,0.8039008416,-1.8910361732,0.0108705
909\H,0,2.4179461896,-0.6419822559,0.0141080976\N,0,-2.9372819668,0.40
87973045,-0.0336203086\H,0,-3.2339559743,-0.5462882998,0.1329340161\H,
0,-3.3190394328,0.6876913781,-0.9303840413\H,0,-3.3800175223,0.9866647
489,0.6718651451\\Version=SGI-G98RevA.7\HF=-332.0456197\MP2=-333.08413
26\RMSD=9.950e-09\PG=C01 [X(C2H5F2N1)]\\@

Trifluoroethylene-Ammonia Complex

1\GINC-PC\SP\RMP2-FC\Gen\C2H4F3N1\SDW501\08-Aug-2000\0\\#MP2/GEN GFIN
PUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculat
ion on trifluoroethylene-ammonia complex\\0,1\H,0,-1.05553,0.23775,-0.
00043\N,0,-3.36524,-0.29876,-0.00028\H,0,-3.94299,0.52204,-0.14334\H,0
,-3.59666,-0.95739,-0.73556\H,0,-3.65549,-0.71775,0.87616\C,0,-0.01298
,0.52779,-0.00297\F,0,0.23289,1.84979,-0.01333\C,0,0.99237,-0.32831,0.
00325\F,0,0.82218,-1.63973,0.01345\F,0,2.2706,-0.00898,0.00026\\Versio
n=SGI-G98RevA.7\HF=-430.9316838\MP2=-432.2103153\RMSD=4.573e-09\PG=C01
 [X(C2H4F3N1)]\\@

Ethane-Ammonia Complex

1\GINC-PC\SP\RMP2-FC\Gen\C2H9N1\SDW501\14-Aug-2000\0\\#MP2/GEN GFINP
UT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculati
on on ethane-ammonia complex\\0,1\C,0,0.,0.,0.\C,0,1.52793,0.,0.\H,0,-
0.39755,1.01549,0.\H,0,1.92982,-1.01476,0.\H,0,-0.3952,-0.51156,-0.879
58\H,0,-0.3952,-0.51156,0.87958\H,0,1.92476,0.51001,0.87938\H,0,1.9247
6,0.51001,-0.87938\N,0,-1.46659,3.89974,0.\H,0,-2.47804,3.83567,0.\H,0
,-1.20008,4.43872,-0.81585\H,0,-1.20008,4.43872,0.81584\\Version=SGI64
-G98RevA.9\HF=-135.4756737\MP2=-136.0671178\RMSD=7.906e-09\PG=C01 [X(C
2H9N1)]\\@

Fluoroethane-Ammonia Complex ($X_{\alpha 1}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H8F1N1\SDW501\14-Aug-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calcula
tion on fluoroethane-ammonia complex with Xa1 = F\\0,1\H,0,-0.24871588
81,-0.1438902011,-0.258998768\C,0,0.841561155,-0.1390105086,-0.2547757
527\F,0,1.2516923771,1.2042704269,-0.2522400447\H,0,1.2067544172,-0.57
56599996,-1.1865468581\C,0,1.4065226072,-0.8484283412,0.9530640759\H,0
,2.4964169173,-0.8287653832,0.9461685831\H,0,1.0811322974,-1.890520371
4,0.951916431\H,0,1.0552255356,-0.3831799103,1.8740660669\N,0,-2.92812
32409,-0.1425145966,-0.4090881283\H,0,-2.9980251848,0.8660541956,-0.48
44559598\H,0,-3.3237379736,-0.5332976338,-1.2565493953\H,0,-3.52592140
25,-0.4269392622,0.3584472614\\Version=SGI64-G98RevA.9\HF=-234.3637998
\MP2=-235.1924478\RMSD=3.214e-09\PG=C01 [X(C2H8F1N1)]\\@

Fluoroethane-Ammonia Complex ($X_{\beta 2}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H8F1N1\SDW501\14-Aug-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calcula
tion on fluoroethane-ammonia complex with Xb2 = F\\0,1\H,0,-0.14328677
17,0.6686306836,-0.6479242432\C,0,0.9464921484,0.6571712766,-0.6438517
355\H,0,1.2982894505,1.6911087392,-0.6461850127\H,0,1.3031259308,0.174
8035886,-1.5542936247\C,0,1.477263545,-0.0525790594,0.5781263011\H,0,2
.5685569222,-0.0752385358,0.5994661023\F,0,1.0458093105,-1.3866467607,
0.5876987698\H,0,1.1144870194,0.4024214607,1.501619799\N,0,-2.90715776
31,0.6444108915,-0.4234594798\H,0,-2.8652205743,-0.3146554275,-0.09756
91031\H,0,-3.3909141846,0.6368852937,-1.3141929994\H,0,-3.4897514053,1
.1574355003,0.2283591185\\Version=SGI64-G98RevA.9\HF=-234.3633541\MP2=
-235.1919554\RMSD=4.090e-09\PG=C01 [X(C2H8F1N1)]\\@

Fluoroethane-Ammonia Complex ($X_{\beta 1}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H8F1N1\SDW501\14-Aug-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calcula
tion on fluoroethane-ammonia complex with Xb1 = F\\0,1\H,0,-0.54083120
59,0.3462793573,-0.616739068\C,0,0.5511197397,0.345204697,-0.614246249
\H,0,0.8999915591,1.3781932266,-0.613976186\H,0,0.9015437307,-0.138849
8404,-1.5261910304\C,0,1.0542285653,-0.3871899123,0.6051860017\F,0,2.4
561915788,-0.3948264735,0.6265868038\H,0,0.7329831718,-1.4302636129,0.
6141989846\H,0,0.7272493727,0.0911243919,1.5301603994\N,0,-3.333954088
2,0.3454122543,-0.4876582368\H,0,-3.6265339544,0.3846818709,-1.4574550
628\H,0,-3.8223534788,-0.4336369888,-0.060879387\H,0,-3.6721846172,1.1
899353683,-0.0404307422\\Version=SGI64-G98RevA.9\HF=-234.3635601\MP2=-
235.1920876\RMSD=9.644e-09\PG=C01 [X(C2H8F1N1)]\\@

Difluoroethane-Ammonia Complex ($X_{\beta 2}$, $X_{\beta 3}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H7F2N1\SDW501\15-Aug-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calcula
tion on difluoroethane-ammonia complex with Xb2 and Xb3 = F\\0,1\H,0,-
0.3432282495,0.5475618895,-0.9680845209\C,0,0.7470809257,0.5382564146,
-0.9652740741\H,0,1.1173449904,1.5628908558,-0.9705448358\H,0,1.107327
4301,0.0311302955,-1.8597276534\C,0,1.2553729586,-0.1735783355,0.25476
08599\H,0,2.3433068272,-0.223694754,0.333426245\F,0,0.7895623325,-1.46
42510957,0.2881030382\F,0,0.7972690562,0.4377024819,1.3951173601\N,0,-
2.9501225873,0.5323856039,-0.7853916856\H,0,-3.0417281575,-0.418047216
6,-0.4446702265\H,0,-3.6800867923,0.6762010201,-1.4736820403\H,0,-3.14
8283741,1.148127732,-0.0048794692\\Version=SGI64-G98RevA.9\HF=-333.265
1198\MP2=-334.3327825\RMSD=4.151e-09\PG=C01 [X(C2H7F2N1)]\\@

Difluoroethane-Ammonia Complex ($X_{\alpha 1}$, $X_{\beta 1}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H7F2N1\SDW501\14-Aug-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT MAXDISK=5242880000\\e\\0,1\H,0,-0.7669989221,0.06707321
68,-0.4335774981\C,0,0.3254757086,0.0695617113,-0.4297914959\F,0,0.758
0896775,1.3962287517,-0.428271771\H,0,0.7036630939,-0.3980028044,-1.34
06729411\C,0,0.8304579247,-0.6524805443,0.7858574786\F,0,2.2004054247,
-0.8881993814,0.6994235708\H,0,0.3299042395,-1.6199598158,0.8713111556
\H,0,0.6519668561,-0.0664862373,1.6888034106\N,0,-3.3393340615,0.06843
61522,-0.518789547\H,0,-3.4753136758,1.0658626714,-0.6405836489\H,0,-3
.7057768024,-0.3842184035,-1.348660017\H,0,-3.924164078,-0.218073027,0
.258144274\\Version=SGI64-G98RevA.9\HF=-333.2471153\MP2=-334.3126581\R
MSD=4.868e-09\PG=C01 [X(C2H7F2N1)]\\@

