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**Table S1.** Calculated Total Energies (Hartrees)

		Sym	State	UHF <sup>a</sup>	PMP4 <sup>b</sup>	G2(MP2,SVP) 0 K <sup>c</sup>	G2(MP2,SVP) 298 K <sup>c</sup>
<u>Components</u>							
1	Cl	K <sub>h</sub>	<sup>2</sup> P	-459.44796	-459.57027	-459.66759	-459.66520
2	CH <sub>3</sub>	D <sub>3h</sub>	<sup>2</sup> A <sub>2</sub> "	-39.55899	-39.69057	-39.74215	-39.73790
3	NH <sub>3</sub>	C <sub>3v</sub>	<sup>1</sup> A <sub>1</sub>	-56.18436	-56.37126	-56.45667	-56.45286
4	NMe <sub>3</sub>	C <sub>3v</sub>	<sup>1</sup> A <sub>1</sub>	-173.26930	-173.89366	-174.09622	-174.08974
5	NCl <sub>3</sub>	C <sub>3v</sub>	<sup>1</sup> A <sub>1</sub>	-1432.73551	-1433.36450	-1433.75673	-1433.75132
6	HN=CH <sub>2</sub>	C <sub>s</sub>	<sup>1</sup> A'	-94.02846	-94.34554	-94.46083	-94.45696
7	HN-CH <sub>2</sub>	C <sub>s</sub>	<sup>3</sup> A"	-93.96268	-94.23644	-94.34960	-94.34546
8	pyridine	C <sub>2v</sub>	<sup>1</sup> A <sub>1</sub>	-246.69582	-247.55302	-247.81777	-247.81247
9	pyridine	C <sub>s</sub>	<sup>3</sup> A'	-246.59325	-247.40072	-247.67627	-247.67016
<u>Cl-adducts</u>							
10	ClNH <sub>3</sub>	C <sub>3v</sub>	<sup>2</sup> A <sub>1</sub>	-515.63874	-515.95733	-516.13808	-516.13253
11	ClNMe <sub>3</sub>	C <sub>3v</sub>	<sup>2</sup> A <sub>1</sub>	-632.72759	-633.49478	-633.79817	-633.78982
12	ClNCl <sub>3</sub>	C <sub>3v</sub>	<sup>2</sup> A <sub>1</sub>	-1892.18460	-1892.93953	-1893.43232	-1893.42425
13a	ClNH=CH <sub>2</sub>	C <sub>s</sub>	<sup>2</sup> A'	-553.48102	-553.92558	-554.14040	-554.13426
13b	ClNH-CH <sub>2</sub>	C <sub>1</sub>	<sup>2</sup> A	-553.44396	-553.89406	-554.11701	-554.11199
14	N-chloropyridinyl	C <sub>2v</sub>	<sup>2</sup> A <sub>1</sub>	-706.14836	-707.13953	-707.50347	-707.49563
<u>Me-adducts</u>							
15	MeNH-CH <sub>2</sub>	C <sub>1</sub>	<sup>2</sup> A	-133.61524	-134.06753	-134.22925	-134.22385
16	MeCH <sub>2</sub> -NH	C <sub>s</sub>	<sup>2</sup> A"	-133.63012	-134.07468	-134.23058	-134.22526
17	N-methylpyridinyl	C <sub>s</sub>	<sup>2</sup> A'	-286.26892	-287.25931	-287.57952	-287.57187
18	4-methylpyridinyl	C <sub>s</sub>	<sup>2</sup> A'	-286.27863	-287.26221	-287.57214	-287.56463

<sup>a</sup> UHF/6-31G(d) total energies at the UHF/6-31G(d) optimized geometries.<sup>b</sup> PMP4/6-31G(d) total energies calculated at the MP2(fc)/6-31G(d) optimized geometries.<sup>c</sup> Calculated at the MP2(full)/6-31G(d) optimized geometries.

**Table S2.** GAUSSIAN Archive Entries for UMP2/(full)6-31G(d) Optimized Geometries for Species 1–18 and UHF/6-31G(d) Frequency Calculations for the 2c–3e Cl Adducts 10–14

## Cl (1)

```
1\1\GINC-RSCQC9\SP\UMP2-FU\6-31G(d)\Cl1(2)\AXN501\09-Feb-1996\0\#MP2=
FULL/6-31G(D)\chlorine atom\0,2\Cl\Version=IBM-RS6000-G94RevC.2\HF=
-459.4479639\MP2=-459.5620568\PUHF=-459.4503696\PMP2-0=-459.5631595\S2
=0.755\S2-1=0.75\S2A=0.75\RMSD=5.367e-09\PG=KH\@
```

CH<sub>3</sub> (2)

```
1\1\GINC-RSCQC2\FOpt\UMP2-FU\6-31G(d)\C1H3(2)\AXN501\16-Jan-1996\0\#N
GEOM=ALLCHECK GUESS=READ MP2(FULL)/6-31G(D) OPT=RCFC\methyl radical,
G2\0,2\C,0.,0.,0.\H,0.,0.,1.078274815\H,0.9338133821,0.,-0.539137407
5\H,-0.9338133821,0.,-0.5391374075\Version=IBM-RS6000-G94RevC.2\HF=-3
9.5589209\MP2=-39.6730311\PUHF=-39.5620213\PMP2-0=-39.6750374\S2=0.762
\S2-1=0.753\S2A=0.75\RMSD=4.447e-09\RMSF=5.067e-05\Dipole=0.,0.,0.\PG=
D03H [O(C1),3C2(H1)]\@
```

NH<sub>3</sub> (3)

```
1\1\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\H3N1\AXN501\5-Nov-1993\1\# MP2=DIRE
CT/6-31G* FOPT SCF=DIRECT GEOM=CHECK\amonia, structure\0,1\N\X,1,1.\
H,1,nh,2,w\H,1,nh,2,w,3,120.,0\H,1,nh,2,w,3,-120.,0\nh=1.0170451\w=11
2.46412835\Version=Fujitsu-VP-Unix-G92RevE.2\HF=-56.1838218\MP2=-56.3
542116\RMSD=9.211e-09\RMSF=7.157e-06\Dipole=0.,0.,-0.7733075\PG=C03V [
C3(N1),3SGV(H1)]\@
```

NMe<sub>3</sub> (4)

```
1\1\GINC-RSCQC9\FOpt\RMP2-FU\6-31G(d)\C3H9N1\AXN501\14-Nov-1995\0\#MP
2=FULL/6-31G* GEOM=CHECK MAXDISK=460000000 FOPT\NMe3 C3v structure\0
,1\N,0.,0.,-0.3965901884\C,1.3780249294,0.,0.065360005\C,-0.6890124647
,1.1934045959,0.065360005\C,-0.6890124647,-1.1934045959,0.065360005\H,
1.460217466,0.,1.1680142209\H,-0.730108733,1.2645854206,1.1680142209\H
,-0.730108733,-1.2645854207,1.1680142209\H,1.8908306394,0.8862250878,-
0.3173985722\H,1.8908306394,-0.8862250878,-0.3173985722\H,-1.712908759
2,1.1943948241,-0.3173985722\H,-0.1779218802,2.0806199119,-0.317398572
2\H,-0.1779218802,-2.0806199119,-0.3173985722\H,-1.7129087592,-1.19439
48241,-0.3173985722\Version=IBM-RS6000-G94RevC.2\HF=-173.2682753\MP2=
-173.846463\RMSD=4.021e-09\RMSF=8.488e-05\Dipole=0.,0.,0.2919384\PG=C0
3V [C3(N1),3SGV(C1H1),X(H6)]\@
```

