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CH3Cl

RHF/6-31+G* OPT

optimization of CH3Cl

0 1

C11

C2 C11 r1

H3 C2 r2 C11 a1

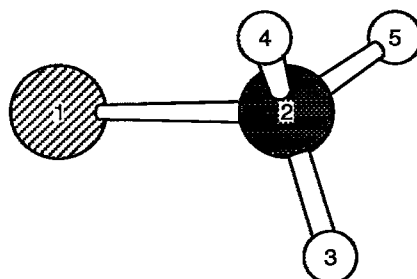
H4 C2 r2 C11 a1 H3 -120.0

H5 C2 r2 C11 a1 H3 120.0

r1=1.78542407

r2=1.0779256

a1=108.44977903



Version=SGI-G92RevG.

HF=-499.094158

RMSD=1.727e-09

RMSF=8.936e-05

Dipole=0. 0. 0.91032

PG=C03V [C3(C1C11) 3

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FEB 23 1998
Journal of Organic Chemistry

NH3.crd
RHF/6-31+G* OPT

optimization of NH3

0 1
X1
N2 X1 1.
H3 N2 r1 X1 a1
H4 N2 r1 X1 a1 H3 120. 0
H5 N2 r1 X1 a1 H3 -120.0

r1=1.00210032
a1=110.76323264

Version=SGI-G92RevG.
HF=-56.1894994
RMSD=9.173e-09
RMSF=5.020e-05
Dipole=0. 0. 0.73132
PG=C03V [C3(N1) 3SGV

NH4+.crd
MP2/6-31+G* GEOM=CHECK

MP2/6-31+G* calculation

1 1
H01
N02 1 1.0133588928
H03 2 1.0133588928 1 109.48
H04 2 1.0133588928 1 109.48 3 120. 0
H05 2 1.0133588928 1 109.48 3 -120. 0

Version=SGI-G94RevC.2
HF=-56.5312766
MP2= -56.7004066

TS(CH3Cl+NH3)

MP4/6-31+G* GEOM=CHECK

TS for NH3 as a nucleophile

0 1

H01

C02 H01 1.0645471858

Cl03 C02 2.4741977553 H01 83.92759505

H04 C02 1.0645436674 Cl03 83.93052369 H01 120.00026272

H05 C02 1.0645202630 Cl03 83.95723542 H01 -119.99840419

N06 C02 1.8995786430 H01 96.08260715 Cl03 179.99093370

H07 N06 1.0052732083 C02 111.03663717 H04 -59.88035483

H08 N06 1.0052782779 C02 111.07406348 H07 119.94809902

H09 N06 1.0052880410 C02 111.13924218 H07 -120.01085660

Version=SGI-G92RevG.2

HF=-555.2259759

MP2=-555.6602421

MP3=-555.6933655

MP4D=-555.7033452

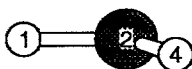
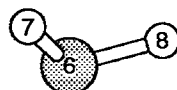
MP4DQ=-555.6968018

MP4SDQ=-555.7016508

MP4SDTQ=-555.7129522

RMSD=2.554e-09

PG=C01 [X(C1H6Cl1N1.)]



NH3CH3+

MP4/6-31+G*

OptiMP4 of NH2CH3

1 1

N01	-0.0181169966	-0.0000000009	-0.0055585262
C02	-0.0016197296	-0.0000000009	1.5014059542
H03	1.0262159855	0.0000000019	1.8268385757
H04	-0.5104019026	0.8872499106	1.8421990439
H05	-0.5104019028	-0.8872499115	1.8421990458
H06	0.4482799780	-0.8139320741	-0.3833176916
H07	0.4482799781	0.8139320732	-0.3833176895
H08	-0.9617257038	0.0000000019	-0.3687946581

Version=DEC-AXP-OSF/1-G94RevC.2

HF=-95.5741589

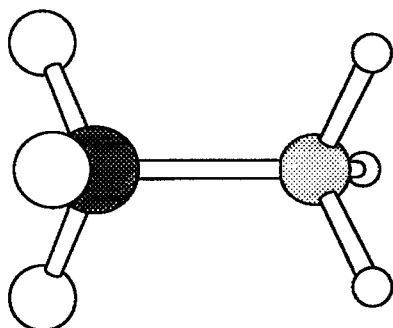
MP2=-95.8691522

MP3=-95.8929898

MP4D=-95.9003645

MP4DQ=-95.8965013

MP4SDTQ=-95.9040889



NH2CH3

MP4/6-31+G*

OptiMP4 of NH2CH3

0 1

N01

C02 N01 1.4595772900

H03 C02 1.0847095100 N01 110.52677142

H04 C02 1.0854855500 N01 111.64142778 H03 119.92262190

H05 C02 1.0854855500 N01 111.64142778 H03 -119.92262190

H06 N01 0.9988299500 C02 112.32792276 H03 119.18846077

H07 N01 0.9988299500 C02 112.32792276 H03 -119.18846077

Version=SGI-G92RevG.2

State=1-A'

HF=-95.2106912

MP2=-95.5113198

MP3=-95.5321846

MP4D=-95.5394936

MP4DQ=-95.53555

MP4SDQ=-95.5376223

MP4SDTQ=-95.5445427

RMSD=7.315e-09

PG=CS [SG(C1H1N1),X(H4)]

TS(CH3Cl+NH2CH3)

MP4/6-31+G* GEOM=CHECK

mp4 calculation

0 1

H01

C02 H01 1.0641645010

Cl03 C02 2.4218939187 H01 85.38709707

H04 C02 1.0642925131 Cl03 85.54731341 H01 120.00885762

H05 C02 1.0641673800 Cl03 85.38812569 H01 -119.97928142

N06 C02 1.9426533093 H01 94.34158153 Cl03 179.53434161

H07 N06 1.0044188129 C02 107.92670367 H04 -57.38854092

H08 N06 1.0044157689 C02 107.92135229 H07 114.75596518

C09 N06 1.4682424943 C02 112.97242969 H07 -122.63197100

H10 C09 1.0813987831 N06 108.97964336 C02 59.15553959

H11 C09 1.0834117549 N06 112.10059179 H10 120.89172619

H12 C09 1.0813782132 N06 108.97642171 H10 -118.21863915

Version=SGI-G92RevG.2

HF=-594.2553493

MP2=-594.8210541

MP3=-594.8633228

MP4D=-594.8769191

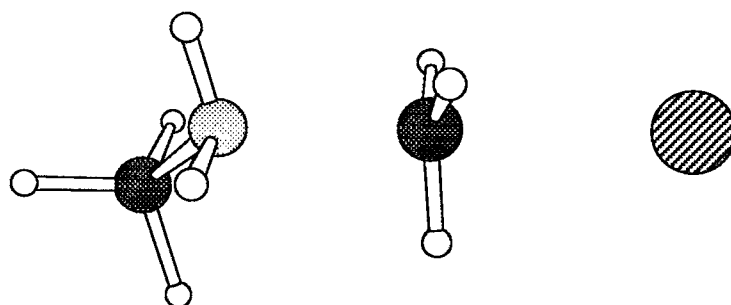
MP4DQ=-594.8678102

MP4SDQ=-594.8741936

MP4SDTQ=-594.8905207

RMSD=1.649e-09

PG=C01 [X(C2H8Cl1N1)]



NH(CH₃)₂

MP4/6-31+G*

optimization of NH(CH₃)₂

0 1

C01

N02	1	1.44740756			
C03	2	1.44751798	1	113.59404712	
H04	3	1.08387741	2	109.66902526	182.15309967 0
H05	3	1.09320724	2	113.56475676	121.44688733 0
H06	3	1.08499543	2	109.44652469	-118.02012014 0
H07	1	1.08387281	2	109.66762504	177.77613905 0
H08	1	1.08497797	2	109.4365586	118.02991348 0
H09	1	1.09320177	2	113.55499756	-121.43702145 0
H10	2	1.00048896	3	110.08973348	123.95026957 0

HF=-134.242641

MP2=-134.673942

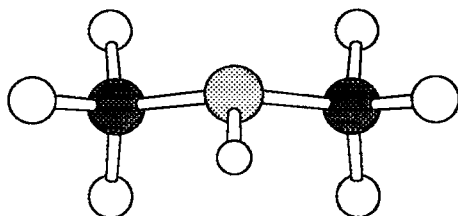
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MP4D=-134.714736

MP4DQ=-134.7083243

MP4SDQ=-134.7116794

MP4SDTQ=-134.7234393



TS(CH3Cl+NH(CH3)2)