Difluoroethane-Ammonia Complex ($X_{\alpha 1}$, $X_{\alpha 2}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H7F2N1\SDW501\15-Aug-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calcula
tion on difluoroethane-ammonia complex with Xa1 and Xa2 = F\\0,1\H,0,-
0.5344345126,0.004420807,-0.0220287732\C,0,0.5560722987,0.004595153,-0
.0243094188\F,0,0.9735990434,1.3147148883,-0.0250330126\F,0,0.97202432
08,-0.5370268022,-1.2177159022\C,0,1.1842378436,-0.7350920031,1.123653
8083\H,0,2.2696057902,-0.6865130453,1.0459261588\H,0,0.8683427513,-1.7
772017942,1.1070454917\H,0,0.8703251349,-0.2874855821,2.0655503882\N,0
,-3.0319722769,-0.0006091164,0.0556594083\H,0,-3.3152191703,-0.3045654
956,-0.8691511058\H,0,-3.5786849849,-0.5310529309,0.7244400092\H,0,-3.
3086002019,0.9704501813,0.1472758691\\Version=SGI64-G98RevA.9\HF=-333.
2662843\MP2=-334.3340022\RMSD=3.103e-09\PG=C01 [X(C2H7F2N1)]\\@

Trifluoroethane-Ammonia Complex ($X_{\beta 1}$, $X_{\beta 2}$, $X_{\beta 3}$ = F)

1\GINC-PC\SP\RMP2-FC\Gen\C2H6F3N1\SDW501\15-Aug-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calcula
tion on trifluoroethane-ammonia complex with Xb1, Xb2 and Xb3 = F\\0,1
\H,0,-1.1050741442,0.8143848671,-0.002936392\C,0,-0.07648704,1.1738808
544,-0.0042937257\H,0,0.1027939531,1.7797175101,0.8813270697\H,0,0.102
4779238,1.7739577696,-0.893885822\C,0,0.8684595545,0.0088188017,-0.000
6161675\F,0,2.1618285753,0.399997412,-0.003222308\F,0,0.7012379904,-0.
7835475784,-1.081600352\F,0,0.7030494835,-0.7753270006,1.086434589\N,0
,-3.4961630948,-0.0485023085,0.0025240598\H,0,-4.2450357396,0.52078876
68,-0.3752711158\H,0,-3.4575659922,-0.8964751876,-0.5519287361\H,0,-3.
7713338676,-0.3191609992,0.9399785764\\Version=SGI64-G98RevA.9\HF=-432
.1735584\MP2=-433.4800113\RMSD=4.034e-09\PG=C01 [X(C2H6F3N1)]\\@

Trifluoroethane-Ammonia Complex ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$ = F)

```
@1\GINC-SC11\SP\ROMP2-FC\GTMP2Large\C2H6F3N1\SDW501\02-May-2001\0\\#RO
MP2/GTMP2LARGE SCF=TIGHT GFINPUT MAXDISK=104857600\\RMP2/G3MP2Large si
ngle-point calculation on a,a,b-trifluoroethane ammonia complex\\0,1\H
,0,0.7199916022,-0.2328325129,-0.0066919231\C,0,-0.3470185246,-0.46247
19238,0.0025080769\F,0,-0.7176286833,-0.7498217191,1.2843280769\F,0,-0
.5685391457,-1.5872818015,-0.7488719231\C,0,-1.2212179152,0.6410785589
,-0.5546519231\H,0,-2.2731880491,0.3986291398,-0.3996219231\H,0,-1.014
5478438,0.7704684448,-1.6172619231\F,0,-0.9353872597,1.8283084011,0.09
91080769\N,0,3.0874318602,0.2343261798,-0.0497819231\H,0,3.6542515739,
-0.2840441332,-0.7113919231\H,0,3.2846524036,1.2184760709,-0.192761923
1\H,0,3.4202317289,-0.003464004,0.8779880769\\Version=DEC-AXP-OSF/1-G9
8RevA.9\HF=-432.1452849\MP2=-433.4494421\RMSD=8.436e-09\PG=C01 [X(C2H6
F3N1)]\\@
```

Tetrafluoroethane-Ammonia Complex ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$, $X_{\beta3}$ = F)

```
@150\GINC-SC15\SP\RMP2-FC\GTMP2Large\C2H5F4N1\SDW501\01-May-2001\0\\#M
P2/GTMP2LARGE SCF=TIGHT MAXDISK=131072000\\RMP2/G3MP2Large single poin
t calculation on a,a,b,b-tetrafluoroethane ammonia complex\\0,1\H,0,0.
9104298799,0.2895862156,-0.0084469833\C,0,-0.1172791673,0.6617300851,-
0.0003249833\F,0,-0.3322682662,1.4408850578,-1.0956389833\F,0,-0.31749
92652,1.4328000597,1.1034610167\C,0,-1.1584790256,-0.4550650471,0.0025
670167\H,0,-2.1804710742,-0.0717121768,0.0098650167\F,0,-0.9671169266,
-1.2349500228,1.0974020167\F,0,-0.9802489274,-1.2281360244,-1.09932998
33\N,0,3.1247159769,-0.4748805034,-0.0072339833\H,0,3.5878619556,-0.30
69154446,0.8788820167\H,0,3.143241104,-1.475808501,-0.1682009833\H,0,3
.6946759226,-0.046368431,-0.7279599833\\Version=DEC-AXP-OSF/1-G98RevA.
9\HF=-531.0403025\MP2=-532.5833956\RMSD=3.725e-09\PG=C01 [X(C2H5F4N1)]
\\@
```

Pentafluoroethane-Ammonia Complex

```
1\GINC-PC\SP\RMP2-FC\Gen\C2H4F5N1\SDW501\03-Oct-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calcula
tion on pentafluoroethane-ammonia complex\\0,1\H,0,-1.0603099025,0.325
5591866,-0.5286660415\C,0,0.0310660407,0.3611419777,-0.5893583761\F,0,
0.4521436249,1.6486946093,-0.5611593878\F,0,0.4493027342,-0.2002610588
,-1.7493348241\C,0,0.6839487742,-0.3927489274,0.582864772\F,0,2.015188
6092,-0.3530245687,0.5244134813\F,0,0.2960930074,-1.6750683677,0.56939
97654\F,0,0.2933675331,0.149411898,1.7442559922\N,0,-3.3655604688,0.36
91078314,-0.4222971738\H,0,-3.7883665099,0.0412182648,-1.2836391162\H,
0,-3.7379536348,-0.202837415,0.327663663\H,0,-3.6993951407,1.314174233
6,-0.2684919073\\Version=SGI64-G98RevA.9\HF=-629.9416231\MP2=-631.7242
58\RMSD=7.982e-09\PG=C01 [X(C2H4F5N1)]\\@
```

Methane-Ammonia Complex

```
1\GINC-PC\SP\RMP2-FC\Gen\C1H7N1\RXS501\23-Feb-2000\0\\#MP2/GEN SCF=T
IGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculation on me
thane-ammonia complex\\0,1\C,0,0.,0.,0.\H,0,0.,0.,1.088637\H,0,1.02507
4,0.,-0.366542\H,0,-0.512537,-0.88774,-0.366542\H,0,-0.512537,0.88774,
-0.366542\N,0,0.,0.,4.059085\H,0,-0.942038,0.,4.432905\H,0,0.471019,0.
815829,4.432905\H,0,0.471019,-0.815829,4.432905\\Version=SGI-G98RevA.6
\State=1-A1\HF=-96.4305389\MP2=-96.8537425\RMSD=7.903e-09\PG=C03V [C3(
C1H1N1),3SGV(H2)]\\@
```

Fluoromethane-Ammonia Complex (∠(C–H•••N) = 180.0°)

1\GINC-PC\SP\RMP2-FC\Gen\C1H6F1N1\RXS501\02-Mar-2000\0\\#MP2/GEN SCF
=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single-point calculation on
fluoromethane-ammonia complex with hydrogen-bond angle fixed to be equ
al to 180 degs.\\0,1\H,0,0.,0.,0.\C,0,1.088998,0.,0.\F,0,1.541207,0.,1
.318987\H,0,1.471871,-0.892744,-0.494433\H,0,1.471871,0.892744,-0.4944
33\N,0,-2.655922,0.,0.\H,0,-2.776404,0.000063,1.006626\H,0,-3.139602,0
.815525,-0.358332\H,0,-3.139602,-0.815525,-0.358332\\Version=SGI-G98Re
vA.6\HF=-195.3103252\MP2=-195.9695342\RMSD=9.043e-09\PG=C01 [X(C1H6F1N
1)]\\@

Fluoromethane-Ammonia Complex (∠(C–H•••N) = 121.8°)