NCl<sub>3</sub> (5)

```
1\1\GINC-RSCQC8\FOpt\RMP2-FU\6-31G(d)\Cl3N1\AXN501\23-Nov-1995\1\# MP
2=FULL/6-31G* SCF=DIRECT FOPT=Z-MATRIX\nc13\0,1\X\N,1,1.\Cl,2,r1,1,a
1\Cl,2,r1,1,a1,3,120.,0\Cl,2,r1,1,a1,3,240.,0\r1=1.77251457\al=111.25
879799\Version=IBM-RS6000-G94RevC.2\HF=-1432.7320341\MP2=-1433.338309
3\RMSD=3.585e-09\RMSF=3.181e-05\Dipole=0.,0.,0.2773441\PG=C03V [C3(N1)
,3SGV(Cl1)]\@
```

HN=CH<sub>2</sub> (6)

```
1\1\GINC-RSCQC2\FOpt\RMP2-FU\6-31G(d)\C1H3N1\AXN501\25-Oct-1995\1\# M
P2=FULL/6-31G* FOPT=Z-MATRIX SCF=DIRECT\formaldimine HN=CH2 structure
\0,1\C\N,1,r1\H,2,r2,1,a1\H,1,r3,2,a2,3,0.\H,1,r4,2,a3,3,180.,0\r1
=1.28093277\r2=1.02637719\r3=1.09440539\r4=1.08890475\al=109.73928772\
a2=125.46279997\al=118.39289704\Version=IBM-RS6000-G94RevC.2\State=1-
A'\HF=-94.0265361\MP2=-94.3230776\RMSD=3.853e-09\RMSF=5.799e-05\Dipole
=0.5866445,0.,-0.5755192\PG=CS [SG(C1H3N1)]\@
```

HN-CH<sub>2</sub> (7)

1\1\GINC-RSCQC9\FOpt\UMP2-FU\6-31G(d)\C1H3N1(3)\AXN501\26-Oct-1995\0\#\  
 # UMP2=FULL/6-31G\* FOPT SCF=DIRECT FREQ\HN=CH2 triplet structure\0,3  
 \C,-0.0186823585,0.,-0.6605887185\N,-0.0183125131,0.,0.7291787097\H,0.  
 9330448474,0.,1.1176586745\H,-0.3463815523,-0.9246664864,-1.1291886658  
 \H,-0.3463815523,0.9246664864,-1.1291886658\Version=IBM-RS6000-G94Rev  
 C.2\State=3-A\HF=-93.9621921\MP2=-94.2087077\PUHF=-93.9655632\PMP2=0=  
 -94.2105989\S2=2.012\S2-1=2.001\S2A=2.\RMSD=7.609e-09\RMSF=1.281e-04\D  
 ipole=0.4047946,0.,-0.2039806\PG=CS [SG(C1H1N1),X(H2)]\@

#### Pyridine (8)

1\1\GINC-RSCQC8\FOpt\RMP2-FU\6-31G(d)\C5H5N1\ROOT\13-Oct-1995\0\#\# MP2  
 =FULL/6-31G\* FOPT SCF=DIRECT MAXDISK=460000000\Pyridine structure\0,  
 1\N,0.,0.,-1.4249604615\C,0.,0.,1.3861168541\C,1.1440844254,0.,-0.7200  
 886482\C,-1.1440844254,0.,-0.7200886482\C,-1.1961773942,0.,0.672891071  
 6\C,1.1961773942,0.,0.6728910716\H,0.,0.,2.4729370387\H,-2.1550440648,  
 0.,1.1830497012\H,2.1550440648,0.,1.1830497012\H,2.0603848887,0.,-1.30  
 73217082\H,-2.0603848887,0.,-1.3073217082\Version=IBM-RS6000-G94RevC.  
 2\State=1-A1\HF=-246.6937746\MP2=-247.5106788\RMSD=3.377e-09\RMSF=9.61  
 4e-05\Dipole=0.,0.,0.9108545\PG=C02V [C2(H1C1N1),SGV(C4H4)]\@

#### Triplet pyridine (9)

1\1\GINC-RSCQC8\FOpt\UMP2-FU\6-31G(d)\C5H5N1(3)\ROOT\12-Oct-1995\0\#\#  
 MP2=FULL/6-31G\* FOPT SCF=DIRECT MAXDISK=460000000\pyridine 3A' Cs str  
 ucture\0,3\N,-0.5098704728,0.,-1.2429713902\C,-0.5088628585,1.1906119  
 68,-0.5008959001\C,-0.5088628585,-1.190611968,-0.5008959001\C,0.319522  
 1795,1.226685034,0.5400465726\C,0.3195221795,-1.226685034,0.5400465726  
 \C,0.9108237206,0.,0.9986369979\H,-1.0898295236,2.0216945617,-0.883880  
 6613\H,-1.0898295236,-2.0216945617,-0.8838806613\H,0.4881051543,2.1539  
 988986,1.0783864901\H,0.4881051543,-2.1539988986,1.0783864901\H,1.5796  
 878728,0.,1.8501580163\Version=IBM-RS6000-G94RevC.2\State=3-A'\HF=-24  
 6.5898159\MP2=-247.3317331\PUHF=-246.6079186\PMP2=0=-247.347401\S2=2.3  
 09\S2-1=2.219\S2A=2.042\RMSD=2.079e-09\RMSF=8.579e-05\Dipole=-0.260659  
 9,0.,0.4146723\PG=CS [SG(C1H1N1),X(C4H4)]\@

#### ClNH<sub>3</sub> (10)

1\1\GINC-IX\FREQ\UHF\6-31G(D)\C1H3N1(2)\AXN501\23-Oct-1995\1\#\# HF/6-  
 31G(D) FREQ SCF=DIRECT GEOM=CHECK GUESS=READ\clnh3 at C3v symmetry\0  
 ,2\C1\N,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,120.,0\H,2,r2,1,a1,3,240.,0\r1  
 =2.68365137\r2=1.00177245\A1=110.54957432\Version=HP-PARisc-HPUX-G92/  
 DFT-RevG.1\HF=-515.6387434\S2=0.758\S2-1=0.\S2A=0.75\RMSD=8.389e-10\RM  
 SF=6.125e-05\Dipole=0.,0.,1.1726342\DipoleDeriv=-0.0973616,0.,0.,0.,-0.  
 0973616,0.,0.,0.,0.4716816,-0.36988,0.,0.,0.,-0.36988,0.,0.,0.,-0.911  
 1742,0.1167488,0.,-0.022024,0.,0.1947456,0.,-0.1385502,0.,0.1464975,0.  
 1752464,0.0337736,0.011012,0.0337736,0.136248,-0.0190733,0.0692751,-0.  
 119988,0.1464975,0.1752464,-0.0337736,0.011012,-0.0337736,0.136248,0.0  
 190733,0.0692751,0.119988,0.1464975\Polar=13.8146178,0.,13.8146178,0.,  
 0.,28.3607528\PolarDeriv=0.0078001,0.,-0.0078001,-3.4226978,0.,-0.0000  
 002,0.,-0.0078,0.,0.,-3.4226978,0.,-0.2578881,0.,-0.2578883,0.,0.,19.2  
 817341,-3.4196731,0.,3.419673,-3.4064474,0.,0.0000008,0.,3.4196731,0.,  
 0.,-3.4064468,0.,-4.0618527,0.,-4.0618527,-0.0000003,0.,0.7549362,7.06  
 5555,0.,0.0073537,3.1974092,0.,4.8277345,0.,1.2545185,0.,0.,1.3553545,  
 0.,2.2777094,0.,0.6021178,2.764126,0.,-6.6788899,-1.826841,2.0713678,-  
 1.7096133,1.815868,-0.7976331,-2.4138676,0.9912915,-2.3331958,5.134027  
 2,-0.7976329,2.736895,4.1809408,1.0210157,-0.7255524,1.8588116,-1.3820  
 629,2.3938029,-6.6788902,-1.826841,-2.0713678,-1.7096133,1.815868,0.79  
 76331,-2.4138676,-0.9912915,-2.3331958,-5.1340272,0.7976329,2.736895,-  
 4.1809408,1.0210157,0.7255524,1.8588116,-1.3820629,-2.3938029,-6.67889  
 02\HyperPolar=19.7191489,0.,-19.7191489,0.,22.298154,0.,22.2981598,-0.  
 0000005,0.,-1168.7934342\PG=C03V [C3(N1C11),3SGV(H1)]\NIMAG=0\0.00053  
 227,0.0,0.00053227,0.0,0.0,0.00779400,-0.00103896,0.0,0.0,0.76544968,0.  
 0,-0.00103896,0.0,0.0,0.76544968,0.0,0.0,-0.01373820,0.0,0.0,0.270860  
 51,0.00043020,0.0,-0.00123478,-0.43095196,0.0,-0.12934012,0.46395076,0