MP4/6-31+G* GEOM=CHECK

TS for NH2CH3 as a nucleophile

0 1

H01
C02 H01 1.0640253872
Cl03 C02 2.3937206555 H01 86.16757817
H04 C02 1.0640211528 Cl03 86.16486478 H01 120.02949005
H05 C02 1.0642012983 Cl03 86.19649163 H01 -119.98557635
N06 C02 1.9647906718 H01 94.06557704 Cl03 179.61141250
H07 N06 1.0038386910 C02 104.98100150 H04 -60.03771270
C08 N06 1.4632791936 C02 110.31362348 H07 117.23404227
H09 C08 1.0818972804 N06 109.56159478 C02 -58.18283924
H10 C08 1.0825839283 N06 109.12124808 H09 118.68339034
H11 C08 1.0855909836 N06 111.76183595 H09 -120.99804735
C12 N06 1.4633032337 C02 110.33641519 H07 -117.25287282
H13 C12 1.0818979284 N06 109.56075908 C02 58.14130206
H14 C12 1.0855921910 N06 111.76316166 H13 120.99613680
H15 C12 1.0825824163 N06 109.12171741 H13 -118.68663699

Version=SGI-G92RevG.2

HF=-633.2858089

MP2=-633.9861696

MP3=-634.0366857

MP4D=-634.0540005

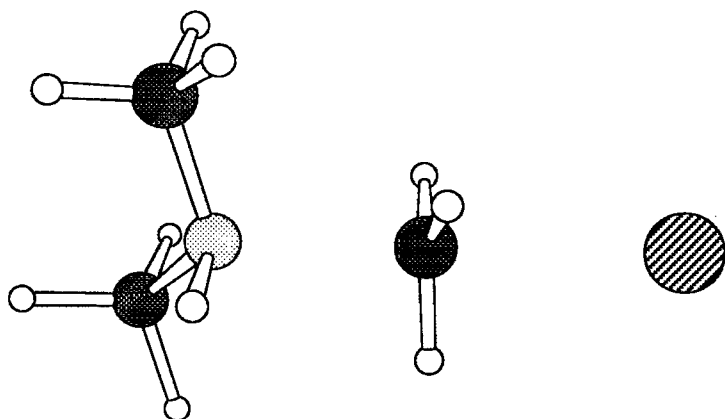
MP4DQ=-634.0421807

MP4SDQ=-634.0501516

MP4SDTQ=-634.071963

RMSD=2.081e-09

PG=C01 [X(C3H10C11N1)]



NH₂(CH₃)₂⁺

MP4/6-31+G*

MP4 of H(+)NH(CH₃)₂

1 1

C01	-0.4599257651	0.0103567997	-1.2037748362
N02	-0.4499709224	-0.0205293312	0.2944828762
C03	0.9190416949	0.0105715599	0.9033074013
H04	0.8215794199	-0.0145706599	1.9777739193
H05	1.4667545264	-0.8510984639	0.5547411291
H06	1.4104522525	0.9188369170	0.5910716708
H07	-1.4835673214	-0.0151135143	-1.5445363737
H08	0.0226553576	0.9187078324	-1.5292514565
H09	0.0789681964	-0.8512167711	-1.5660556995
H10	-0.9353340041	-0.8468214267	0.6122110192
H11	-0.9864075487	0.7594112470	0.6454702672

Version=DEC-AXP-OSF/1-G94RevC.2

HF=-134.6142655

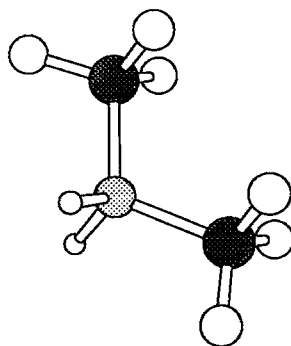
MP2=-135.0387342

MP3=-135.0722332

MP4D=-135.0830847

MP4DQ=-135.0768533

MP4SDTQ=-135.0900657



NH(CH₃)₃⁺

RHF/6-31+G* OPT OPTCYC=100

optimizationofproducts

1 1

C01	-1.3896871467	-0.1658477255	0.3062138644
N02	0.1052251425	-0.1524792385	0.2819717809
C03	0.6466606487	1.2409852310	0.3070185323
C04	0.6470696401	-0.9360935389	-0.8703657413
H05	-1.7310421457	0.3672695462	1.1804222695
H06	-1.7515562950	0.3179923496	-0.5884445862
H07	-1.7307912124	-1.1893608864	0.3384831752
H08	0.4197735264	-0.6082399234	1.1248484815
H09	0.3229119049	-0.4667763423	-1.7869506682
H10	1.7250463655	-0.9394906487	-0.8162298511
H11	0.2691889844	-1.9456896116	-0.8165553807
H12	0.2681760379	1.7486465680	1.1810927890
H13	1.7246325775	1.1978455210	0.3400671283
H14	0.3228254061	1.7508942973	-0.5877357560

Version=DEC-AXP-OSF/1-G94RevD.2

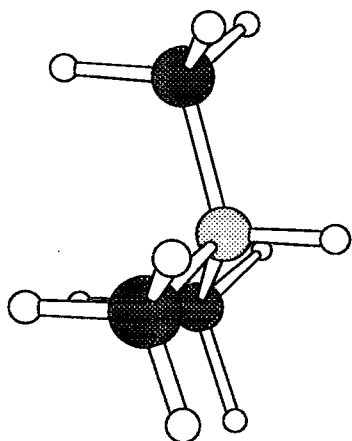
HF=-173.6516132

RMSD=5.452e-09

RMSF=1.936e-05

Dipole=0.1117632,-0.1619489,0.2994909

PG=C01 [X(C3H10N1)]



mp2nn.zmt 1
MP2=MAXDISK=200000000/6-31+G* SCF=DIRECT

optimization of nn

0 1

C01

C02 C01 1.5540860000

C03 C02 1.5354620600 C01 108.04410858

C04 C03 1.5354244300 C02 108.59843972 C01 58.97254763

C05 C04 1.5540913100 C03 108.03278285 C02 -58.97040759

N06 C01 1.4587661400 C02 111.45341221 C03 -0.00126513

C07 N06 1.4587884800 C01 109.77571161 C02 60.37006043

C08 C03 1.5355224700 C02 108.60181849 C01 -58.95936619

H09 C01 1.0845434900 C02 111.09909734 C03 120.59741111

H10 C01 1.0845436500 C02 111.09421893 C03 -120.60130789

H11 C02 1.0869788400 C01 110.97020832 N06 120.75884334

H12 C02 1.0869641600 C01 110.96872509 N06 -120.75168433

H13 C03 1.0858315800 C02 110.32845202 C01 -180.00006030

H14 C04 1.0869821400 C03 110.07495791 C02 62.34484168

H15 C04 1.0869748100 C03 110.06528839 C02 179.71621896

H16 C05 1.0845435600 C04 111.09469532 C03 120.60550780

H17 C05 1.0845422900 C04 111.09356434 C03 -120.59844037

H18 C07 1.0845439800 N06 108.08021382 C01 61.98756489

H19 C07 1.0845593200 N06 108.08513433 C01 177.27980963

H20 C08 1.0869760500 C03 110.07136608 C02 -62.35040928

H21 C08 1.0869755400 C03 110.06934066 C02 -179.71778614

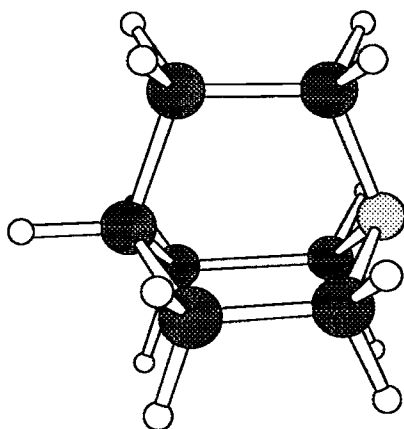
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MP2=-328.1686701

RMSD=1.513e-09

PG=C01 [X(C7H13N1)]