@29\GINC-PC\SP\RMP2-FC\Gen\C1H6F1N1\SDW501\21-Nov-2000\0\\#MP2/GEN SCF
=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single point calculation on
fluoromethane-ammonia complex with non-linear hydrogen bond (C-H...N a
ngle = 121.8 deg.)\\0,1\H,0,-0.1865648084,1.3044799471,0.\C,0,-1.19638
50088,0.8991876926,0.\F,0,-1.106882542,-0.4947441577,0.\H,0,-1.7373691
613,1.2068251189,0.8936869593\H,0,-1.7373691613,1.2068251189,-0.893686
9593\N,0,2.0659106931,-0.3551668504,0.\H,0,1.1766623046,-0.8439429693,
0.\H,0,2.5817594528,-0.6652239994,-0.8151389634\H,0,2.5817594528,-0.66
52239994,0.8151389634\\Version=SGI64-G98RevA.9\State=1-A'\HF=-195.3111
236\MP2=-195.9712422\RMSD=3.871e-09\PG=CS [SG(C1H2F1N1),X(H4)]\\@

Difluoromethane-Ammonia Complex

@30\GINC-PC\SP\RMP2-FC\Gen\C1H5F2N1\SDW501\21-Nov-2000\0\\#MP2/GEN SCF
=TIGHT MAXDISK=5242880000\\MP2/G3MP2Large single point calculation on
difluoromethane-ammonia complex\\0,1\H,0,0.2920747736,-0.0295311199,0.
4207993796\C,0,-0.7974892405,-0.0199714677,0.4364740357\H,0,-1.2318118
869,-0.0801742335,1.4349759892\F,0,-1.2389839547,1.1299212891,-0.15317
92422\F,0,-1.260341762,-1.0758529094,-0.2954934193\N,0,2.7170232407,-0
.0272828703,-0.0020955381\H,0,3.4129026374,-0.0807568952,0.7330754634\
H,0,2.8851087555,-0.8062728381,-0.6289284536\H,0,2.9014299291,0.820928
5672,-0.5260438722\\Version=SGI64-G98RevA.9\HF=-294.2079069\MP2=-295.1
0583\RMSD=3.354e-09\PG=C01 [X(C1H5F2N1)]\\@

Trifluoromethane-Ammonia Complex

1\GINC-PC\SP\RMP2-FC\Gen\C1H4F3N1\RXS501\02-Mar-2000\0\\#MP2/GEN GFI
NPUT SCF=TIGHT TEST MAXDISK=5242880000\\MP2/G3MP2Large single-point ca
lculation on trifluoromethane-ammonia complex\\0,1\N,0,0.,0.,0.\H,0,0.
,0.,2.32574\H,0,0.941355,0.,-0.376846\H,0,-0.470678,-0.815238,-0.37684
6\H,0,-0.470678,0.815238,-0.376846\C,0,0.,0.,3.416515\F,0,1.254489,0.,
3.896864\F,0,-0.627244,1.086419,3.896864\F,0,-0.627244,-1.086419,3.896
864\\Version=SGI-G98RevA.6\State=1-A'\HF=-393.1159925\MP2=-394.2531822
\RMSD=3.868e-09\PG=CS [SG(C1H2F1N1),X(H2F2)]\\@

TABLE S3: GAUSSIAN 98 Archive Entries for the Optimized Geometries of the Anions (Table 6) at the B3-LYP/6-311+G(3df,2p) level

HCCH

```
@122\GINC-PC\SP\RMP2-FC\Gen\C2H1(1-)\SDW501\29-Nov-2000\0\\#MP2/GEN SC
F=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point on acetylene a
nion\\-1,1\C,0,0.,0.,0.\H,0,0.,0.,1.067636\C,0,0.,0.,-1.238822\\Versio
n=SGI64-G98RevA.9\State=1-SG\HF=-76.2320544\MP2=-76.5426746\RMSD=6.742
e-09\PG=C*V [C*(H1C1C1)]\\@
```

FCCH

```
@123\GINC-PC\SP\RMP2-FC\Gen\C2F1(1-)\SDW501\29-Nov-2000\0\\#MP2/GEN SC
F=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation on
 fluoroacetylene anion\\-1,1\C,0,0.,0.,0.\C,0,1.238083,0.,0.\F,0,2.573
727,0.,0.\\Version=SGI64-G98RevA.9\State=1-SG\HF=-175.0962241\MP2=-175
.6500887\RMSD=9.451e-09\PG=C*V [C*(C1C1F1)]\\@
```

H_2CCH_2

```
@124\GINC-PC\SP\RMP2-FC\Gen\C2H3(1-)\SDW501\29-Nov-2000\0\\#MP2/GEN SC
F=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation on
 the ethylene anion\\-1,1\C,0,0.,0.1106465298,0.7730264042\C,0,0.,0.03
59191598,-0.5757060223\H,0,0.,-0.9176394428,1.1979145178\H,0,0.,-0.895
2287872,-1.1771618249\H,0,0.,0.9334740927,-1.2046749839\\Version=SGI64
-G98RevA.9\State=1-A'\HF=-77.3890573\MP2=-77.7281527\RMSD=8.292e-09\PG
=CS [SG(C2H3)]\\@
```

H_2CCFH (X_{a1} = F)

```
@125\GINC-PC\SP\RMP2-FC\Gen\C2H2F1(1-)\SDW501\29-Nov-2000\0\\#MP2/GEN
SCF=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation
on fluoroethylene anion (Xa1=F)\\-1,1\C,0,-0.0182415487,0.6348655152,0
.\C,0,1.1442128728,-0.0471823117,0.\F,0,-1.1158077619,-0.3217873902,0.
\H,0,2.0753914294,0.5096453754,0.\H,0,1.2110504826,-1.1396580845,0.\\V
ersion=SGI64-G98RevA.9\State=1-A'\HF=-176.3035773\MP2=-176.8816028\RMS
D=6.581e-09\PG=CS [SG(C2H2F1)]\\@
```

$HFCCH_2$ (X_{b1} = F)

```
@127\GINC-PC\SP\RMP2-FC\Gen\C2H2F1(1-)\SDW501\30-Nov-2000\0\\#MP2/GEN
SCF=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation
on fluoroethylene anion (Xb1=F)\\-1,1\C,0,0.1253176832,0.3866800171,0.
\C,0,1.2664590557,-0.257946331,0.\F,0,-1.1421871988,-0.3000113832,0.\H
,0,-0.1519169018,1.4442569503,0.\H,0,2.0809412577,0.4834433819,0.\\Ver
sion=SGI64-G98RevA.9\State=1-A'\HF=-176.2959402\MP2=-176.8780595\RMSD=
2.522e-09\PG=CS [SG(C2H2F1)]\\@
```

$HFCCH_2$ (X_{b2} = F)

```
@126\GINC-PC\SP\RMP2-FC\Gen\C2H2F1(1-)\SDW501\29-Nov-2000\0\\#MP2/GEN
SCF=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation
on fluoroethylene anion (Xb1=F)\\-1,1\C,0,0.1714891308,0.452634762,0.\
C,0,1.3532246471,-0.0967471938,0.\F,0,-1.1503523985,-0.2703156004,0.\H
,0,-0.1366276658,1.4915548135,0.\H,0,1.341516585,-1.1940398193,0.\\Ver
sion=SGI64-G98RevA.9\State=1-A'\HF=-176.2945244\MP2=-176.8798301\RMSD=
5.587e-09\PG=CS [SG(C2H2F1)]\\@
```

HFCCFH (X_{a1}, X_{b1} = F)

```
@128\GINC-VPP07\SP\ROMP2-FC\Gen\C2H1F2(1-)\SDW501\30-Nov-2000\0\\#ROMP
2/GEN SCF=TIGHT MAXDISK=19660800\\mp2/g3mp2large single point calculat
ion on difluoroethylene anion (Xa1,Xb1=F)\\-1,1\C,0,-0.1390405557,0.78
32110327,0.\C,0,-0.0359513754,-0.5460389671,0.\F,0,1.2079488933,1.3112
14942,0.\F,0,-1.1859431263,-1.3387888178,0.\H,0,0.8518996831,-1.174867
5105,0.\\Version=Fujitsu-VP-Unix-G98RevA.7\State=1-A'\HF=-275.1926627\
MP2=-276.0085839\RMSD=2.659e-09\PG=CS [SG(C2H1F2)]\\@
```

HFCCFH (X_{a1}, X_{b2} = F)

```
@129\GINC-VPP07\SP\ROMP2-FC\Gen\C2H1F2(1-)\SDW501\30-Nov-2000\0\\#ROMP
2/GEN SCF=TIGHT MAXDISK=19660800\\mp2/g3mp2large single point calculat
ion on difluoroethylene anion (Xa1,Xb2=F)\\-1,1\C,0,0.,-0.7408764501,0
.7548901191\C,0,0.,-0.6450769587,-0.5774014458\F,0,0.,0.5482112133,1.3
705998484\H,0,0.,-1.5033416024,-1.2342816083\F,0,0.,0.5427956817,-1.35
17832297\\Version=Fujitsu-VP-Unix-G98RevA.7\State=1-A'\HF=-275.1929803
\MP2=-276.0102429\RMSD=8.571e-09\PG=CS [SG(C2H1F2)]\\@
```