.0,-0.00009240,0.0,0.0,-0.07865518,0.0,0.0,0.07151677,-0.00088469,0.0,  
0.00198140,-0.18907441,0.0,-0.08570744,0.15030296,0.0,0.07711953,0.000  
03825,-0.00022629,0.00061739,-0.16672938,0.15254898,0.06467006,-0.0167  
1449,0.03915955,0.01982807,0.16962527,-0.00022629,0.00029955,-0.001069  
35,0.15254898,-0.34287777,-0.11201183,-0.00394713,0.00361540,0.0000577  
4,-0.16992890,0.36584226,0.00044234,-0.00076616,0.00198140,0.09453720,  
-0.16374324,-0.08570744,-0.00986403,0.01720048,0.00330325,-0.07515148,  
0.13016618,0.07711953,0.00003825,0.00022629,0.00061739,-0.16672938,-0.  
15254898,0.06467006,-0.01671449,-0.03915955,0.01982807,0.01378035,0.02  
155334,-0.00996404,0.16962527,0.00022629,0.00029955,0.00106935,-0.1525  
4898,-0.34287777,0.11201183,0.00394713,0.00361540,-0.00005774,-0.02155  
334,-0.02687944,0.01714274,0.16992890,0.36584226,0.00044234,0.00076616  
,0.00198140,0.09453720,0.16374324,-0.08570744,-0.00986403,-0.01720048,  
0.00330325,-0.00996404,-0.01714274,0.00330325,-0.07515148,-0.13016618,  
0.07711953\0.0,0.0,-0.00001025,0.0,0.0,0.00005040,0.00013302,0.0,-0.0  
0001338,-0.00006651,0.00011520,-0.00001338,-0.00006651,-0.00011520,-0.  
00001338\\@

1\1\ ANU-VP\FOpt\UMP2-FU\6-31G(d)\Cl1H3N1(2)\AXN501\12-Oct-1995\1\# U  
MP2=FULL/6-31G(D) FOPT=Z-MATRIX SCF=DIRECT\clnh3 C3v structure (10)\  
0,2\Cl\N,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,120.,0\H,2,r2,1,a1,3,240.,0\ r  
1=2.38318897\ r2=1.01426742\ a1=108.09783626\ Version=Fujitsu-VP-Unix-G9  
4RevC.2\HF=-515.6358114\MP2=-515.9359968\PUHF=-515.6397312\ PMP2-0=-515  
.938104\ S2=0.762\ S2-1=0.751\ S2A=0.75\ RMSD=5.388e-09\ RMSF=3.117e-05\ Dip  
ole=0.,0.,1.78412\ PG=C03V [C3(N1C11),3SGV(H1)]\\@

ClNMe<sub>3</sub> (11)

1\1\ ANU-VP\Freq\UHF\6-31G(d)\C3H9Cl1N1(2)\AXN501\25-Oct-1995\0\#N GE  
OM=ALLCHECK GUESS=READ UHF/6-31G(D) FREQ\clnme3 C3v structure (11) +f  
rq. anl.\0,2\Cl,0.,0.,-1.8152201699\N,0.,0.,0.5869347989\C,1.40197883  
94,0.,0.9607260779\C,-0.7009894197,1.2141492905,0.9607260779\C,-0.7009  
894197,-1.2141492905,0.9607260779\H,1.5170239514,0.,2.0451420174\H,-0.  
7585119757,1.3137812801,2.0451420174\H,-0.7585119757,-1.3137812801,2.0  
451420174\H,1.8835308,0.8773695418,0.5536173069\H,1.8835308,-0.8773695  
418,0.5536173069\H,-1.7015897117,1.1925007507,0.5536173069\H,-0.181941  
0883,2.0698702925,0.5536173069\H,-0.1819410882,-2.0698702925,0.5536173  
069\H,-1.7015897117,-1.1925007507,0.5536173069\ Version=Fujitsu-VP-Uni  
x-G94RevC.2\HF=-632.7275889\ S2=0.768\ S2-1=0.\ S2A=0.75\ RMSD=1.694e-09\ R  
MSF=2.396e-05\ Dipole=0.,0.,1.8361675\ DipoleDeriv=-0.3223425,0.,-0.0000  
003,0.,-0.3223426,0.0000004,-0.0000003,0.0000001,1.0089174,-0.5568699,  
0.,0.0000017,0.,-0.5568698,-0.0000024,-0.0000005,0.0000002,0.7863102,0.  
5250996,0.0000002,1.2655501,0.,0.1380193,0.0000019,0.0727929,-0.00000  
01,-0.3115103,0.2347896,-0.1676107,-0.632788,-0.1676108,0.4283295,1.09  
60056,-0.0363965,0.0630406,-0.311493,0.2347895,0.1676107,-0.6327821,0.  
1676105,0.4283297,-1.0960076,-0.0363966,-0.0630402,-0.3114951,-0.03055  
32,0.,-0.4372418,0.,0.0502549,0.0000001,-0.0803907,0.,-0.3530399,0.030  
0528,0.0349909,0.2186196,0.034991,-0.0103512,-0.3786606,0.0401955,-0.0  
696204,-0.3530456,0.0300529,-0.0349909,0.2186206,-0.0349909,-0.0103512  
,0.3786652,0.0401954,0.0696204,-0.3530448,0.0077604,-0.0394165,-0.1392  
302,-0.0943583,-0.0561,-0.0553874,0.0166283,0.0601333,0.0330693,0.0077  
604,0.0394165,-0.139229,0.0943584,-0.0561,0.0553844,0.0166283,-0.06013  
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 3,-0.00000653,-0.00000045,0.00000697,-0.00000099,-0.00000045,0.0000069  
 7,0.00000099,-0.00000045,-0.00000263,0.00000653,-0.00000045\\\@