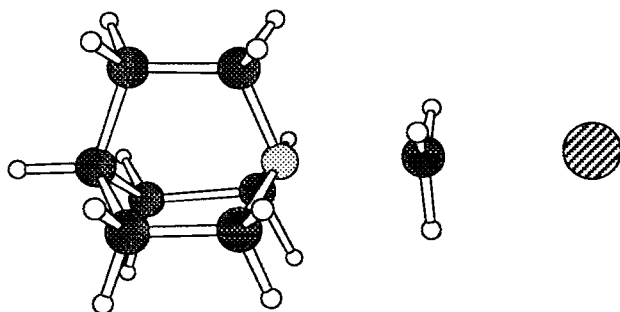
mp2ch3clnn.zmt 1 (TS)
MP2=MAXDISK=200000000/6-31+G* GEOM=CHECK SCF=DIRECT

optimization of TS of CH3Cl+NC5N(CH3)

0 1

C01
C02 C01 1.5488300984
C03 C02 1.5338093413 C01 108.42854459
C04 C03 1.5338073952 C02 108.65712345 C01 56.70219668
C05 C04 1.5488308577 C03 108.42883995 C02 -61.35298334
N06 C01 1.4723025081 C02 110.89683215 C03 4.06641722
C07 N06 1.4723014329 C01 109.76254926 C02 57.91633075
C08 C03 1.5338084197 C02 108.65627173 C01 -61.35478690
H09 C01 1.0831302651 C02 111.55309387 C03 124.39817244
H10 C01 1.0831862017 C02 111.46152481 C03 -115.87081323
H11 C02 1.0851752645 C01 110.43485012 N06 125.12442557
H12 C02 1.0854333201 C01 110.56371865 N06 -116.79435820
H13 C03 1.0843948808 C02 110.27428099 C01 -182.32580634
H14 C04 1.0854338645 C03 110.15741155 C02 59.75878981
H15 C04 1.0851749579 C03 110.38206365 C02 177.55619491
H16 C05 1.0831299248 C04 111.55320929 C03 124.39574067
H17 C05 1.0831865067 C04 111.46148712 C03 -115.87312589
H18 C07 1.0831862574 N06 107.66134901 C01 59.37545308
H19 C07 1.0831303261 N06 107.92512601 C01 174.73062297
H20 C08 1.0851751640 C03 110.38247258 C02 -64.38787770
H21 C08 1.0854336284 C03 110.15718689 C02 -182.18542812
C22 N06 1.9974902580 C07 109.17838655 C05 119.64011060
H23 C22 1.0636257083 N06 92.68604226 C07 57.89961223
H24 C22 1.0636256544 N06 92.68605120 H23 120.00042364
H25 C22 1.0636259101 N06 92.68602210 H23 -119.99957102
Cl26 C22 2.3583396232 H23 87.31401375 N06 180.00000767

Version=SGI-G92RevG.2
HF=-826.1303194
MP2=-827.4901926
RMSD=6.680e-09
FG=



1(H+)

MP2=MAXDISK=600000000/6-31+G* GEOM=CHECK

optimization of HN(CH3)2NC5+

1 1

C01	-1.4580735896	-0.0000616681	-0.6959011116
C02	-1.4120404816	-0.0001124019	0.8465198988
C03	0.0513749768	-0.0000480027	1.3076145896
C04	0.7525596382	1.2506861337	0.7615654583
C05	0.6846070429	1.2382309959	-0.7799649290
N06	-0.0480281159	0.0000454044	-1.2213861545
C07	0.6847579258	-1.2380879573	-0.7800587509
C08	0.7526999565	-1.2506603380	0.7614712443
H09	-1.9441876030	-0.8758867852	-1.1012101868
H10	-1.9442963564	0.8757312103	-1.1011493278
H11	-1.9285888027	0.8709819170	1.2301505305
H12	-1.9284929131	-0.8712902624	1.2300898365
H13	0.0938464810	-0.0000861885	2.3888258995
H14	0.2784241873	2.1462571021	1.1435962698
H15	1.7860499264	1.2750252514	1.0842223603
H16	0.1446293511	2.0829789494	-1.1830396349
H17	1.6605381121	1.2074075253	-1.2428388216
H18	0.1448878837	-2.0828690027	-1.1832080433
H19	1.6606882025	-1.2071029000	-1.2429233586
H20	0.2786593691	-2.1463133582	1.1434274438
H21	1.7861903411	-1.2749120943	1.0841343239
H22	-0.0874641727	0.0000808697	-2.2278526067

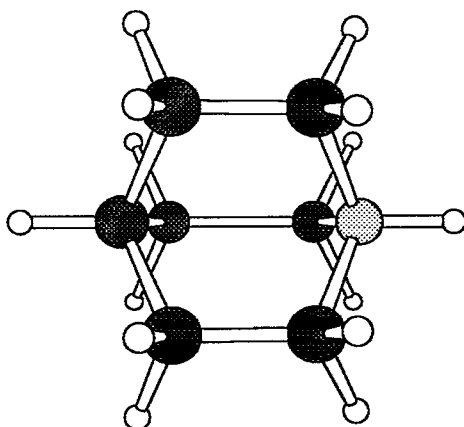
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HF=-327.4770041

MP2=-328.5513526

RMSD=7.739e-09

PG=C01 [X(C7H14N1)]



1(CH3+)

MP2=MAXDISK=400000000/6-31+G*

optimizationofproducts ch3qp-ca+

1 1

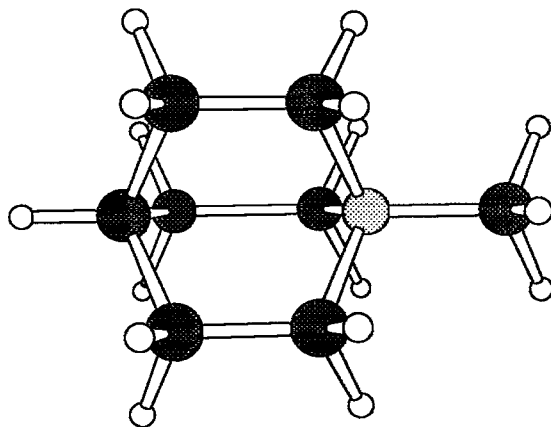
N01	-0.3184968006	-0.8687014244	-0.0001713574
C02	1.1893450441	-0.8803673684	-0.0001640139
C03	1.7381741117	0.5609143139	-0.0002240090
C04	0.5675223170	1.5479166585	0.0003057611
C05	-0.2879461961	1.3035182342	1.2465167092
C06	-0.8100774489	-0.1475495786	1.2294674636
C07	-0.2884891194	1.3042086594	-1.2456679544
C08	-0.8100610606	-0.1470705905	-1.2295352215
C09	-0.8308430482	-2.2661247103	-0.0004458972
H10	-0.4668656851	-0.7187134339	2.0801211279
H11	-1.8892636785	-0.1966144806	1.2052595577
H12	0.2944833026	1.4734924999	2.1436323938
H13	-1.1223134195	1.9934859451	1.2730506680
H14	0.9400093984	2.5638692252	0.0005051180
H15	2.3623812086	0.7159212072	-0.8715855043
H16	2.3630125186	0.7157207894	0.8707176177
H17	1.4936863680	-1.4369367570	-0.8749448008
H18	1.4936601860	-1.4368530545	0.8746800127
H19	-1.8892338197	-0.1965703699	-1.2056409881
H20	-0.4664015506	-0.7176427310	-2.0804061753
H21	0.2934214393	1.4750994513	-2.1429449839
H22	-1.1231103471	1.9939075087	-1.2712254237
H23	-0.4745646273	-2.7756520071	0.8822392908
H24	-1.9103772822	-2.2490570183	-0.0003026805
H25	-0.4747940056	-2.7752205133	-0.8834727551

Version=DEC-AXP-OSF/1-G94RevD.2

HF=-366.5106195

MP2=-367.723622

RMSD=2.887e-09



MP2/6-31+G* GEOM=CHECK

NC5H5 nucleophile

0 1

N01

C02	N01	1.3190496924			
C03	C02	1.3880284052	N01	121.68569539	
N04	C03	1.3190933691	C02	121.69304859	N01 0.00000000
C05	N01	1.3193385559	C02	116.62347776	C03 0.00000000
C06	C05	1.3877307707	N01	121.68654773	C02 0.00000000
H07	C02	1.0746231985	N01	117.40072841	C05 180.00000000
H08	C03	1.0746205986	C02	120.90981206	N01 180.00000000
H09	C05	1.0746051586	N01	117.39000011	C02 180.00000000
H10	C06	1.0746063967	C05	120.92293248	N01 180.00000000