F_2CCH_2 (X_{b1}, X_{b2} = F)

```
@130\GINC-VPP07\SP\ROMP2-FC\Gen\C2H1F2(1-)\SDW501\30-Nov-2000\0\\#ROMP
2/GEN SCF=TIGHT MAXDISK=19660800\\mp2/g3mp2large single point calculat
ion on difluoroethylene anion (Xb1,Xb2=F)\\-1,1\C,0,0.,-0.0312913261,0
.2065659038\C,0,0.,-0.0848151313,1.5059298574\F,0,0.,1.0684617796,-0.6
83417227\F,0,0.,-1.0937889878,-0.6725751552\H,0,0.,0.9245836174,1.9289
568732\\Version=Fujitsu-VP-Unix-G98RevA.7\State=1-A'\HF=-275.1979294\M
P2=-276.0214768\RMSD=7.269e-09\PG=CS [SG(C2H1F2)]\\@
```

F_2CCFH

```
@131\GINC-PC\SP\ROMP2-FC\Gen\C2F3(1-)\SDW501\01-Dec-2000\0\\#ROMP2/GEN
 SCF=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation
 on trifluoroethylene anion\\-1,1\C,0,-0.8783899049,-0.7099851784,0.\C
,0,-0.0960595245,0.3644644718,0.\F,0,-0.0528677285,-1.8819209351,0.\F,
0,-0.5729054234,1.6394969392,0.\F,0,1.275406105,0.4727711335,0.\\Versi
on=SGI64-G98RevA.9\State=1-A'\HF=-374.0863541\MP2=-375.1427291\RMSD=8.
811e-09\PG=CS [SG(C2F3)]\\@
```

H_3CCH_3

```
@132\GINC-PC\SP\RMP2-FC\Gen\C2H5(1-)\SDW501\29-Nov-2000\0\\#MP2/GEN SC
F=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation on
 ethane anion\\-1,1\C,0,0.,0.0782113227,0.8397454353\C,0,0.,0.03969990
21,-0.688900954\H,0,0.,-0.9616258425,-1.196504817\H,0,-0.8857739119,-0
.4369501783,1.2456380921\H,0,0.8857739119,-0.4369501783,1.2456380921\H
,0,-0.8736072951,0.5640294251,-1.0999191276\H,0,0.8736072951,0.5640294
251,-1.0999191276\\Version=SGI64-G98RevA.9\State=1-A'\HF=-78.5596779\M
P2=-78.9358612\RMSD=5.031e-09\PG=CS [SG(C2H1),X(H4)]\\@
```

H_3CCFH_2 (X_{a1} = F)

```
@133\GINC-VPP07\SP\RMP2-FC\Gen\C2H4F1(1-)\SDW501\29-Nov-2000\0\\#MP2/G
EN SCF=TIGHT MAXDISK=19660800\\mp2/g3mp2large single point calculation
 on fluoroethane (Xa1=F)\\-1,1\C,0,0.0269122869,0.6701170581,0.1374907
574\C,0,1.1176703417,-0.3835277649,0.0546354399\F,0,-1.2469649872,-0.1
099305994,-0.0512373818\H,0,2.0862743228,0.1305389517,-0.0025139111\H,
0,0.0636807266,1.23255581,-0.8138652873\H,0,1.1497858816,-1.0197841181
,0.9462871152\H,0,1.0554481829,-1.0734710076,-0.8215286647\\Version=Fu
jitsu-VP-Unix-G98RevA.7\HF=-177.460837\MP2=-178.0717936\RMSD=1.492e-09
\PG=C01 [X(C2H4F1)]\\@
```

H_3CCF_2H (X_{a1}, X_{a2} = F)

```
@134\GINC-PC\SP\RMP2-FC\Gen\C2H3F2(1-)\SDW501\04-Dec-2000\0\\#MP2/GEN
SCF=TIGHT GUESS=READ MAXDISK=5242880000\\mp2/g3mp2large single point c
alculations on difluoroethane anion (Xa1,Xa2=F)\\-1,1\C,0,-0.016728796
9,0.5512320134,0.\C,0,-1.3121453918,-0.2511776221,0.\H,0,-1.132330231,
-1.3436357804,0.\F,0,0.7167909938,-0.0262630305,1.1213786175\F,0,0.716
7909938,-0.0262630305,-1.1213786175\H,0,-1.8983312629,0.0080219908,0.8
846402829\H,0,-1.8983312629,0.0080219908,-0.8846402829\\Version=SGI64-
G98RevA.9\State=1-A'\HF=-276.3816763\MP2=-277.2315571\RMSD=4.356e-09\P
G=CS [SG(C2H1),X(H2F2)]\\@
```

F_3CCH_3 (X_{b1}, X_{b2}, X_{b3} = F)

```
@135\GINC-VPP02\SP\RMP2-FC\Gen\C2H2F3(1-)\SDW501\04-Dec-2000\0\\#MP2/G
EN SCF=TIGHT MAXDISK=30146560\\mp2/g3mp2large single point on trifluor
oethane anion (Xb1,Xb2,Xb3=F)\\-1,1\C,0,0.,-0.0490534325,0.129831304\C
,0,0.,0.0060773163,1.5338551302\F,0,0.,1.2335836643,-0.6659964169\F,0,
1.1043100609,-0.6466328829,-0.439983237\F,0,-1.1043100609,-0.646632882
9,-0.439983237\H,0,0.9151444118,0.3974978059,1.9657737058\H,0,-0.91514
44118,0.3974978059,1.9657737058\\Version=Fujitsu-VP-Unix-G98RevA.7\Sta
te=1-A'\HF=-375.3027787\MP2=-376.4002764\RMSD=3.724e-09\PG=CS [SG(C2F1
),X(H2F2)]\\@
```

FH_2CCF_2H ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$ = F)

```
@2\GINC-SC39\SP\ROMP2-FC\GTMP2Large\C2H2F3(1-)\SDW501\01-May-2001\0\\#
ROMP2/GTMP2LARGE SCF=TIGHT MAXDISK=117964800\\RMP2/G3MP2large single-p
oint calculation on a,a,b-ethane anion\\-1,1\H,0,-1.2855927687,-0.8404
338216,0.0292776106\C,0,-0.1933382335,-0.8835216527,0.1729945797\C,0,0
.4705412284,0.4736818732,0.1210950498\H,0,0.0440842676,-1.357569509,1.
1266369434\F,0,0.2899756658,-1.7399088592,-0.8457403434\F,0,-0.0168050
071,1.0544508001,1.3681028943\F,0,-0.3200272663,1.202907171,-0.8468572
543\\Version=DEC-AXP-OSF/1-G98RevA.9\HF=-375.2762049\MP2=-376.3615612\
RMSD=5.459e-09\PG=C01 [X(C2H2F3)]\\@
```

F_2HCCF_2H ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$, $X_{\beta3}$ = F)

@5\GINC-SC3\SP\ROMP2-FC\GTMP2Large\C2H1F4(1-)\SDW501\01-May-2001\0\\#R
OMP2/GTMP2LARGE SCF=TIGHT MAXDISK=131072000\\RMP2/6-31G(d) single-poin
t calculation on a,a,b,b-tetrafluoroethane anion\\-1,1\C,0,-0.47688845
95,-0.7226386131,0.\C,0,0.2141653523,0.62455023,0.\H,0,1.3145339496,0.
5925431158,0.\F,0,0.1765509606,-1.3650374923,1.1172273449\F,0,0.176550
9606,-1.3650374923,-1.1172273449\F,0,-0.1620062554,1.364814558,1.10311
83031\F,0,-0.1620062554,1.364814558,-1.1031183031\\Version=DEC-AXP-OSF
/1-G98RevA.9\State=1-A'\HF=-474.1852786\MP2=-475.5082083\RMSD=7.905e-0
9\PG=CS [SG(C2H1),X(F4)]\\@

F_3CCF_2H

@136\GINC-VPP07\SP\RMP2-FC\Gen\C2F5(1-)\SDW501\05-Dec-2000\0\\#MP2/GEN
SCF=TIGHT MAXDISK=4194304000\\mp2/g3mp2large single point calculation
on pentafluoroethane \\-1,1\C,0,0.6054463897,-0.879993623,0.\C,0,0.06
76455095,0.5393463165,0.\F,0,-1.3021533094,0.7157491676,0.\F,0,-0.0733
655549,-1.470480551,1.1145644854\F,0,-0.0733655549,-1.470480551,-1.114
5644854\F,0,0.5000782432,1.2261550694,1.08858008\F,0,0.5000782432,1.22
61550694,-1.08858008\\Version=Fujitsu-VP-Unix-G98RevA.7\State=1-A'\HF=
-573.0971924\MP2=-574.6584248\RMSD=4.036e-09\PG=CS [SG(C2F1),X(F4)]\\@