1\1\ ANU-VP\FOp\t\UMP2-FU\6-31G(d)\C3H9C11N1(2)\AXN501\12-Oct-1995\0\#



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MP2=FULL/6-31G* SCF=DIRECT FOPT\\c1nme3 C3v structure (11)\\0,2\\C1,0.
,0.,-1.774978704\\N,0.,0.,0.5741597299\\C,1.4078328852,0.,0.9409311711\\C
,-0.7039164426,1.2192190429,0.9409311711\\C,-0.7039164426,-1.2192190429
,0.9409311711\\H,1.527767642,0.,2.0339285632\\H,-0.763883821,1.323085589
1,2.0339285632\\H,-0.763883821,-1.3230855891,2.0339285632\\H,1.882905709
5,0.8860795729,0.519495515\\H,1.8829057095,-0.8860795729,0.519495515\\H,
-1.7088202747,1.1876043909,0.519495515\\H,-0.1740854348,2.0736839638,0.
519495515\\H,-0.1740854348,-2.0736839638,0.519495515\\H,-1.7088202747,-1
.1876043909,0.519495515\\Version=Fujitsu-VP-Unix-G94RevC.2\\HF=-632.726
6327\\MP2=-633.4408344\\PUHF=-632.7320815\\PMP2-0=-633.4439533\\S2=0.768\\S
2-1=0.753\\S2A=0.75\\RMSD=4.858e-09\\RMSF=8.400e-05\\Dipole=0.,0.,1.983676
3\\PG=C03V [C3(N1C11),3SGV(C1H1),X(H6)]\\@

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# C1NCl3 (12)

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1\\1\\GINC-RSCQC9\\Freq\\UHF\\6-31G(d)\\C14N1(2)\\AXN501\\17-Jan-1996\\0\\#N GE
OM=ALLCHECK GUESS=READ UHF/6-31G(D) FREQ\\nc14 structure\\0,2\\C1,0.,0.
,-2.9087516755\\N,0.,0.,0.3674062814\\C1,1.6316469534,0.,0.9191555787\\C1
,-0.8158234767,1.4130477116,0.9191555787\\C1,-0.8158234767,-1.413047711
6,0.9191555787\\Version=IBM-RS6000-G94RevC.2\\HF=-1892.1845974\\S2=0.755
\\S2-1=0.\\S2A=0.75\\RMSD=1.819e-09\\RMSF=2.287e-06\\Dipole=0.,0.,0.3630661
\\DipoleDeriv=-0.0095643,0.,-0.0000009,0.,-0.0095616,0.,-0.0000005,0.,0
.0565809,0.5522724,0.,-0.0000003,0.,0.5522857,0.,-0.0000031,0.,-0.1830
824,-0.3112387,0.,0.0243921,0.,-0.050568,0.,-0.1880408,0.,0.0421679,-0
.1157348,0.1129012,-0.0121959,0.1128748,-0.2460777,0.0211235,0.0940221
,-0.1628578,0.0421676,-0.1157348,-0.1129012,-0.0121959,-0.1128748,-0.2
460777,-0.0211235,0.0940221,0.1628578,0.0421676\\Polar=49.2849289,0.,49
.2849624,-0.000028,0.,29.0315152\\PolarDeriv=-0.0071328,0.,0.0070096,-0
.6222625,0.,0.000026,0.,0.0072366,0.,0.,-0.6224822,0.,-0.3381469,0.,-0
.338175,0.0000093,0.,2.6399966,-10.3938402,0.,10.3938909,-5.2464651,0.
,-0.0000095,0.,10.3937582,0.,0.,-5.2466186,0.,-9.3882775,0.,-9.3879079
,-0.0000023,0.,-6.6359402,26.3547851,0.,1.3101711,3.3117043,0.,0.37314
68,0.,5.5884122,0.,0.,0.6008148,0.,5.597164,0.,0.8877815,6.5351809,0.,
1.3319711,-7.9769377,7.8422748,-5.8555789,1.2785268,-1.1738519,-0.1865
687,4.13705,-7.9947005,19.8216711,-1.17383,2.6340369,0.3231518,2.06483
01,-2.0391961,4.4192136,-3.2675929,5.6596815,1.3319659,-7.9769377,-7.8
422748,-5.8555789,1.2785268,1.1738519,-0.1865687,-4.13705,-7.9947005,-
19.8216711,1.17383,2.6340369,-0.3231518,2.0648301,2.0391961,4.4192136,
-3.2675929,-5.6596815,1.3319659\\HyperPolar=44.4968938,0.,-44.500482,0.
,31.7873724,0.,31.7947995,-0.0008928,0.,-90.4445827\\PG=C03V [C3(N1C11)
,3SGV(C11)]\\NImag=0\\0.00019521,0.,0.00019507,0.00000002,0.,0.00133442
,-0.00017262,0.,0.,0.33292277,0.,-0.00017307,0.,0.,0.33292283,0.000000
11,0.,-0.00133240,0.,0.,0.13666739,-0.00006575,0.,0.00012291,-0.181719
80,0.,-0.04540864,0.24357887,0.,0.00005072,0.,0.,-0.04011366,0.,0.,0.0
4839881,-0.00026654,0.,-0.00000068,-0.07478136,0.,-0.04511173,0.056163
58,0.,0.03231326,0.00002157,0.00004948,-0.00006145,-0.07551518,0.06131
735,0.02270431,-0.03089667,0.03034884,0.00944214,0.09719382,0.00005040
,-0.00003639,0.00010644,0.06131727,-0.14631827,-0.03932501,0.01594670,
-0.00416792,-0.00082890,-0.08451545,0.19478385,0.00013321,-0.00023049,
-0.00000069,0.03739069,-0.06476259,-0.04511172,-0.00543892,0.00776268,
0.00639961,-0.02808179,0.04863909,0.03231326,0.00002157,-0.00004948,-0
.00006145,-0.07551518,-0.06131735,0.02270431,-0.03089667,-0.03034884,0
.00944214,0.00919645,0.00720107,-0.00400322,0.09719382,-0.00005040,-0
.00003639,-0.00010644,-0.06131727,-0.14631827,0.03932501,-0.01594670,-0
.00416792,0.00082890,-0.00720107,-0.04426104,0.00859158,0.08451545,0.1
9478385,0.00013321,0.00023049,-0.00000069,0.03739069,0.06476259,-0.045
11172,-0.00543892,-0.00776268,0.00639961,-0.00400322,-0.00859158,0.006
39961,-0.02808179,-0.04863909,0.03231326\\0.,0.,-0.00000015,0.,0.,-0.0
000636,0.00000282,0.,0.00000217,-0.00000141,0.00000244,0.00000217,-0.
00000141,-0.00000244,0.00000217\\@

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1\\1\\GINC-RSCQC9\\FOpt\\UMP2-FU\\6-31G(d)\\C14N1(2)\\AXN501\\19-Jan-1996\\1\\#
MP2=FULL/6-31G(D) OPT=Z-MATRIX\\nc14 structure\\0,2\\C1\\N,1,r1\\C1,2,r2,

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1,a1\Cl,2,r2,1,a1,3,120.,0\Cl,2,r2,1,a1,3,240.,0\\r1=2.60478104\r2=1.7
6510681\al=110.63932311\\Version=IBM-RS6000-G94RevC.2\HF=-1892.1782285
\MP2=-1892.9054419\PUHF=-1892.1809022\PM2=0=-1892.9067816\S2=0.756\S2
-1=0.75\S2A=0.75\RMSD=6.145e-09\RMSF=3.702e-05\Dipole=0.,0.,0.6655572\
PG=C03V [C3(N1Cl1),3SGV(Cl1)]\\@
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ClNH=CH<sub>2</sub> (13a)