Version=SGI-G92RevG.2

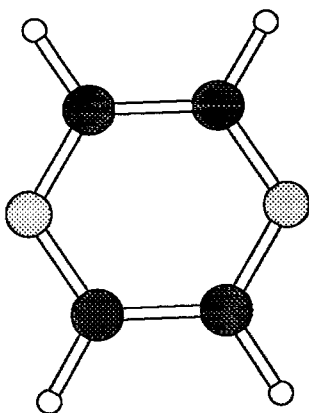
State=1-A'

HF=-262.6904798

MP2=-263.5170806

RMSD=3.363e-09

PG=CS [SG(C4H4N2)]



2 (TS)

MP2/6-31+G* GEOM=CHECK

N2C4H4 nucleophile

0 1

H01					
C02	H01	1.0646623299			
C103	C02	2.4630657604	H01	84.15997620	
H04	C02	1.0645957429	C103	84.06689590	H01 119.83315436
H05	C02	1.0646609810	C103	84.15968960	H01 -120.33828083
N06	C02	1.8861448998	H01	95.78353271	C103 179.89812137
C07	N06	1.3194874938	C02	121.63339056	H04 -0.17231858
C08	C07	1.3871272216	N06	120.23780166	C02 180.01064929
N09	C08	1.3171994882	C07	121.57734025	N06 0.00015239
C10	N06	1.3214870904	C07	118.76091551	C08 -0.00083566
C11	C10	1.3850505263	N06	120.26701270	C07 0.00067264
H12	C07	1.0736070100	N06	117.81782167	C10 179.99875370
H13	C08	1.0734327188	C07	120.72340737	N06 180.00034434
H14	C10	1.0740522459	N06	117.59982669	C07 180.00134116
H15	C11	1.0733691095	C10	120.79021950	N06 179.99993787

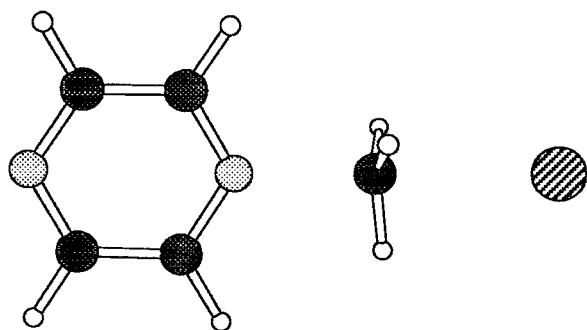
Version=SGI-G92RevG.2

HF=-761.7201625

MP2=-762.8144398

RMSD=3.401e-09

PG=C01 [X(C5H7C11N2)]



2(H+)

MP2=MAXDISK=200000000/6-31+G* GEOM=CHECK

NC5H6+ nucleophile

1 1

N01	-1.0902609558	0.0000000000	-0.6718821086
C02	-1.1562771839	0.0000000000	0.6572524558
C03	0.0345948806	0.0000000000	1.3595965967
N04	1.1976915090	0.0000000000	0.7380843178
C05	0.0673377216	0.0000000000	-1.3283150543
C06	1.2300467325	0.0000000000	-0.5802506802
H07	-2.1258474541	0.0000000000	1.1143372907
H08	0.0364769196	0.0000000000	2.4321525353
H09	0.0398079832	0.0000000000	-2.3998738336
H10	2.1889769200	0.0000000000	-1.0606991495
H11	-1.9456411459	0.0000000000	-1.1990322160

Version=SGI-G94RevC.2

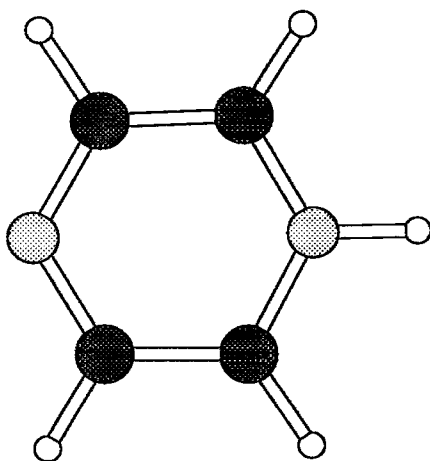
State=1-A'

HF=-263.0364746

MP2=-263.8548814

RMSD=9.532e-09

PG=CS [SG(C4H5N2)]



2(CH3)+

RHF/6-31+G* OPT OPTCYC=100

optimization CH3-2+

1 1

N01	-0.9482480565	-1.6322972146	0.0000000000
C02	0.3710724556	-1.6140831065	0.0000000000
C03	1.0793658595	-0.4289268921	0.0000000000
N04	0.4141189369	0.7275223267	0.0000000000
C05	-0.9154450924	0.7262479483	0.0000000000
C06	-1.5896729733	-0.4845281165	0.0000000000
C07	1.1756595943	2.0023910762	0.0000000000
H08	-2.6625014398	-0.5050601313	0.0000000000
H09	-1.4197422211	1.6717326468	0.0000000000
H10	2.1509624743	-0.3868024054	0.0000000000
H11	0.8875554874	-2.5544911836	0.0000000000
H12	1.7888747175	2.0387336998	-0.8875588685
H13	0.4790010381	2.8239724325	0.0000000000
H14	1.7888747175	2.0387336998	0.8875588685

Version=DEC-AXP-OSF/1-G94RevD.2

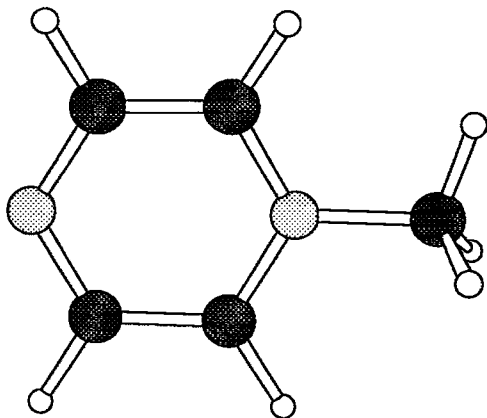
State=1-A'

HF=-302.0765311

RMSD=7.907e-09

RMSF=1.759e-04

Dipole=0.7556331,1.3244524,0.



NC5H5 **3a**

MP2/6-31+G* GEOM=CHECK

NC5H5 nucleophile

0 1

N01

C02 N01 1.3216189205

C03 C02 1.3872341759 N01 123.55422959

C04 C03 1.3851618493 C02 118.23310600 N01 0.00000000

C05 N01 1.3219634173 C02 117.80648711 C03 0.00000000

C06 C05 1.3869114328 N01 123.55055520 C02 0.00000000

H07 C02 1.0756786426 N01 116.12490118 C05 180.00000000

H08 C03 1.0745172217 C02 120.33072653 N01 180.00000000

H09 C04 1.0755646210 C03 120.69654437 C02 180.00000000

H10 C05 1.0756571103 N01 116.11143694 C02 180.00000000

H11 C06 1.0745185269 C05 120.34071683 N01 180.00000000

Version=SGI-G92RevG.2

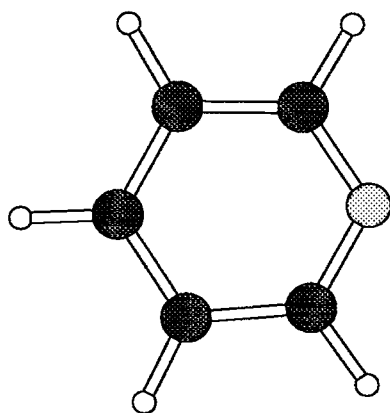
State=1-A'

HF=-246.7034911

MP2=-247.4960717

RMSD=7.669e-09

PG=CS [SG(C5H5N1)]



TS(3a + CH3Cl)