CH_4

@137\GINC-PC\SP\RMP2-FC\Gen\C1H3(1-)\SDW501\30-Nov-2000\0\\#MP2/GEN SC
F=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point on methane ani
on\\-1,1\C,0,0.0721783959,-0.0721783959,-0.0721783959\H,0,0.7008803431
,0.5669753593,0.5669753593\H,0,-0.5669753593,-0.7008803431,0.566975359
3\H,0,-0.5669753593,0.5669753593,-0.7008803431\\Version=SGI64-G98RevA.
9\State=1-A1\HF=-39.5213319\MP2=-39.7267378\RMSD=6.196e-09\PG=C03V [C3
(C1),3SGV(HI)]\\@

FCH_3

@138\GINC-PC\SP\RMP2-FC\Gen\C1H2F1(1-)\SDW501\30-Nov-2000\0\\#MP2/GEN
SCF=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation
on fluoromethane anion\\-1,1\C,0,0.,0.1295139319,-0.7628132721\F,0,0.,
0.0244095409,0.7379831379\H,0,0.8751431389,-0.4983847297,-1.0324843042
\H,0,-0.8751431389,-0.4983847297,-1.0324843042\\Version=SGI64-G98RevA.
9\State=1-A'\HF=-138.4101263\MP2=-138.8494884\RMSD=8.847e-10\PG=CS [SG
(C1F1),X(H2)]\\@

F_2CH_2

@139\GINC-PC\SP\RMP2-FC\Gen\C1H1F2(1-)\SDW501\01-Dec-2000\0\\#MP2/GEN
SCF=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation
on difluoromethane anion\\-1,1\H,0,0.892905833,0.,1.0787973274\C,0,-0.
1367897971,0.,0.6486643857\F,0,-0.0040092806,1.1324303516,-0.276154646
7\F,0,-0.0040092806,-1.1324303516,-0.2761546467\\Version=SGI64-G98RevA
.9\State=1-A'\HF=-237.3234377\MP2=-238.0012034\RMSD=7.966e-09\PG=CS [S
G(C1H1),X(F2)]\\@

F_3CH

@140\GINC-PC\SP\RMP2-FC\Gen\C1F3(1-)\SDW501\01-Dec-2000\0\\#MP2/GEN SC
F=TIGHT MAXDISK=5242880000\\mp2/g3mp2large single point calculation on
 trifluoromethane anion\\-1,1\C,0,0.,0.,0.5465846034\F,0,-0.0000003065
,1.2641676591,-0.1214632452\F,0,-1.0948011541,-0.632084095,-0.12146324
52\F,0,1.0948014606,-0.6320835641,-0.1214632452\\Version=SGI64-G98RevA
.9\State=1-A1\HF=-336.2589331\MP2=-337.1769691\RMSD=6.143e-09\PG=C03V
[C3(C1),3SGV(F1)]\\@

TABLE S4: Total Energies and BSSE Contributions Used For Tables 2 - 5 Obtained From B3-LYP/6-311+G(3df,2p) Geometries[a]

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
$HCCH\cdots NH_3$			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{HCCH}	-77.092770	-77.154156	-77.065885
$E_{HCCH\cdots NH_3}$	-133.473102	-133.608609	-133.428657
$E_{NH_3}^{monomer}$	-56.371902	-56.448262	-56.354160
$E_{HCCH}^{monomer}$	-77.092960	-77.154174	-77.066021
$E_{NH_3}^{full}$	-56.374108	-56.448954	-56.356228
E_{HCCH}^{full}	-77.093216	-77.154334	-77.066272
BSSE	-0.002463	-0.000852	-0.002319
$FCCH\cdots NH_3$			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{FCCH}	-176.085786	-176.254340	-176.059046
$E_{FCCH\cdots NH_3}$	-232.466811	-232.709332	-232.422470
$E_{NH_3}^{monomer}$	-56.371900	-56.448262	-56.354159
$E_{FCCH}^{monomer}$	-176.086139	-176.254316	-176.059318
$E_{NH_3}^{full}$	-56.374133	-56.448980	-56.356251
E_{FCCH}^{full}	-176.086448	-176.254664	-176.059622
BSSE	-0.002542	-0.001065	-0.002396

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
H_2CCH_2•••NH_3			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{H_2CCH_2}$	-78.321524	-78.390916	-78.284855
$E_{H_2CCH_2\cdots NH_3}$	-134.696663	-134.841409	-134.642288
$E_{NH_3}^{monomer}$	-56.371880	-56.448262	-56.354147
$E_{H_2CCH_2}^{monomer}$	-78.321566	-78.390908	-78.284870
$E_{NH_3}^{full}$	-56.373322	-56.448598	-56.355556
$E_{H_2CCH_2}^{full}$	-78.321727	-78.390999	-78.285024
BSSE	-0.001602	-0.000427	-0.001563
H_2CCFH•••NH_3 ($X_{\alpha 1}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{H_2CCFH}	-177.339828	-177.517076	-177.303166
$E_{H_2CCFH\cdots NH_3}$	-233.717670	-233.969904	-233.663356
$E_{NH_3}^{monomer}$	-56.371899	-56.448264	-56.354160
$E_{H_2CCFH}^{monomer}$	-177.339940	-177.516996	-177.303213
$E_{NH_3}^{full}$	-56.373584	-56.448760	-56.355764
$E_{H_2CCFH}^{full}$	-177.340135	-177.517205	-177.303390
BSSE	-0.001879	-0.000704	-0.001782
$HFCCH_2$•••NH_3 ($X_{\beta 1}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{HFCCH_2}	-177.339828	-177.517076	-177.303166
$E_{HFCCH_2\cdots NH_3}$	-233.716235	-233.968688	-233.661837
$E_{NH_3}^{monomer}$	-56.371888	-56.448265	-56.354153
$E_{HFCCH_2}^{monomer}$	-177.339862	-177.516987	-177.303161
$E_{NH_3}^{full}$	-56.373444	-56.448676	-56.355652
$E_{HFCCH_2}^{full}$	-177.340078	-177.517142	-177.303364
BSSE	-0.001772	-0.000566	-0.001702

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
$HFCCH_2\cdots NH_3$ ($X_{\beta 2}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{HFCCH_2}	-177.339828	-177.517076	-177.303166
$E_{HFCCH_2\cdots NH_3}$	-233.7164656	-233.9687555	-233.6620733
$E_{NH_3}^{monomer}$	-56.37189943	-56.4482648	-56.35416015
$E_{HFCCH_2}^{monomer}$	-177.3398973	-177.5170083	-177.3032093
$E_{NH_3}^{full}$	-56.3734293	-56.4486704	-56.35563433
$E_{HFCCH_2}^{full}$	-177.3401039	-177.5171529	-177.3034043
BSSE	-0.00173646	-0.0005502	-0.00166923
$HFCCFH\cdots NH_3$ ($X_{\alpha 1}$, $X_{\beta 1}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{HFCCFH}	-276.347754	-276.630361	-276.310017
$E_{HFCCFH\cdots NH_3}$	-332.726775	-333.084133	-332.671365
$E_{NH_3}^{monomer}$	-56.371900	-56.448263	-56.354160
$E_{HFCCFH}^{monomer}$	-276.347944	-276.630230	-276.310129
$E_{NH_3}^{full}$	-56.373671	-56.448828	-56.355831
E_{HFCCFH}^{full}	-276.348191	-276.630523	-276.310356
BSSE	-0.002018	-0.000859	-0.001898
$HFCCFH\cdots NH_3$ ($X_{\alpha 1}$, $X_{\beta 2}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{HFCCFH}	-276.347193	-276.632190	-276.309720
$E_{HFCCFH\cdots NH_3}$	-332.726450	-333.086076	-332.671305
$E_{NH_3}^{monomer}$	-56.371914	-56.448262	-56.354168
$E_{HFCCFH}^{monomer}$	-276.347382	-276.632075	-276.309855
$E_{NH_3}^{full}$	-56.373676	-56.448803	-56.355836
E_{HFCCFH}^{full}	-276.347617	-276.632364	-276.310069
BSSE	-0.001996	-0.000831	-0.001882