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1\1\GINC-RSCQC2\Freq\UHF\6-31G(d)\ClH3Cl1N1(2)\AXN501\24-Oct-1995\0\\#
N GEOM=ALLCHECK GUESS=READ UHF/6-31G(D) FREQ\HClN=CH2 Cs all-in-plane
structure (13a) + frq.anl.\0,2\C,1.2141371873,0.,-1.7227150756\N,1.1
931254239,0.,-0.4707946584\H,2.1154378982,0.,-0.0703884208\H,2.1191087
848,0.,-2.3176494762\H,0.282011836,0.,-2.2653781249\Cl,-1.1854858594,0
.,1.0756040638\\Version=IBM-RS6000-G94RevC.2\State=2-A'\HF=-553.481021
4\S2=0.779\S2-1=0.\S2A=0.75\RMSD=6.173e-10\RMSF=8.633e-06\Dipole=0.855
6487,0.,-0.8243268\DipoleDeriv=0.4119777,0.,0.0635807,0.,0.0220824,0.,
-0.1282202,0.,0.4172825,-0.3952336,0.,0.2032854,0.,-0.4992634,0.,0.176
7522,0.,-0.5989533,-0.0137619,0.,-0.0974372,0.,0.289368,0.,0.0535882,0
.,0.2024031,-0.1114042,0.,0.1030587,0.,0.1511733,0.,0.0933357,0.,-0.07
05026,-0.0728589,0.,-0.0797762,0.,0.0903625,0.,-0.0451784,0.,-0.015522
3,0.1812809,0.,-0.1927114,0.,-0.0537227,0.,-0.1502774,0.,0.0652927\Pol
ar=27.5634864,0.,12.7138286,-4.3730813,0.,34.8650476\PolarDeriv=-4.429
6498,0.,0.4464006,7.7896397,0.,-3.8874446,0.,0.4317599,0.,0.,-5.378706
4,0.,0.0409508,0.,-1.3417826,-0.0314076,0.,-19.5691557,-8.1053651,0.,-
0.2985233,0.4496765,0.,-3.6272822,0.,-0.3712565,0.,0.,5.0162116,0.,3.0
620015,0.,1.5634593,-1.9132893,0.,22.1233626,5.9544143,0.,0.042134,6.1
385972,0.,0.9888696,0.,1.459526,0.,0.,0.6201984,0.,5.5055735,0.,-0.113
2606,-0.8180358,0.,6.1483901,6.3426615,0.,0.2712425,-4.8728859,0.,2.70
04556,0.,1.5897719,0.,0.,-0.6224308,0.,-1.7173455,0.,-0.1199982,2.1153
671,0.,-4.07107,-4.8156161,0.,-0.4345082,-3.8894228,0.,-1.6626549,0.,-
1.61242,0.,0.,-0.9057795,0.,-1.7575709,0.,-0.0226514,-2.4031346,0.,-3.
67258,5.0535553,0.,-0.0267456,-5.6156047,0.,5.4880565,0.,-1.4973812,0.
,0.,1.2705067,0.,-5.1336094,0.,0.0342335,3.0505002,0.,-0.958947\HyperP
olar=-261.6125779,0.,0.9662119,0.,233.0316672,0.,-7.4801816,-190.06202
25,0.,127.077303\PG=CS [SG(ClH3Cl1N1)]\NImag=0\\0.74068159,0.,0.173753
33,0.01553282,0.,0.97431075,-0.14440854,0.,-0.03431294,0.55263084,0.,-
0.05985838,0.,0.07652508,0.04013089,0.,-0.67103672,0.14248626,0.,0.
84369562,-0.00200940,0.,0.01422493,-0.42365608,0.,-0.18010086,0.417564
74,0.,0.00420933,0.,0.,-0.04612990,0.,0.,0.03629564,-0.05513463,0.,-0.
02539702,-0.11113301,0.,-0.11013211,0.16688052,0.,0.13686156,-0.286491
25,0.,0.11999781,0.01037636,0.,0.00447492,0.00443286,0.,-0.00040844,0.
29084398,0.,-0.06252446,0.,0.,0.03807877,0.,0.,-0.01548257,0.,0.,0.028
54413,0.11463760,0.,-0.14399539,0.03893840,0.,-0.03369451,0.00097756,0
.,0.00327465,-0.14019871,0.,0.16225802,-0.31044708,0.,-0.12140848,0.01
182505,0.,-0.00621438,0.00279300,0.,0.00169213,-0.01912038,0.,-0.01336
102,0.31504025,0.,-0.05576921,0.,0.,-0.00813654,0.,0.,0.02110255,0.,0.
,0.01106443,0.,0.,0.03200181,-0.11399358,0.,-0.12976537,-0.03960087,0.
,-0.02886739,-0.00133875,0.,-0.00617927,0.01608055,0.,0.01152466,0.139
19317,0.,0.15299956,0.00267468,0.,0.00596586,-0.00676762,0.,-0.0007768
3,0.00087489,0.,-0.00189656,-0.0004156,0.,-0.00099383,-0.00009084,0.,
-0.00034053,0.00335046,0.,0.00018939,0.,0.,-0.00047902,0.,0.,0.0000049
5,0.,0.,0.00031970,0.,0.,-0.00026304,0.,0.,0.00022801,-0.00117311,0.,-
0.00411624,0.00362217,0.,0.00003511,-0.00064340,0.,0.00157219,0.000053
88,0.,0.00063257,0.00009858,0.,0.00028781,-0.00195811,0.,0.00158856\\-
0.00000342,0.,0.00001710,0.00001716,0.,0.00000424,-0.00002050,0.,-0.00
001001,-0.00000673,0.,-0.00000411,0.00000981,0.,-0.00000542,0.00000368
,0.,-0.00000181\\@
```

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1\1\ ANU-VP\FOpt\UMP2-FU\6-31G(d)\ClH3Cl1N1(2)\AXN501\12-Oct-1995\0\\#
UMP2=FULL/6-31G* FOPT SCF=DIRECT\HClN=CH2 Cs all-in-plane structure
(13a)\0,2\C,1.0856696164,0.,-1.5757434749\N,1.0866283107,0.,-0.334754
917\H,2.0176094912,0.,0.0881581009\H,1.9835159771,0.,-2.202959961\H,0.
1304654824,0.,-2.099963505\Cl,-1.0736474602,0.,0.9419123902\\Version=F
```

ujitsu-VP-Unix-G94RevC.2\State=2-A'\HF=-553.4788255\MP2=-553.89266\PUHF=-553.4842851\PMF2=0=-553.8971171\S2=0.797\S2-1=0.779\S2A=0.751\RMSD=9.318e-09\RMSF=1.048e-05\Dipole=1.1649915,0.,-1.0948341\PG=CS [SG(C1H3C11N1)]\@

#### ClNH-CH<sub>2</sub> (13b)

1\1\GINC-RSCQC2\FOpt\UMP2-FU\6-31G(d)\C1H3C11N1(2)\AXN501\15-Nov-1995\0\# MP2=FULL/6-31G\* SCF=DIRECT FOPT\HClN=CH2 2c-2e, C1 "perpendicular" (13b) structure\0,2\C,1.5550378668,-0.343433283,-0.287892143\N,0.5692792164,0.5460361676,0.1364063906\H,0.5428879985,1.393446888,-0.430020518\H,2.481875708,0.1282613048,-0.5874161992\H,1.5735701152,-1.3063238059,0.2033551384\C1,-1.0537362081,-0.1162963448,0.093328806\Version=IBM-RS6000-G94RevC.2\HF=-553.4433414\MP2=-553.8645057\PUHF=-553.4470393\PMF2=0=-553.8672678\S2=0.772\S2-1=0.761\S2A=0.75\RMSD=4.453e-09\RMSF=1.857e-05\Dipole=-0.4710124,0.2952,0.3489364\PG=C01 [X(C1H3C11N1)]\@