MP2/6-31+G* GEOM=CHECK SCF=DIRECT

optimization of TS of CH3Cl+NC5

0 1

H01

C02 H01 1.0638371069

C103 C02 2.4321659268 H01 85.32859582

H04 C02 1.0639677421 C103 85.21081844 H01 119.81332630

H05 C02 1.0638379004 C103 85.32848241 H01 -120.37610241

N06 C02 1.9266254735 H01 94.63558608 C103 179.93660548

C07 N06 1.3236738829 C02 121.28023138 H04 -0.09862708

C08 C07 1.3827380093 N06 122.24956008 C02 180.00820191

C09 C08 1.3855255164 C07 118.34710801 N06 0.00021265

C10 N06 1.3251862822 C07 119.64913875 C08 -0.00060386

C11 C10 1.3813057928 N06 122.27819119 C07 0.00053907

H12 C07 1.0745430408 N06 116.54650830 C02 0.00790744

H13 C08 1.0734084418 C07 120.07557836 N06 180.00027000

H14 C09 1.0747205858 C08 120.42978328 C07 -179.99989522

H15 C10 1.0750176341 N06 116.34998383 C02 -0.00762643

H16 C11 1.0734123230 C09 121.56359264 C08 179.99976011

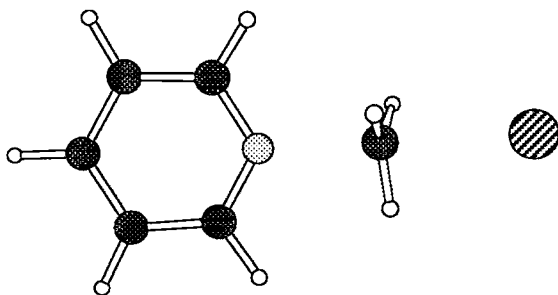
Version=SGI-G92RevG.2

HF=-745.7408382

MP2=-746.8005388

RMSD=9.559e-09

PG=C01 [X(C6H8C11N1)]



HNC5H5+ **3a**(H+)

MP2=MAXDISK=200000000/6-31+G* GEOM=CHECK

NC5H6+ nucleophile

1 1

N01	-1.1118368139	0.0000000000	-0.6695486088
C02	-1.1733737505	0.0000000000	0.6670775019
C03	-0.0139672905	0.0000000000	1.4002650477
C04	1.2017629943	0.0000000000	0.7236963951
C05	0.0407918183	0.0000000000	-1.3490941592
C06	1.2311695395	0.0000000000	-0.6672771434
H07	-2.1521194881	0.0000000000	1.1049523122
H08	-0.0609197455	0.0000000000	2.4717293038
H09	2.1220788366	0.0000000000	1.2778966426
H10	-0.0299332232	0.0000000000	-2.4189910157
H11	2.1562710893	0.0000000000	-1.2098903749
H12	-1.9708196389	0.0000000000	-1.1868624596

Version=SGI-G94RevC.2

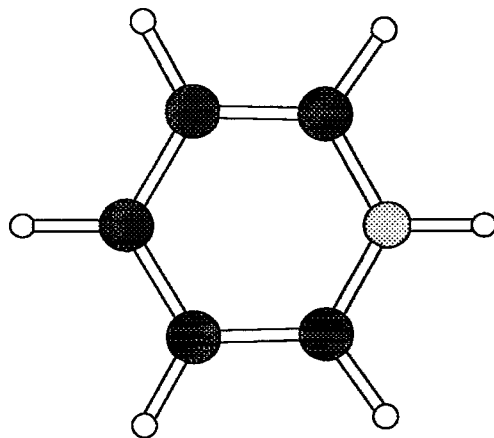
State=1-A'

HF=-247.0736721

MP2=-247.8550019

RMSD=6.063e-09

PG=CS [SG(C5H6N1)]



3a (CH3+)

RHF/6-31+G* OPT OPTCYC=100

optimization CH3-3a+

1 1

C01	-0.1817197268	-1.1687777448	-0.0000135123
C02	1.1932839285	-1.1940066906	-0.0000201723
C03	1.8840578741	0.0085083824	-0.0000000249
C04	1.1744230172	1.2043325754	0.0000200433
C05	-0.1962755971	1.1582885191	0.0000135313
N06	-0.8512865411	-0.0114847756	0.0000001309
C07	-2.3323324019	0.0020254310	0.0000000739
H08	-0.7691654650	-2.0652983870	-0.0000284405
H09	1.7034255303	-2.1376754926	-0.0000386878
H10	2.9583421353	0.0164751280	-0.0000000743
H11	1.6720474104	2.1546785026	0.0000384300
H12	-0.8023164679	2.0435604172	0.0000282916
H13	-2.6802649346	0.5101420713	-0.8868313811
H14	-2.6914195986	-1.0138332872	-0.0000117712
H15	-2.6802653863	0.5101216421	0.8868430832

Version=DEC-AXP-OSF/1-G94RevD.2

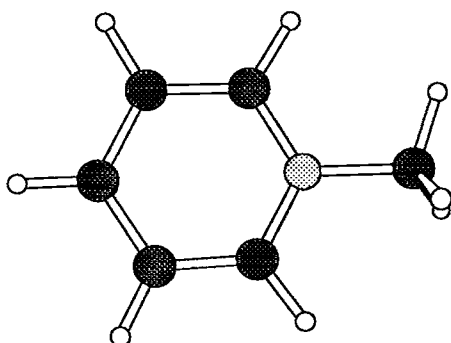
HF=-286.1101954

RMSD=3.125e-09

RMSF=1.034e-04

Dipole=-0.3897489,-0.0035792,-0.0000002

PG=C01 [X(C6H8N1)]



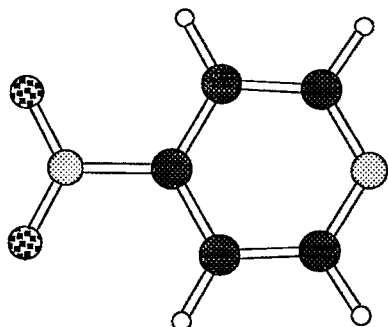
nc5no2.crd **3b**
MP2/6-31+G* GEOM=CHECK GUESS=READ

NC5H5 nucleophile

0 1

N01	-2.1375389161	0.0000000000	-1.2985624016
C02	-2.1496044549	0.0000000000	0.0217222094
C03	-0.9998804676	0.0000000000	0.7982753254
C04	0.2018513076	0.0000000000	0.1226338790
C05	-0.9713637531	0.0000000000	-1.9177177096
C06	0.2476664332	0.0000000000	-1.2552489621
H07	-3.1158951123	0.0000000000	0.4914783631
H08	-1.0424053361	0.0000000000	1.8682639337
N09	1.4557753988	0.0000000000	0.8843863328
H10	-0.9997820911	0.0000000000	-2.9917635406
H11	1.1776661626	0.0000000000	-1.7860778553
O12	1.3739401380	0.0000000000	2.0738074167
O13	2.4736531878	0.0000000000	0.2636104743

Version=Sun-SVR4-Unix-G94RevC.2
State=1-A'
HF=-450.1743705
MP2=-451.5091806
RMSD=2.612e-09
PG=CS [SG(C5H4N2O2)]



TS(3b +CH3Cl)

MP2=MAXDISK=400000000/6-31+G* GEOM=CHECK GUESS=READ

no2 TS

0 1

H01	2.6489831970	-0.0342538141	-1.2590965229
C02	2.6220976989	-0.0341313240	-0.1946928827
C103	5.0824383274	-0.0311572886	-0.3974643735
H04	2.7818070702	-0.9522413696	0.3201309004
H05	2.7788148741	0.8792144656	0.3296328545
N06	0.7489362246	-0.0321075718	-0.0427829248
C07	0.1158057960	-1.0150553628	0.5745598542
C08	-1.2622044515	-1.0389629188	0.7009697428
C09	-1.9551770797	0.0171344572	0.1499477833
C10	0.0692193983	0.9758882619	-0.5672100063
C11	-1.3091864140	1.0502512859	-0.4973114195
H12	0.7214121347	-1.8039408104	0.9789738848
H13	-1.7636578202	-1.8406920000	1.2032744891
N14	-3.4214513000	0.0437453732	0.2545043134
H15	0.6431285263	1.7418342143	-1.0548461505
H16	-1.8479291297	1.8706612156	-0.9253277078
O17	-3.9379333726	-0.8666353713	0.8205547212
O18	-3.9795334498	0.9737454961	-0.2349891649

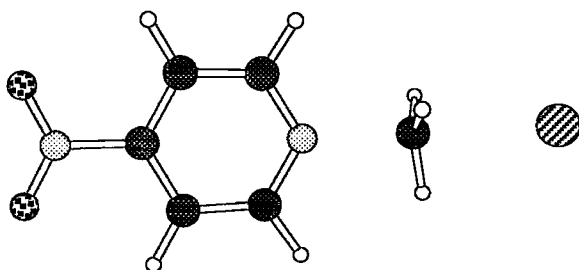
Version=Sun-SVR4-Unix-G94RevC.2

HF=-949.2014279

MP2=-950.805351

RMSD=1.516e-09

PG=C01 [X(C6H7Cl1N2O2)]



3b(H+)