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
F_2CCH_2•••NH_3 ($X_{\beta1}$, $X_{\beta2}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{F_2CCH_2}$	-276.364999	-276.648621	-276.329053
$E_{F_2CCH_2\cdots NH_3}$	-332.742582	-333.101109	-332.688861
$E_{NH_3}^{monomer}$	-56.371899	-56.448264	-56.354159
$E_{F_2CCH_2}^{monomer}$	-276.365110	-276.648495	-276.329118
$E_{NH_3}^{full}$	-56.373508	-56.448734	-56.355694
$E_{F_2CCH_2}^{full}$	-276.365371	-276.648707	-276.329368
BSSE	-0.001870	-0.000682	-0.001785
F_2CCFH•••NH_3 ($X_{\alpha1}$, $X_{\beta1}$, $X_{\beta2}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{F_2CCFH}	-375.365842	-375.755695	-375.328385
$E_{F_2CCFH\cdots NH_3}$	-431.746012	-432.210315	-431.690833
$E_{NH_3}^{monomer}$	-56.371911	-56.448262	-56.354166
$E_{F_2CCFH}^{monomer}$	-375.366106	-375.755505	-375.328572
$E_{NH_3}^{full}$	-56.373732	-56.448868	-56.355880
$E_{F_2CCFH}^{full}$	-375.366396	-375.755882	-375.328841
BSSE	-0.002110	-0.000983	-0.001982
H_3CCH_3•••NH_3			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{H_3CCH_3}$	-79.534310	-79.617688	-79.494707
$E_{H_3CCH_3\cdots NH_3}$	-135.908151	-136.067118	-135.850837
$E_{NH_3}^{monomer}$	-56.371878	-56.448267	-56.354148
$E_{H_3CCH_3}^{monomer}$	-79.534321	-79.617677	-79.494708
$E_{NH_3}^{full}$	-56.373067	-56.448515	-56.355355
$E_{H_3CCH_3}^{full}$	-79.534422	-79.617734	-79.494807
BSSE	-0.001289	-0.000304	-0.001306

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
H_3CCFH_2•••NH_3 ($X_{\alpha 1}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{H_3CCFH_2}$	-178.549127	-178.741140	-178.508606
$E_{H_3CCFH_2 \cdots NH_3}$	-234.925118	-235.192448	-234.866855
$E_{NH_3}^{monomer}$	-56.371895	-56.448265	-56.354157
$E_{H_3CCFH_2}^{monomer}$	-178.549130	-178.741075	-178.508597
$E_{NH_3}^{full}$	-56.373387	-56.448613	-56.355616
$E_{H_3CCFH_2}^{full}$	-178.549318	-178.741239	-178.508770
BSSE	-0.001680	-0.000512	-0.001632
H_2FCCH_3•••NH_3 ($X_{\beta 2}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{H_2FCCH_3}$	-178.549127	-178.741140	-178.508606
$E_{H_2FCCH_3 \cdots NH_3}$	-234.924521	-235.191955	-234.866289
$E_{NH_3}^{monomer}$	-56.371892	-56.448264	-56.354155
$E_{H_2FCCH_3}^{monomer}$	-178.549093	-178.741085	-178.508561
$E_{NH_3}^{full}$	-56.373307	-56.448567	-56.355557
$E_{H_2FCCH_3}^{full}$	-178.549289	-178.741212	-178.508746
BSSE	-0.001612	-0.000429	-0.001587
H_2FCCH_3•••NH_3 ($X_{\beta 1}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{H_2FCCH_3}$	-178.5491273	-178.7411401	-178.5086062
$E_{H_2FCCH_3 \cdots NH_3}$	-234.9247648	-235.1920876	-234.8665328
$E_{NH_3}^{monomer}$	-56.37190441	-56.4482648	-56.3541633
$E_{H_2FCCH_3}^{monomer}$	-178.5491153	-178.7410934	-178.5085901
$E_{NH_3}^{full}$	-56.37329381	-56.4485914	-56.35553682
$E_{H_2FCCH_3}^{full}$	-178.5492737	-178.7412002	-178.5087364
BSSE	-0.00154778	-0.0004334	-0.00151983

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
HF_2CCH_3•••NH_3 ($X_{\beta1}$, $X_{\beta2}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{HF_2CCH_3}$	-277.583943	-277.880928	-277.543254
$E_{HF_2CCH_3\cdots NH_3}$	-333.960447	-334.332783	-333.902063
$E_{NH_3}^{monomer}$	-56.371892	-56.448264	-56.354155
$E_{HF_2CCH_3}^{monomer}$	-277.583884	-277.880823	-277.543182
$E_{NH_3}^{full}$	-56.373424	-56.448644	-56.355644
$E_{HF_2CCH_3}^{full}$	-277.584149	-277.881039	-277.543427
BSSE	-0.001797	-0.000597	-0.001734
H_2FCCFH_2•••NH_3 ($X_{\alpha1}$, $X_{\beta1}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{H_2FCCFH_2}$	-277.559643	-277.859860	-277.518040
$E_{H_2FCCFH_2\cdots NH_3}$	-333.937328	-334.312658	-333.878006
$E_{NH_3}^{monomer}$	-56.371916	-56.448262	-56.354169
$E_{H_2FCCFH_2}^{monomer}$	-277.559630	-277.859748	-277.518021
$E_{NH_3}^{full}$	-56.373496	-56.448690	-56.355694
$E_{H_2FCCFH_2}^{full}$	-277.559859	-277.859748	-277.518225
BSSE	-0.001808	-0.000427	-0.001728
H_3CCF_2H•••NH_3 ($X_{\alpha1}$, $X_{\alpha2}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{H_3CCF_2H}$	-277.583943	-277.880928	-277.543254
$E_{H_3CCF_2H\cdots NH_3}$	-333.961784	-334.334002	-333.903351
$E_{NH_3}^{monomer}$	-56.371903	-56.448263	-56.354162
$E_{H_3CCF_2H}^{monomer}$	-277.583975	-277.880792	-277.543274
$E_{NH_3}^{full}$	-56.373568	-56.448751	-56.355750
$E_{H_3CCF_2H}^{full}$	-277.584208	-277.881083	-277.543482
BSSE	-0.001897	-0.000779	-0.001797

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
F_3CCH_3•••NH_3 ($X_{\beta1}$, $X_{\beta2}$, $X_{\beta3}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{F_3CCH_3}$	-376.627703	-377.027173	-376.587155
$E_{F_3CCH_3\cdots NH_3}$	-433.005425	-433.480011	-432.947197
$E_{NH_3}^{monomer}$	-56.371907	-56.448263	-56.354164
$E_{F_3CCH_3}^{monomer}$	-376.627701	-377.027052	-376.587145
$E_{NH_3}^{full}$	-56.373475	-56.448731	-56.355670
$E_{F_3CCH_3}^{full}$	-376.627978	-377.027273	-376.587399
BSSE	-0.001845	-0.000688	-0.001760
FH_2CCF_2H•••NH_3 ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{FH_2CCF_2H}$	-376.5912381	-376.9952627	-376.5492549
$E_{FH_2CCF_2H\cdots NH_3}$	-432.9702951	-433.4494421	-432.9105954
$E_{NH_3}^{monomer}$	-56.3719046	-56.4482619	-56.35416225
$E_{FH_2CCF_2H}^{monomer}$	-376.5913055	-376.9950991	-376.5493029
$E_{NH_3}^{full}$	-56.37365122	-56.4488314	-56.35581537
$E_{FH_2CCF_2H}^{full}$	-376.5915994	-376.9954804	-376.5495671
BSSE	-0.00204058	-0.0009508	-0.00191732
F_2HCCF_2H•••NH_3 ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$, $X_{\beta3}$ = F)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{F_2HCCF_2H}$	-475.6199911	-476.1281521	-475.5776496
$E_{F_3CCH_3\cdots NH_3}$	-532.0002016	-532.5833956	-531.9401727
$E_{NH_3}^{monomer}$	-56.37190536	-56.4482613	-56.35416246
$E_{F_2HCCF_2H}^{monomer}$	-475.6200918	-476.1279418	-475.5777227
$E_{NH_3}^{full}$	-56.37374828	-56.4489025	-56.35589814
$E_{F_2HCCF_2H}^{full}$	-475.6204379	-476.1284154	-475.5780347
BSSE	-0.00218906	-0.0011148	-0.00204764

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
$F_3CCF_2H\cdots NH_3$			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{F_3CCF_2H}$	-574.657011	-575.267841	-574.614778
$E_{F_3CCF_2H\cdots NH_3}$	-631.038575	-631.724258	-630.978676
$E_{NH_3}^{monomer}$	-56.371919	-56.448260	-56.354170
$E_{F_3CCF_2H}^{monomer}$	-574.657212	-575.267592	-574.614955
$E_{NH_3}^{full}$	-56.373817	-56.448936	-56.355955
$E_{F_3CCF_2H}^{full}$	-574.657594	-575.268131	-574.615299
BSSE	-0.002280	-0.001216	-0.002129
$CH_4\cdots NH_3$			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{CH_4}	-40.355801	-40.404281	-40.332542
$E_{CH_4\cdots NH_3}$	-96.729820	-96.853743	-96.688842
$E_{NH_3}^{monomer}$	-56.371880	-56.448267	-56.354149
$E_{CH_4}^{monomer}$	-40.355816	-40.404266	-40.332542
$E_{NH_3}^{full}$	-56.373139	-56.448515	-56.355416
$E_{CH_4}^{full}$	-40.355919	-40.404314	-40.332639
BSSE	-0.001362	-0.000295	-0.001364