#### N-Chloropyridinyl (14)

1\1\GINC-PC\Freq\UHF\6-31G(d)\C5H5C11N1(2)\AXN501\23-Jan-1996\0\#N GEOM=ALLCHECK GUESS=READ UHF/6-31G(D) FREQ\cl-pyridine structure+freq. a n1.\0,2\N,0.,0.,0.1759237988\C,0.,1.1337112985,-0.5021105034\C,0.,-1.1337112985,-0.5021105034\C,0.,1.191012896,-1.8855152391\C,0.,-1.191012896,-1.8855152391\C,0.,0.,-2.5904579503\H,0.,2.0360962086,0.0828516745\H,0.,-2.0360962086,0.0828516745\H,0.,2.1400659323,-2.3884815072\H,0.,-2.1400659323,-2.3884815072\H,0.,0.,-3.6657501926\C1,0.,0.,3.0141058752\Version=SGI-G94RevC.3\State=2-A1\HF=-706.1483574\S2=0.758\S2-1=0.\S2A=0.75\RMSD=3.163e-09\RMSF=3.643e-05\Dipole=0.,0.,-1.2747458\DipoleDeriv=-0.3330028,0.,0.,0.,-0.4338927,0.0000007,0.,0.,-0.7674332,0.0738904,0.,0.,0.,0.2862827,-0.0661009,0.,0.3402493,0.3152267,0.0738905,0.,0.,0.,0.2862828,0.0661006,0.,-0.3402493,0.3152267,-0.1555343,0.,0.,0.,-0.100446,-0.1381159,0.,-0.4045188,-0.2778153,-0.1555343,0.,0.,0.,-0.100446,0.1381174,0.,0.4045189,-0.2778164,-0.0490061,0.,0.,0.,0.2946288,0.0000002,0.,0.0000001,0.3090817,0.0996638,0.,0.,0.,-0.0660995,-0.0583865,0.,-0.0852358,0.0307823,0.0996638,0.,0.,0.,-0.0660997,0.0583858,0.,0.0852359,0.0307834,0.1396808,0.,0.,0.,-0.0641722,0.0697434,0.,0.0694304,0.0307185,0.1396806,0.,0.,0.,-0.0641721,-0.0697444,0.,-0.0694305,0.0307174,0.1205536,0.,0.,0.,0.0821437,-0.0000002,0.,0.,-0.1043743,-0.053946,0.,0.,0.,-0.0540101,-0.0000001,0.,0.,0.3649023\Polar=25.4354661,0.,68.9228682,0.,-0.000003,81.1213633\PolarDeriv=0.,-0.0000052,0.,2.188482,0.,0.,-0.0000096,0.,0.0000025,0.,-1.8067369,0.00008,-0.0205002,0.,-0.5226686,0.,-0.0000021,6.7796919,0.,2.0745418,0.,1.8189759,0.,0.,0.1489442,0.,0.2304078,0.,0.6896525,9.5660639,0.1529962,0.,2.7486433,0.,0.7267045,7.6816045,0.,-2.0745389,0.,1.8189183,0.,0.,-0.1489317,0.,-0.2304146,0.,0.689781,-9.5661916,0.1529905,0.,2.7486735,0.,-0.7267661,7.6817906,0.,3.5569327,0.,-1.4502024,0.,0.,-0.1541113,0.,-0.66638,0.,-1.3845733,0.0049698,0.0742979,0.,-1.338102,0.,-2.1842532,5.012465,0.,-3.5569413,0.,-1.4501913,0.,0.,0.1541034,0.,0.6663491,0.,-1.384672,-0.0051421,0.0743025,0.,-1.3381385,0.,2.1844015,5.0123537,0.,0.0000066,0.,-3.6429553,0.,0.,0.000003,0.,0.0000328,0.,3.2924126,0.0003316,-0.2482289,0.,-2.6072943,0.,-0.0001403,-6.5239888,0.,1.2624987,0.,0.5294732,0.,0.,0.3776435,0.,7.3295327,0.,3.1936329,0.6061827,0.2683883,0.,2.9080557,0.,-0.8492683,-1.1465848,0.,-1.2624963,0.,0.529491,0.,0.,-0.3776439,0.,-7.3295345,0.,3.1936254,-0.6061293,0.2683891,0.,2.9080618,0.,0.8492736,-1.1466962,0.,1.0968965,0.,-0.6705655,0.,0.,0.3540965,0.,8.2498607,0.,-3.6625353,1.9793523,-0.1821535,0.,-2.862452,0.,-0.8278883,2.6056447,0.,-1.096896,0.,-0.6705598,0.,0.,-0.3540979,0.,-8.2498588,0.,-3.6625575,-1.9793798,-0.1821542,0.,-2.8624402,0.,0.8278762,2.6056261,0.,0.000006,0.,-1.4523083,0.,0.,0.,0.0000002,0.,-1.4196041,-0.0001518,-0.4663501,0.,-0.273447,0.,0.0000365,-2.6564776,0.,-0.0000004,0.,2.4514411,0.,0.,0.0000003,0.,0.0000005,0.,2.2615916,0.000008,0.1080223,0.,0.4911096,0.,0.0000077,2.6500587\HyperPolar=0.,0.0000077,0.,-0.0000066,-3.588067,0.,-37.3503236,0.,-0.0002267,1026.6847802\PG=C02V [C2(H1C1N1C11)],