MP2/6-31+G* GEOM=CHECK GUESS=READ

NC5H5 nucleophile

1 1

N01	-2.0561965672	0.0000000000	-1.2220968504
C02	-2.1148963807	0.0000000000	0.1124154964
C03	-0.9518232375	0.0000000000	0.8458081182
C04	0.2385814957	0.0000000000	0.1417682256
C05	-0.9120670800	0.0000000000	-1.9114319735
C06	0.2880813325	0.0000000000	-1.2403096053
H07	-3.0903752767	0.0000000000	0.5575873767
H08	-0.9707805301	0.0000000000	1.9171493162
N09	1.5068641105	0.0000000000	0.8955938069
H10	-0.9871996974	0.0000000000	-2.9810577240
H11	1.2200680465	0.0000000000	-1.7690172719
O12	1.4126420482	0.0000000000	2.0780942753
O13	2.5005480244	0.0000000000	0.2476990366
H14	-2.9191627069	0.0000000000	-1.7349884548

Version=Sun-SVR4-Unix-G94RevC.2

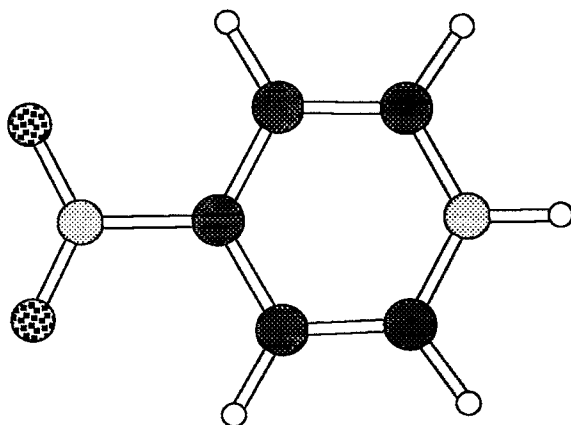
State=1-A'

HF=-450.5164562

MP2=-451.8455683

RMSD=1.004e-09

PG=CS [SG(C5H5N2O2)]



3b(CH3+)

RHF/6-31+G* OPT OPTCYC=100

optimization CH3-3b+

1 1

C01	-0.3593051257	-1.7195889885	0.0000000000
N02	0.9751595291	-1.7112545047	0.0000000000
C03	1.6593324235	-0.5604993928	0.0000000000
C04	1.0141395647	0.6524536399	0.0000000000
C05	-0.3680896654	0.6350660308	0.0000000000
C06	-1.0802082203	-0.5448317353	0.0000000000
N07	-1.0998046646	1.9135276739	0.0000000000
C08	1.7346399547	-2.9885346917	0.0000000000
H09	-0.8404220176	-2.6770088904	0.0000000000
H10	-2.1517353863	-0.5567658759	0.0000000000
H11	1.5655555519	1.5712586034	0.0000000000
H12	2.7291139717	-0.6369574854	0.0000000000
H13	2.3474860845	-3.0286745385	0.8876393185
H14	1.0366976860	-3.8088830441	0.0000000000
H15	2.3474860845	-3.0286745385	-0.8876393185
O16	-2.2843373075	1.8406127976	0.0000000000
O17	-0.4362526444	2.8975627536	0.0000000000

Version=DEC-AXP-OSF/1-G94RevD.2

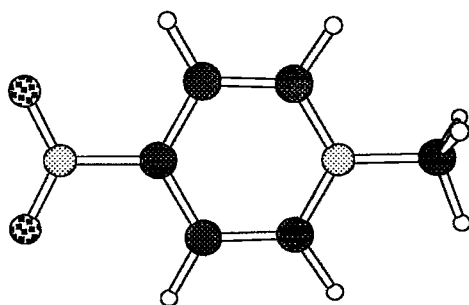
State=1-A'

HF=-489.555101

RMSD=7.160e-09

RMSF=5.712e-05

Dipole=2.0454982,-3.5745824,0.



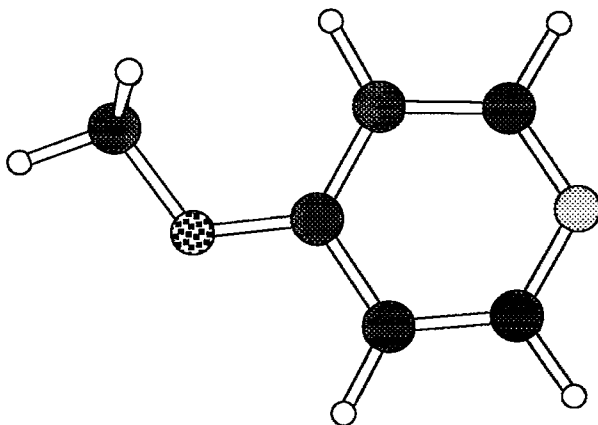
nc5och3.crd **3c**
MP2/6-31+G* GEOM=CHECK GUESS=READ

NC5H5 nucleophile

0 1

N01	-1.8820307268	-0.0092602252	-1.3283327035
C02	-1.8684070574	-0.0046690110	-0.0124856586
C03	-0.7172912674	0.0004496728	0.7670513911
C04	0.5071769718	0.0009177808	0.1139756298
C05	-0.7010597539	-0.0088888855	-1.9369214502
C06	0.5093220591	-0.0039071544	-1.2802185553
H07	-2.8291438489	-0.0051771842	0.4723563659
H08	-0.8016079435	0.0037739355	1.8358851372
O09	1.6991198376	0.0053420756	0.7187095727
H10	-0.7249250154	-0.0125361534	-3.0122040107
H11	1.4396873910	-0.0036855531	-1.8158912168
C12	1.7771875447	0.0143582670	2.1208992482
H13	2.8292370882	0.0194656310	2.3599079925
H14	1.3101390331	0.9021073756	2.5318636289
H15	1.3162987011	-0.8714270970	2.5429308157

Version=Sun-SVR4-Unix-G94RevC.2
HF=-360.5899856
MP2=-361.6925109
RMSD=2.009e-09
PG=C01 [X(C6H7N1O1)]



3c (TS)

MP2=MAXDISK=400000000/6-31+G* GEOM=CHECK GUESS=READ

no2 TS

0 1

H01	2.4076512003	0.0768232049	-1.2969133004
C02	2.4129912898	0.0747971710	-0.2334243281
C103	4.8252662002	0.0675762843	-0.4198704710
H04	2.5325059299	-0.8467168198	0.2842680397
H05	2.5335804006	0.9886264892	0.2970640877
N06	0.4766217692	0.0753693978	-0.0807720973
C07	-0.1742735923	-0.8978026503	0.5273486290
C08	-1.5504985517	-0.9325058650	0.6559263399
C09	-2.2849633822	0.1177437335	0.1131615628
C10	-0.2277581345	1.0808004126	-0.6002767427
C11	-1.5937038579	1.1494631893	-0.5316396150
H12	0.4231400709	-1.6932146546	0.9351620918
H13	-2.0106876594	-1.7561112381	1.1634205053
O14	-3.6031840963	0.2240160071	0.1565114337
H15	0.3374513751	1.8545882458	-1.0875706343
H16	-2.1342905006	1.9714813686	-0.9591654849
C17	-4.3863426129	-0.7674880816	0.7855959048
H18	-5.4085027812	-0.4424756742	0.6804567831
H19	-4.2577761741	-1.7258337847	0.2978597429
H20	-4.1361839546	-0.8457261790	1.8363772925

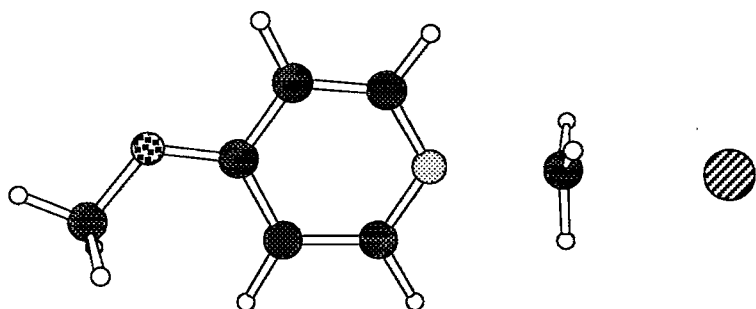
Version=Sun-SVR4-Unix-G94RevC.2

HF=-859.6299771

MP2=-860.9989576

RMSD=3.491e-09

PG=C01 [X(C7H10C11N1O1)]



3c (H+)