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
FCH_3•••NH_3 (fixed linear hydrogen bond)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{FCH_3}	-139.360124	-139.518154	-139.335807
$E_{FCH_3•••NH_3}$	-195.736346	-195.969534	-195.694297
$E_{NH_3}^{monomer}$	-56.371897	-56.448265	-56.354159
$E_{FCH_3}^{monomer}$	-139.360127	-139.518087	-139.335791
$E_{NH_3}^{full}$	-56.373379	-56.448598	-56.355602
$E_{FCH_3}^{full}$	-139.360287	-139.518237	-139.335931
BSSE	-0.001641	-0.000484	-0.001583
FCH_3•••NH_3 (nonlinear hydrogen bond)			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{FCH_3}	-139.360124	-139.518154	-139.335807
$E_{FCH_3•••NH_3}$	-195.739223	-195.971242	-195.697322
$E_{NH_3}^{monomer}$	-56.371873	-56.448258	-56.354141
$E_{FCH_3}^{monomer}$	-139.360059	-139.518061	-139.335731
$E_{NH_3}^{full}$	-56.373190	-56.448549	-56.355464
$E_{FCH_3}^{full}$	-139.362831	-139.518550	-139.338561
BSSE	-0.004089	-0.000780	-0.004153
F_2CH_2•••NH_3			
E_{NH_3}	-56.371769	-56.448198	-56.354050
$E_{F_2CH_2}$	-238.388435	-238.652511	-238.363965
$E_{F_2CH_2•••NH_3}$	-294.766587	-295.105830	-294.724402
$E_{NH_3}^{monomer}$	-56.371907	-56.448263	-56.354164
$E_{F_2CH_2}^{monomer}$	-238.388431	-238.652364	-238.363937
$E_{NH_3}^{full}$	-56.373554	-56.448735	-56.355734
$E_{F_2CH_2}^{full}$	-238.388635	-238.652610	-238.364112
BSSE	-0.001852	-0.000718	-0.001744

	CCSD(T)/6-31G(d)	MP2/G3MP2large	MP2/6-31G(d)
$F_3CH\cdots NH_3$			
E_{NH_3}	-56.371769	-56.448198	-56.354050
E_{F_3CH}	-337.431185	-337.797610	-337.406981
$E_{F_3CH\cdots NH_3}$	-393.812009	-394.253182	-393.770128
$E_{NH_3}^{monomer}$	-56.371917	-56.448260	-56.354170
$E_{F_3CH}^{monomer}$	-337.431232	-337.797331	-337.406996
$E_{NH_3}^{full}$	-56.373779	-56.448866	-56.355919
$E_{F_3CH}^{full}$	-337.431454	-337.797726	-337.407186
BSSE	-0.002084	-0.001000	-0.001940

[a]All energies are given in hartrees.

TABLE S5: Total Energies and ZPVEs of the Anions Used for Table 6[a]

Anion	CCSD(T)/ 6-31G(d)	MP2/ G3MP2large	MP2/ 6-31G(d)	ZPVE
HCCH	-76.449203	-76.542675	-76.422956	0.014465
FCCH	-175.456647	-175.650089	-175.429899	0.008207
H_2CCH_2	-77.621704	-77.728153	-77.586037	0.035436
H_2CCFH ($X_{\alpha1}$ = F)	-176.673804	-176.881603	-176.637517	0.043892
$HFCCH_2$ ($X_{\beta1}$ = F)	-176.666080	-176.878060	-176.630715	0.028846
$HFCCH_2$ ($X_{\beta2}$ = F)	-176.669590	-176.879830	-176.633976	0.028694
HFCCFH ($X_{\alpha1}$, $X_{\beta1}$ = F)	-275.699109	-276.008584	-275.661604	0.021951
HFCCFH ($X_{\alpha1}$, $X_{\beta2}$ = F)	-275.700097	-276.010243	-275.662576	0.022386
F_2CCH_2 ($X_{\beta1}$, $X_{\beta2}$ = F)	-275.708985	-276.021477	-275.674147	0.021969
F_2CCFH	-374.730731	-375.142729	-374.692893	0.014859
H_3CCH_3	-78.806417	-78.935861	-78.768322	0.057276
H_3CCFH_2 ($X_{\alpha1}$ = F)	-177.846990	-178.071794	-177.806505	0.050874
H_3CCF_2H ($X_{\alpha1}$, $X_{\alpha2}$ = F)	-276.905513	-277.231557	-276.864027	0.043965
FH_2CCF_2H ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$ = F)	-375.931185	-376.361561	-375.888517	0.037264
F_2HCCF_2H ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$, $X_{\beta3}$ = F)	-474.975689	-475.508208	-474.932807	0.029818
F_3CCH_3 ($X_{\beta1}$, $X_{\beta2}$, $X_{\beta3}$ = F)	-375.966496	-376.400276	-375.929678	0.035636
F_3CCF_2H	-574.025140	-574.658425	-573.982441	0.021651
CH_4	-39.620891	-39.726738	-39.599392	0.028472
FCH_3	-138.654811	-138.849488	-138.630580	0.022875
F_2CH_2	-237.709557	-238.001203	-237.684230	0.016452
F_3CH	-336.784312	-337.176960	-336.759074	0.008968

[a]All energies are given in hartrees.

TABLE S6: B3-LYP/6-311+G(3df,2p) ZPVEs and Scale Factors of the Monomers Used for Tables 2 – 5[a]

Monomer		Monomer	
$ZPVE^{calc}_{NH_3}$	0.034240		
$ZPVE^{ref}_{NH_3}$	0.033880		
sf_{NH_3}	0.989486		
$ZPVE^{calc}_{HCCH}$	0.026977	$ZPVE^{calc}_{FCCH}$	0.020427
$ZPVE^{ref}_{HCCH}$	0.026227	$ZPVE^{ref}_{FCCH}$	0.020110
sf_{HCCH}	0.972199	sf_{FCCH}	0.984470
$ZPVE^{calc}_{H_2CCH_2}$	0.050874	$ZPVE^{calc}_{H_2CCFH}$	0.043892
$ZPVE^{ref}_{H_2CCH_2}$	0.050358	$ZPVE^{ref}_{H_2CCFH}$	0.043273
$sf_{H_2CCH_2}$	0.989857	sf_{H_2CCFH}	0.985898
$ZPVE^{calc}_{HFCCFH}$ ($X_{\alpha 1}$, $X_{\beta 1}$ = F)	0.036590	$ZPVE^{calc}_{HFCCFH}$ ($X_{\alpha 1}$, $X_{\beta 2}$ = F)	0.036986
$ZPVE^{ref}_{HFCCFH}$ ($X_{\alpha 1}$, $X_{\beta 1}$ = F)	0.036074	$ZPVE^{ref}_{HFCCFH}$ ($X_{\alpha 1}$, $X_{\beta 2}$ = F)	0.036419
sf_{HFCCFH} ($X_{\alpha 1}$, $X_{\beta 1}$ = F)	0.985888	sf_{HFCCFH} ($X_{\alpha 1}$, $X_{\beta 2}$ = F)	0.984680
$ZPVE^{calc}_{F_2CCH_2}$ ($X_{\beta 1}$, $X_{\beta 2}$ = F)	0.036546	$ZPVE^{calc}_{F_2CCFH}$ ($X_{\alpha 1}$, $X_{\beta 1}$, $X_{\beta 2}$ = F)	0.029271
$ZPVE^{ref}_{F_2CCH_2}$ ($X_{\beta 1}$, $X_{\beta 2}$ = F)	0.036074	$ZPVE^{ref}_{F_2CCFH}$ ($X_{\alpha 1}$, $X_{\beta 1}$, $X_{\beta 2}$ = F)	0.028857
$sf_{F_2CCH_2}$ ($X_{\beta 1}$, $X_{\beta 2}$ = F)	0.987075	sf_{F_2CCFH} ($X_{\alpha 1}$, $X_{\beta 1}$, $X_{\beta 2}$ = F)	0.985841
$ZPVE^{calc}_{H_3CCH_3}$	0.074295	$ZPVE^{calc}_{H_3CCFH_2}$	0.067607
$ZPVE^{ref}_{H_3CCH_3}$	0.073259	$ZPVE^{ref}_{H_3CCFH_2}$	0.066692
$sf_{H_3CCH_3}$	0.986061	$sf_{H_3CCFH_2}$	0.986472
$ZPVE^{calc}_{F_2HCCH_3}$ ($X_{\beta 2}$,$X_{\beta 3}$ or $X_{\alpha 1}$,$X_{\alpha 2}$ = F)	0.060125	$ZPVE^{calc}_{H_2FCCFH_2}$ ($X_{\alpha 1}$, $X_{\beta 1}$ = F)	0.060696
$ZPVE^{ref}_{F_2HCCH_3}$ ($X_{\beta 2}$,$X_{\beta 3}$ or $X_{\alpha 1}$,$X_{\alpha 2}$ = F)	0.059335	$ZPVE^{ref}_{H_2FCCFH_2}$ ($X_{\alpha 1}$, $X_{\beta 1}$ = F)	0.059885
$sf_{F_2HCCH_3}$ ($X_{\beta 2}$,$X_{\beta 3}$ or $X_{\alpha 1}$,$X_{\alpha 2}$ = F)	0.986868	$sf_{H_2FCCFH_2}$ ($X_{\alpha 1}$, $X_{\beta 1}$ = F)	0.986639