SGV(C4H4)]\NImag=0\0.11468143,0.,0.75408512,0.,-0.00000002,0.51040968  
,-0.08226062,0.,0.,0.19524690,0.,-0.32821716,0.14336745,0.,0.85578808,  
0.,0.06083690,-0.23308354,0.,0.05747303,0.78640245,-0.08226061,0.,0.,0  
.00412113,0.,0.,0.19524690,0.,-0.32821715,-0.14336744,0.,-0.11644623,0  
.05711018,0.,0.85578808,0.,-0.06083689,-0.23308354,0.,-0.05711018,0.11  
301429,0.,-0.05747303,0.78640245,0.02646687,0.,0.,-0.08430616,0.,0.,-0  
.01149588,0.,0.,0.15722960,0.,0.05801257,0.04052931,0.,-0.17640145,0.0  
5785368,0.,-0.03536878,-0.04485738,0.,0.84582066,0.,0.15465614,-0.0283  
3419,0.,-0.06089288,-0.35876564,0.,-0.07011434,-0.10133376,0.,-0.05038  
284,0.76645471,0.02646688,0.,0.,-0.01149588,0.,0.,-0.08430616,0.,0.,0.  
00786814,0.,0.,0.15722960,0.,0.05801260,-0.04052932,0.,-0.03536878,0.0  
4485738,0.,-0.17640145,-0.05785368,0.,-0.06432406,-0.03894196,0.,0.845  
82066,0.,-0.15465614,-0.02833418,0.,0.07011434,-0.10133376,0.,0.060892  
88,-0.35876564,0.,0.03894196,0.11337993,0.,0.05038284,0.76645471,-0.01  
116490,0.,0.,0.00850857,0.,0.,0.00850858,0.,0.,-0.07710047,0.,0.,-0.07  
710049,0.,0.,0.17628037,0.,-0.14454949,0.,0.,0.07865586,-0.12633144,0.  
0.07865587,0.12633146,0.,-0.32520483,-0.03920431,0.,-0.32520482,0.039  
20430,0.,0.75050202,0.,0.00000003,0.00296676,0.,-0.03735092,-0.0261742  
4,0.,0.03735090,-0.02617423,0.,-0.14487462,-0.22486368,0.,0.14487470,-  
0.22486375,0.,0.,0.86235581,-0.00316751,0.,0.,-0.05354284,0.,0.,0.0120  
7644,0.,0.,0.00906922,0.,0.,0.00005554,0.,0.,0.00855873,0.,0.,0.033657  
34,0.,-0.03572788,-0.01168392,0.,-0.27430059,-0.14350884,0.,-0.0025381  
4,0.00386877,0.,0.00694479,0.00326056,0.,0.00013913,-0.00001534,0.,0.0  
0085170,0.00105155,0.,0.30474365,0.,0.02287525,0.01752628,0.,-0.147678  
12,-0.17440949,0.,0.00463229,-0.00014945,0.,-0.03127518,-0.01069662,0.  
0.00118045,-0.00016025,0.,0.00168792,-0.00712323,0.,0.14890946,0.1743  
3769,-0.00316751,0.,0.,0.01207644,0.,0.,-0.05354284,0.,0.,0.00005554,0  
.,0.,0.00906922,0.,0.,0.00855872,0.,0.,0.00003161,0.,0.,0.03365734,0.,  
-0.03572790,0.01168392,0.,-0.00253814,-0.00386877,0.,-0.27430059,0.143  
50884,0.,0.00013913,0.00001534,0.,0.00694479,-0.00326056,0.,0.00085169  
,-0.00105158,0.,-0.00105830,0.00068090,0.,0.30474365,0.,-0.02287522,0.  
01752628,0.,-0.00463229,-0.00014945,0.,0.14767812,-0.17440949,0.,-0.00  
118045,-0.00016025,0.,0.03127518,-0.01069662,0.,-0.00168792,-0.0071231  
8,0.,-0.00068090,0.00041628,0.,-0.14890946,0.17433769,0.00927002,0.,0.  
0.00161643,0.,0.,-0.00008883,0.,0.,-0.04423297,0.,0.,0.00891249,0.,0.  
0.00390455,0.,0.,-0.00404184,0.,0.,-0.00178928,0.,0.,0.03108541,0.,0.  
00194947,-0.00030838,0.,0.00467152,-0.00266339,0.,0.00018692,-0.001165  
05,0.,-0.31508748,0.12917819,0.,-0.00337332,-0.00454887,0.,-0.01939388  
0.01786075,0.,0.00063759,0.00071379,0.,0.00002877,0.00009433,0.,0.330  
23576,0.,0.00101217,-0.00856657,0.,0.03554060,-0.00616607,0.,-0.002103  
78,-0.00136763,0.,0.12835574,-0.14283185,0.,-0.00410534,-0.00158583,0.  
,-0.01855148,0.01606200,0.,-0.00078647,0.00073995,0.,0.00021052,0.0001  
4239,0.,-0.13957537,0.14165263,0.00926999,0.,0.,-0.00008883,0.,0.,0.00  
161643,0.,0.,0.00891249,0.,0.,-0.04423297,0.,0.,0.00390455,0.,0.,-0.00  
178928,0.,0.,-0.00404184,0.,0.,0.00026665,0.,0.,0.03108541,0.,0.001949  
46,0.00030838,0.,0.00018692,0.00116505,0.,0.00467152,0.00266339,0.,-0.  
00337332,0.00454887,0.,-0.31508748,-0.12917819,0.,-0.01939388,-0.01786  
080,0.,0.00002877,-0.00009433,0.,0.00063759,-0.00071379,0.,-0.00099449  
,-0.00094010,0.,0.33023576,0.,-0.00101219,-0.00856656,0.,0.00210378,-0  
.00136763,0.,-0.03554060,-0.00616607,0.,0.00410534,-0.00158583,0.,-0.1  
2835574,-0.14283185,0.,0.01855148,0.01606195,0.,-0.00021052,0.00014239  
0.,0.00078647,0.00073995,0.,0.00094010,0.00063229,0.,0.13957537,0.141  
65263,-0.00380821,0.,0.,0.01009783,0.,0.,0.01009783,0.,0.,0.00734338,0  
.,0.,0.00734339,0.,0.,-0.05283287,0.,0.,-0.00077068,0.,0.,-0.00077067,  
0.,0.,-0.00491099,0.,0.,-0.00491099,0.,0.,0.03316289,0.,-0.00088455,0.  
0.,-0.00603637,-0.00335639,0.,-0.00603637,0.00335639,0.,0.00878333,-0  
.03222547,0.,0.00878333,0.03222547,0.,-0.07565907,0.,0.,0.00020680,-0.  
00165998,0.,0.00020680,0.00165998,0.,0.00113466,0.00093486,0.,0.001134  
66,-0.00093486,0.,0.06835247,0.,0.,0.00056637,0.,-0.00371346,0.0005758  
4,0.,0.00371346,0.00057584,0.,0.00332594,-0.01153773,0.,-0.00332594,-0  
.01153773,0.,0.,-0.38102358,0.,0.00023296,-0.00073780,0.,-0.00023296,-  
0.00073780,0.,-0.00046896,0.00095531,0.,0.00046896,0.00095531,0.,0.,0.  
40185149,-0.00032581,0.,0.,0.00002704,0.,0.,0.00002703,0.,0.,0.0001902

4,0.,0.,0.00019022,0.,0.,-0.00002534,0.,0.,-0.00013674,0.,0.,-0.00013674,0.,0.,0.00000836,0.,0.,0.00000839,0.,0.,-0.00004092,0.,0.,0.00021427,0.,-0.00068515,0.00000001,0.,0.00000635,0.00043264,0.,0.00000634,-0.00043263,0.,0.00005933,0.00010261,0.,0.00005933,-0.00010262,0.,-0.0001117,0.,0.,0.00007253,0.00002761,0.,0.00007255,-0.00002763,0.,0.00000455,0.00000857,0.,0.00000455,-0.00000856,0.,0.00001432,0.,0.,0.00049649,0.,-0.00000002,-0.00902678,0.,0.00277866,0.00145724,0.,-0.00277866,0.00145724,0.,-0.00054149,0.00027490,0.,0.00054144,0.00027494,0.,0.,-0.0010063,0.,-0.00043732,0.00011425,0.,0.00043734,0.00011421,0.,-0.00005714,0.00033339,0.,0.00005718,0.00033343,0.,0.,0.00009448,0.,0.,0.00467333\\0.,0.,0.00012917,0.,0.00001070,-0.00000019,0.,-0.00001070,-0.00000019,0.,-0.00006894,-0.00006928,0.,0.00006894,-0.00006928,0.,0.,-0.00008565,0.,-0.00002510,0.00003628,0.,0.00002510,0.00003628,0.,0.00000775,0.00001372,0.,-0.00000775,0.00001372,0.,0.,0.00000096,0.,0.,-0.00000533\\\\@