MP2/6-31+G* GEOM=CHECK GUESS=READ

optimization of HNC5OCH3+

1 1

N01	-1.7749171141	-0.0015410652	-1.2950829696
C02	-1.8397869818	-0.0008925870	0.0414667361
C03	-0.7073678445	-0.0000097905	0.8024322601
C04	0.5410009452	0.0002027031	0.1519655009
C05	-0.5944514096	-0.0013857103	-1.9484315791
C06	0.5729386639	-0.0005419348	-1.2607177657
H07	-2.8210138380	-0.0011171903	0.4745527030
H08	-0.7946322750	0.0004402095	1.8694800117
O09	1.6877742960	0.0009526786	0.7522581264
H10	-0.6399587279	-0.0019533671	-3.0196555647
H11	1.5163643285	-0.0004120942	-1.7699180178
C12	1.8105481201	0.0025494582	2.1759929134
H13	2.8694047078	0.0040258846	2.3664589362
H14	1.3581744213	0.8943798298	2.5863118421
H15	1.3603248754	-0.8895574153	2.5880788636
H16	-2.6237270211	-0.0021726614	-1.8240413925

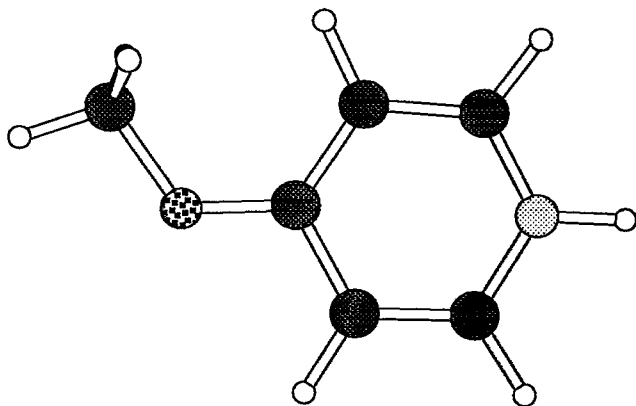
Version=Sun-SVR4-Unix-G94RevC.2

HF=-360.9721071

MP2=-362.0615043

RMSD=1.980e-09

PG=C01 [X(C6H8N1O1)]



3c (CH3+)

RHF/6-31+G* OPT OPTCYC=100

optimization CH3-3c+

1 1

C01	-0.5957662712	-1.5840692926	-0.0000074333
N02	0.7520721903	-1.5877867061	0.0000054233
C03	1.4134113898	-0.4235135544	0.0000126710
C04	0.7748259354	0.7837230215	0.0000083848
C05	-0.6297050337	0.8030734179	-0.0000036297
C06	-1.3101435756	-0.4287534789	-0.0000113524
O07	-1.3617527610	1.8748536365	-0.0000095492
C08	-0.7946934553	3.1841639793	-0.0000098211
C09	1.5111730944	-2.8552208284	0.0000138735
H10	-1.0764291036	-2.5419740003	-0.0000120869
H11	-2.3822430080	-0.4464788714	-0.0000207101
H12	1.3601221160	1.6804632641	0.0000152915
H13	2.4846758035	-0.4863487813	0.0000232809
H14	2.1260227616	-2.9056857063	0.8864285979
H15	0.8154698502	-3.6782845363	-0.0000082115
H16	2.1260623888	-2.9056728701	-0.8863740652
H17	-0.2016173969	3.3337889019	-0.8915723934
H18	-1.6355231026	3.8556539018	-0.0000214154
H19	-0.2016360568	3.3337969622	0.8915639870

Version=DEC-AXP-OSF/1-G94RevD.2

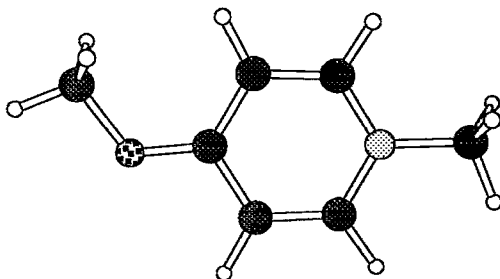
HF=-400.006741

RMSD=7.183e-09

RMSF=4.983e-05

Dipole=1.0039861,-0.8148477,0.000007

PG=C01 [X(C7H10N1O1)]



3d

MP2=MAXDISK=200000000/6-31+G* SCF=DIRECT

optimization of N(CH3)2NC5

0 1

C01

N02 C01 1.4483852400

C03 N02 1.4483697600 C01 117.82107291

H04 C03 1.0830403300 N02 110.93576478 C01 141.14997379

H05 C03 1.0889919800 N02 112.45442603 H04 121.74279239

H06 C03 1.0800769900 N02 109.01842459 H04 -118.10983015

H07 C01 1.0830555700 N02 110.94023031 C03 218.94349493

H08 C01 1.0800715300 N02 109.01852978 H07 118.11626672

H09 C01 1.0889812200 N02 112.45050361 H07 -121.74204456

C10 N02 1.3721421300 C03 119.29468053 C01 158.49550591

C11 C10 1.4043216500 N02 122.18246220 C03 11.14614874

C12 C11 1.3812403600 C10 119.31619913 N02 178.67185258

C13 C10 1.4043156400 N02 122.17828840 C11 179.46424806

C14 C13 1.3812430600 C10 119.31638025 C11 0.82809735

N15 C14 1.3223196300 C13 125.00895026 C10 -0.36069688

H16 C11 1.0712240700 C10 121.94366791 C13 179.19885076

H17 C12 1.0763933600 C11 118.98984595 C10 180.18513907

H18 C13 1.0712255400 C10 121.94278432 C11 180.79271831

H19 C14 1.0763933300 C13 118.98964449 C10 179.81136034

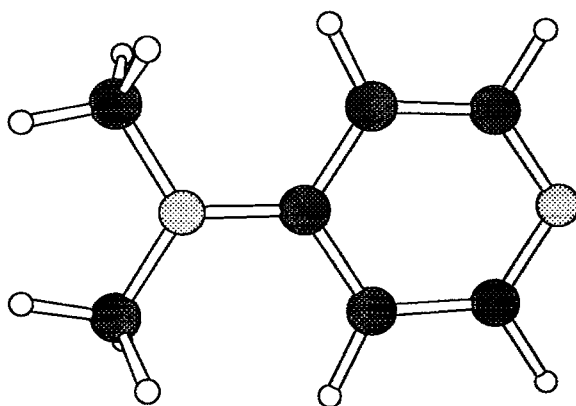
Version=SGI-G92RevG.2

HF=-379.7896231

MP2=-381.0162608

RMSD=6.905e-09

PG=C01 [X(C7H10N2)]



3d(TS)

MP2=MAXDISK=240000000/6-31+G* SCF=DIRECT

optimization of TS of CH3Cl+NC5N(CH3)

0 1

H01					
C02	H01	1.0634927000			
Cl03	C02	2.4018809000	H01	86.40963706	
H04	C02	1.0630731100	Cl03	86.52497594	H01 -119.79517750
H05	C02	1.0630728000	Cl03	86.52507275	H04 -120.40903191
N06	C02	1.9655395500	H01	93.54116213	Cl03 179.99999213
C07	N06	1.3276624300	C02	120.29367461	H01 180.01883869
C08	C07	1.3717254200	N06	123.96862099	C02 180.00441989
C09	C08	1.4120310500	C07	119.45416477	N06 0.00033706
C10	N06	1.3265807000	C02	122.39257229	C07 180.00537318
C11	C09	1.4111559000	C08	115.83732701	C07 0.00027641
N12	C09	1.3516133600	C08	122.06154290	C07 -180.00017725
C13	N12	1.4522831800	C09	120.26121473	C08 0.00360000
C14	N12	1.4522412600	C09	120.23574854	C08 -180.00006613
H15	C07	1.0758140900	N06	116.15701820	C02 0.00430134
H16	C08	1.0704822300	C07	118.71572565	N06 -179.99992501
H17	C10	1.0754289000	N06	116.31059794	C02 -0.00422174
H18	C11	1.0704746700	C09	121.83595888	C08 -180.00029750
H19	C13	1.0786617700	N12	109.04749976	C09 179.99673467
H20	C13	1.0851821400	N12	111.46218292	C09 60.86577717
H21	C13	1.0851821500	N12	111.46219165	C09 -60.87231169
H22	C14	1.0786622600	N12	109.05309751	C09 -180.00079519
H23	C14	1.0851901800	N12	111.45657496	C09 -60.86358302
H24	C14	1.0851892000	N12	111.45621684	C09 60.86246320