Monomer		Monomer	
$ZPVE^{calc}_{FH_2CCF_2H}$ ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$ = F)	0.053178	$ZPVE^{calc}_{F_2HCCF_2H}$ ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$, $X_{\beta3}$ = F)	0.045432
$ZPVE^{ref}_{FH_2CCF_2H}$ ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$ = F)	0.052476	$ZPVE^{ref}_{F_2HCCF_2H}$ ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$, $X_{\beta3}$ = F)	0.0448500
$sf_{FH_2CCF_2H}$ ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$ = F)	0.986797	$sf_{F_2HCCF_2H}$ ($X_{\alpha1}$, $X_{\alpha2}$, $X_{\beta2}$, $X_{\beta3}$ = F)	0.987190
$ZPVE^{calc}_{F_3CCH_3}$ ($X_{\beta1}$, $X_{\beta2}$, $X_{\beta3}$ = F)	0.052005	$ZPVE^{calc}_{F_3CCF_2H}$	0.037273
$ZPVE^{ref}_{F_3CCH_3}$ ($X_{\beta1}$, $X_{\beta2}$, $X_{\beta3}$ = F)	0.051336	$ZPVE^{ref}_{F_3CCF_2H}$	0.036808
$sf_{F_3CCH_3}$ ($X_{\beta1}$, $X_{\beta2}$, $X_{\beta3}$ = F)	0.987140	$sf_{F_3CCF_2H}$	1.002576
$ZPVE^{calc}_{CH_4}$	0.044570	$ZPVE^{calc}_{FCH_3}$	0.039105
$ZPVE^{ref}_{CH_4}$	0.043983	$ZPVE^{ref}_{FCH_3}$	0.039207
sf_{CH_4}	0.986830	sf_{FCH_3}	1.002607
$ZPVE^{calc}_{F_2CH_2}$	0.032577	$ZPVE^{calc}_{F_3CH}$	0.025022
$ZPVE^{ref}_{F_2CH_2}$	0.032160	$ZPVE^{ref}_{F_3CH}$	0.024755
$sf_{F_2CH_2}$	0.987207	$sf_{F_3CH_2}$	0.989330

[a]All energies are given in hartrees.

TABLE S7: B3-LYP/6-311+G(3df,2p) ZPVEs and Scale Factors of the Ammonia Complexes Used for Tables 2 – 5[a]

Dimer		Dimer	
$ZPVE^{calc}_{HCCH\cdots NH_3}$	0.063061	$ZPVE^{calc}_{FCCH\cdots NH_3}$	0.056402
$sf_{HCCH\cdots NH_3}$	0.981868	$sf_{FCCH\cdots NH_3}$	0.987612
$ZPVE^{calc}_{H_2CCH_2\cdots NH_3}$	0.086277	$ZPVE^{calc}_{H_2CCFH\cdots NH_3}$ ($X_{\alpha 1}$ = F)	0.079504
$sf_{H_2CCH_2\cdots NH_3}$	0.989708	$sf_{H_2CCFH\cdots NH_3}$	0.987470
$ZPVE^{calc}_{HFCCH_2\cdots NH_3}$ ($X_{\beta 1}$ = F)	0.079325	$ZPVE^{calc}_{HFCCH_2\cdots NH_3}$ ($X_{\beta 2}$ = F)	0.079331
$sf_{HFCCH_2\cdots NH_3}$	0.987470	$sf_{HFCCH_2\cdots NH_3}$	0.987470
$ZPVE^{calc}_{HFCCFH\cdots NH_3}$ ($X_{\alpha 1}$, $X_{\beta 1}$ = F)	0.072323	$ZPVE^{calc}_{HFCCFH\cdots NH_3}$ ($X_{\alpha 1}$, $X_{\beta 2}$ = F)	0.072648
$sf_{HFCCFH\cdots NH_3}$	0.987627	$sf_{HFCCFH\cdots NH_3}$	0.986991
$ZPVE^{calc}_{F_2CCH_2\cdots NH_3}$ ($X_{\beta 1}$, $X_{\beta 2}$ = F)	0.072075	$ZPVE^{calc}_{F_2CCFH\cdots NH_3}$ ($X_{\alpha 1}$, $X_{\beta 1}$, $X_{\beta 2}$ = F)	0.065012
$sf_{F_2CCH_2\cdots NH_3}$	0.988241	$sf_{F_2CCFH\cdots NH_3}$	0.987806
$ZPVE^{calc}_{H_3CCH_3\cdots NH_3}$	0.109305	$ZPVE^{calc}_{H_3CCFH_2\cdots NH_3}$ ($X_{\alpha 1}$ = F)	0.102901
$sf_{H_3CCH_3\cdots NH_3}$	0.987141	$sf_{H_3CCFH_2\cdots NH_3}$ ($X_{\alpha 1}$ = F)	0.987485
$ZPVE^{calc}_{H_2FCCH_3\cdots NH_3}$ ($X_{\beta 1}$ = F)	0.102763	$ZPVE^{calc}_{H_2FCCH_3\cdots NH_3}$ ($X_{\beta 2}$ = F)	0.102783
$sf_{H_2FCCH_3\cdots NH_3}$ ($X_{\beta 1}$ = F)	0.987485	$sf_{H_2FCCH_3\cdots NH_3}$ ($X_{\beta 2}$ = F)	0.987485
$ZPVE^{calc}_{F_2HCCH_3\cdots NH_3}$ ($X_{\beta 1}$, $X_{\beta 2}$ = F)	0.095422	$ZPVE^{calc}_{H_2FCCFH_2\cdots NH_3}$ ($X_{\alpha 1}$, $X_{\beta 1}$ = F)	0.096185
$sf_{F_2HCCH_3\cdots NH_3}$ ($X_{\beta 1}$, $X_{\beta 2}$ = F)	0.987818	$sf_{H_2FCCFH_2\cdots NH_3}$ ($X_{\alpha 1}$, $X_{\beta 1}$ = F)	0.987666
$ZPVE^{calc}_{H_3CCF_2H\cdots NH_3}$ ($X_{\alpha 1}$, $X_{\alpha 2}$ = F)	0.095680	$ZPVE^{calc}_{F_3CCH_3\cdots NH_3}$ ($X_{\beta 1}$, $X_{\beta 2}$, $X_{\beta 3}$ = F)	0.087438
$sf_{H_3CCF_2H\cdots NH_3}$ ($X_{\alpha 1}$, $X_{\alpha 2}$ = F)	0.987818	$sf_{F_3CCH_3\cdots NH_3}$ ($X_{\beta 1}$, $X_{\beta 2}$, $X_{\beta 3}$ = F)	0.988072

Dimer		Dimer	
$ZPVE^{calc}_{FH_2CCF_2H\cdots NH_3}$	0.088776	$ZPVE^{calc}_{F_2HCCF_2H\cdots NH_3}$	0.081205
$sf_{FH_2CCF_2H\cdots NH_3}$	0.987850	$sf_{F_2HCCF_2H\cdots NH_3}$	0.988177
$ZPVE^{calc}_{F_3CCF_2H\cdots NH_3}$	0.073062	$ZPVE^{calc}_{CH_4\cdots NH_3}$	0.079673
$sf_{F_3CCF_2H\cdots NH_3}$	0.996308	$sf_{CH_4\cdots NH_3}$	0.987984
$ZPVE^{calc}_{FCH_3\cdots NH_3}$ ($\angle$(C–H•••N = 180°)	0.074528	$ZPVE^{calc}_{FCH_3\cdots NH_3}$ ($\angle$(C–H•••N = 127°)	0.075110
$sf_{FCH_3\cdots NH_3}$	0.996482	$sf_{FCH_3\cdots NH_3}$	0.996482
$ZPVE^{calc}_{F_2CH_2\cdots NH_3}$	0.068300	$ZPVE^{calc}_{F_3CH\cdots NH_3}$	0.060811
$sf_{F_2CH_2\cdots NH_3}$	0.988375	$sf_{F_2CH_2\cdots NH_3}$	0.989420

[a]All energies are given in hartrees.