1\\1\GINC-RSCQC9\FOpt\UMP2-FU\6-31G(d)\C5H5Cl1N1(2)\AXN501\19-Jan-1996\0\\# UMP2=FULL/6-31G\* SCF=DIRECT FOPT MAXDISK=920000000\\c1-pyridine structure\\0,2\N,-0.3058369725,0.,0.\C,0.3632472034,1.162218664,0.\C,0.3632472034,-1.162218664,0.\C,1.7606732106,1.2027777849,0.\C,1.7606732106,-1.2027777849,0.\C,2.4716782962,0.,0.\H,-0.2450353692,2.0623723841,0.\H,-0.2450353692,-2.0623723841,0.\H,2.2744610899,2.1593910229,0.\H,2.2744610899,-2.1593910229,0.\H,3.5579856426,0.,0.\Cl,-2.6937113542,0.,0.\\Version=IBM-RS6000-G94RevC.2\State=2-A1\HF=-706.1422858\MP2=-707.0880065\PUHF=-706.1464965\PMP2-0=-707.091125\S2=0.774\S2-1=0.762\S2A=0.751\RMSD=9.657e-09\RMSF=2.750e-05\Dipole=2.0954325,0.,0.\PG=C02V [C2(H1C1N1C11),SGV(C4H4)]\\@

#### MeNH-CH<sub>2</sub> (15)

1\\1\GINC-RSCQC9\FOpt\UMP2-FU\6-31G(d)\C2H6N1(2)\AXN501\15-Nov-1995\1\\# MP2=FULL/6-31G(D) FOPT=Z-MATRIX SCF=DIRECT GEOM=CHECK\\CH3-N(H)=CH2 2c-2e, C1 structure (15)\\0,2\C\N,1,r1\H,2,r2,1,a1\H,1,r3,2,a2,3,aa1,0\H,1,r4,2,a3,3,aa2,0\C,2,r5,1,a4,3,aa3,0\H,6,r6,2,a5,1,aa4,0\H,6,r7,2,a6,1,aa5,0\H,6,r8,2,a7,1,aa6,0\\r1=1.392451\r2=1.01458455\r3=1.08360617\r4=1.08448718\r5=1.45383066\r6=1.09255983\r7=1.09184854\r8=1.09821327\aa1=112.93244707\aa2=115.65839059\aa3=115.23232847\aa4=117.11805974\aa5=108.56629122\aa6=109.37118229\aa7=113.40551413\aa1=40.6658715\aa2=182.94835315\aa3=133.22514696\aa4=56.87010902\aa5=174.62629352\aa6=296.56676185\\Version=IBM-RS6000-G94RevC.2\HF=-133.6146869\MP2=-134.0316485\PUHF=-133.6175527\PMP2-0=-134.0333641\S2=0.76\S2-1=0.752\S2A=0.75\RMSD=9.155e-09\RMSF=3.131e-05\Dipole=0.1141626,0.1794633,0.3575886\PG=C01 [X(C2H6N1)]\\@

#### MeCH<sub>2</sub>-NH (16)

1\\1\GINC-RSCQC2\FOpt\UMP2-FU\6-31G(d)\C2H6N1(2)\AXN501\18-Jan-1996\1\\# UMP2=(FULL)/6-31G\* FOPT=Z-MATRIX\\HN-ch2ch3 ncf structure for aces2\\0,2\C\C,1,r1\N,2,r2,1,a1\H,3,r3,2,a2,1,180.,0\H,1,r4,2,a3,3,180.,0\H,1,r5,2,a4,3,aa1,0\H,1,r5,2,a4,3,-aa1,0\H,2,r6,1,a5,3,aa2,0\H,2,r6,1,a5,3,-aa2,0\\r1=1.51824125\r2=1.44929073\r3=1.02917917\r4=1.09338533\r5=1.09193823\r6=1.10170394\aa1=110.81412632\aa2=106.62818383\aa3=111.08541072\aa4=110.16929665\aa5=110.56259115\aa1=59.5723515\aa2=121.73224733\\Version=IBM-RS6000-G94RevC.2\State=2-A\HF=-133.6295291\MP2=-134.0343527\PUHF=-133.6329226\PMP2-0=-134.0364505\S2=0.76\S2-1=0.752\S2A=0.75\RMSD=8.335e-09\RMSF=7.662e-05\Dipole=-0.6619608,0.,0.3557218\PG=CS [SG(C2H2N1),X(H4)]\\@

#### N-Methylpyridinyl (17)

1\\1\GINC-EIGEN\FOpt\UMP2-FU\6-31G(d)\C6H8N1(2)\AXN501\30-Jan-1996\0\\# UMP2=FULL/6-31G\* FOPT\\N-methyl-pyridine, 2A', (me17b), structure\\0,2\N,-0.8955175716,0.,0.0299426435\C,-0.1792214197,1.1916512625,0.0338685427\C,-0.1792214197,-1.1916512625,0.0338685427\C,1.1575840047,1.2001912789,0.1271348992\C,1.1575840047,-1.2001912789,0.1271348992\C,1.9040

860171,0.,0.1853546201\H,-0.7798677067,2.0930622849,-0.0080581478\H,-0.7798677067,-2.0930622849,-0.0080581478\H,1.6599479989,2.1623436139,0.157268397\H,1.6599479989,-2.1623436139,0.157268397\H,2.9838912353,0.,0.2464702545\C,-2.2829871409,0.,-0.3896533204\H,-2.3827080897,0.,-1.4826210542\H,-2.779832503,-0.8858147459,0.0109413477\H,-2.779832503,0.8858147459,0.0109413477\\Version=IBM-RS6000-G94RevC.2\State=2-A'\HF=-286.2662206\MP2=-287.1820253\PUHF=-286.2886971\PMP2-0=-287.20156\S2=1.049\S2-1=0.962\S2A=0.807\RMSD=9.227e-09\RMSF=1.467e-05\Dipole=-0.8583896,0.,-0.1835908\PG=CS [SG(C2H2N1),X(C4H6)]\\@

#### 4-Methylpyridinyl (18)

1\1\GINC-PC\FOpt\UMP2-FU\6-31G(d)\C6H8N1(2)\AXN501\25-Jan-1996\0\\# UMP2=FULL/6-31G\* FOPT SCF=DIRECT\\4-me-pyridine (me18), 2A', structure\\0,2\N,-0.2237860171,-1.8670738956,0.\C,-0.2282022017,-1.1439413854,1.1523073288\C,-0.2282022017,-1.1439413854,-1.1523073288\C,-0.2282022017,0.1990506923,1.2230566303\C,-0.2282022017,0.1990506923,-1.2230566303\C,-0.19585382,1.0502311509,0.\H,-0.2337235444,-1.7400643915,2.0616581877\H,-0.2337235444,-1.7400643915,-2.0616581877\H,-0.2275279198,0.6923813375,2.1914902327\H,-0.2275279198,0.6923813375,-2.1914902327\H,-1.0842645232,1.7068673678,0.\C,1.0350013555,1.9790650343,0.\H,1.9503537554,1.3835110407,0.\H,1.0324417214,2.6187080874,-0.8871527543\H,1.0324417214,2.6187080874,0.8871527543\\Version=SGI-G94RevC.3\State=2-A'\HF=-286.2763202\MP2=-287.1744411\PUHF=-286.3075083\PMP2-0=-287.2020717\S2=1.167\S2-1=1.056\S2A=0.862\RMSD=8.004e-09\RMSF=1.041e-04\Dipole=1.1094638,0.,0.053451\PG=CS [SG(C2H2N1),X(C4H6)]\\@