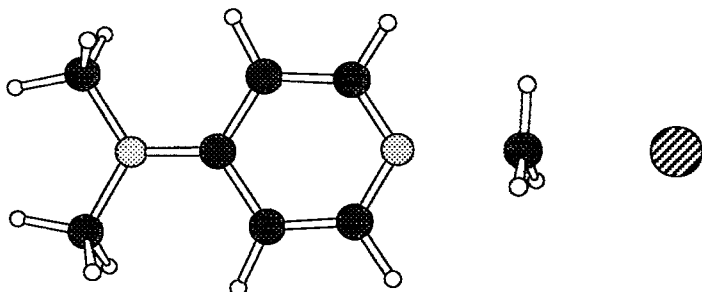
Version=SGI-G92RevG.2

HF=-878.8338018

MP2=-880.326564

RMSD=3.977e-09

PG=C01 [X(C8H13C11N2)]



3d(H+)

MP2=MAXDISK=400000000/6-31+G* GEOM=CHECK

optimization of HN(CH3)2NC5+

1 1

C01	1.2561040992	0.6134050002	-2.2254349106
N02	1.2876829509	0.4141872339	-0.7742851560
C03	2.5550359108	0.6118697154	-0.0662844705
H04	2.4692335896	1.4054058109	0.6655995942
H05	2.8713313697	-0.3012861775	0.4224157263
H06	3.3113062486	0.8917097959	-0.7796886772
H07	0.5702943937	1.4080818453	-2.4916662970
H08	2.2410243118	0.8923041448	-2.5591244377
H09	0.9713476500	-0.2988733372	-2.7347266251
C10	0.1958614323	0.0631506917	-0.1177342292
C11	0.1957104789	-0.1391481267	1.2990730807
C12	-0.9436655242	-0.4983664102	1.9333482914
C13	-1.0560278222	-0.1373133967	-0.7817039541
C14	-2.1505109840	-0.4965900533	-0.0728038508
N15	-2.0979108310	-0.6746890402	1.2614751608
H16	1.0830802389	-0.0131605449	1.8820831203
H17	-0.9793556920	-0.6580804582	2.9931682873
H18	-1.1552003651	-0.0098276680	-1.8386425783
H19	-3.1036462122	-0.6549328499	-0.5380565368
H20	-2.9228659168	-0.9398724391	1.7575486489

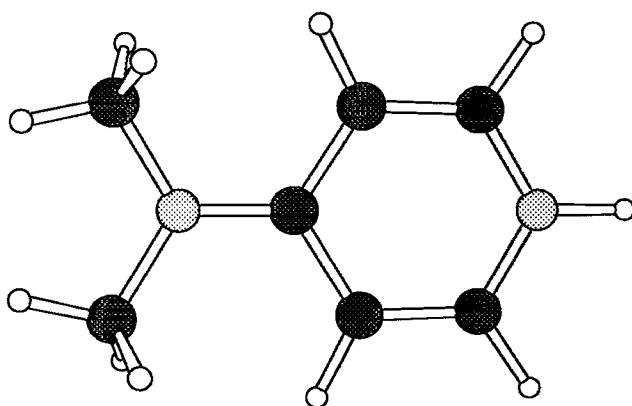
Version=SGI-G94RevC.2

HF=-380.1879162

MP2=-381.4016625

RMSD=8.612e-10

PG=C01 [X(C7H11N2)]



3d(CH3+)

RHF/6-31+G* OPT OPTCYC=100

optimization CH3-3d+

1 1

C01	-0.2892486173	-1.8136229999	0.0007864003
N02	1.0560170359	-1.8284471326	0.0011293717
C03	1.7122405885	-0.6509100159	0.0007483180
C04	1.0758853776	0.5444324204	-0.0000007678
C05	-0.3507422976	0.5976462264	-0.0004082354
C06	-1.0111382132	-0.6652081079	0.0000921059
N07	-1.0144292572	1.7440819846	-0.0011383498
C08	-0.2982841748	3.0203297018	-0.0028533007
C09	-2.4777105541	1.7564288887	0.0000397351
C10	1.8151986550	-3.0892409059	0.0017927878
H11	-0.7754426086	-2.7692301774	0.0010575847
H12	-2.0779504286	-0.7412677425	-0.0002522881
H13	1.6707519494	1.4333089651	-0.0000379061
H14	2.7837893910	-0.7085300671	0.0011560929
H15	2.4323899347	-3.1421254159	0.8871413642
H16	1.1222249096	-3.9152881366	0.0027564256
H17	2.4316623052	-3.1435332170	-0.8839817142
H18	0.3200911014	3.1169831847	-0.8869528023
H19	-1.0171220276	3.8222639117	-0.0060201442
H20	0.3172788480	3.1211051826	0.8827950223
H21	-2.8687494333	1.2686093245	0.8846444203
H22	-2.8169771270	2.7785553800	0.0015830766
H23	-2.8702658494	1.2705735968	-0.8850085446

Version=DEC-AXP-OSF/1-G94RevD.2

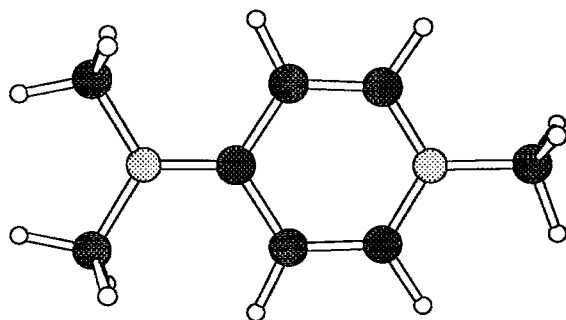
HF=-419.2212958

RMSD=5.949e-09

RMSF=3.002e-05

Dipole=0.3891464,-0.6582126,0.0004612

PG=C01 [X(C8H13N2)]



4a

MP2=MAXDISK=200000000/6-31+G* SCF=DIRECT

optimization of N(CH3)2Ph

0 1

C01					
N02	C01	1.4456590100			
C03	N02	1.4533570400	C01	111.98091449	
H04	C03	1.0798552100	N02	110.89509008	C01 174.75512223
H05	C03	1.0925372200	N02	112.11166358	H04 121.03908648
H06	C03	1.0836503000	N02	109.15888385	H04 -118.84485222
H07	C01	1.0822309400	N02	110.22637012	C03 186.11883668
H08	C01	1.0834927600	N02	108.64547977	H07 118.12915161
H09	C01	1.0927662800	N02	113.41777863	H07 -122.08676648
C10	N02	1.4142207000	C03	115.37115071	C01 137.34388574
C11	C10	1.3995376300	N02	118.84004068	C03 62.54827493
C12	C11	1.3809457400	C10	120.99276452	N02 179.45050394
C13	C10	1.3918381100	N02	123.10668781	C11 178.50911885
C14	C13	1.3918396500	C10	120.69762554	C11 -0.17902633
C15	C14	1.3815851900	C13	120.83736351	C10 -0.55188369
H16	C11	1.0746751700	C10	119.31266836	C13 182.33882267
H17	C12	1.0759408100	C11	119.37589250	C10 180.23327817
H18	C13	1.0731317100	C10	120.55312650	C11 179.92409696
H19	C14	1.0759955200	C13	119.09078894	C10 179.88191185
H20	C15	1.0751618700	C14	120.67386802	C13 180.16332344

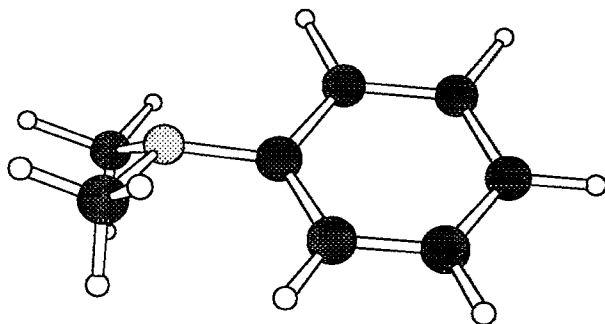
Version=SGI-G92RevG.2

HF=-363.7903429

MP2=-364.9868074

RMSD=4.009e-09

PG=C01 [X(C8H11N1)]



4a (TS)

MP2=MAXDISK=240000000/6-31+G* SCF=DIRECT

TS calculation

0 1

H01						
C02	H01	1.0636067700				
C103	C02	2.4106000600	H01	85.73698278		
H04	C02	1.0630571400	C103	85.49764458	H01	119.56296140
H05	C02	1.0630586200	C103	85.49990477	H04	120.87262348
N06	C02	1.9693279700	H01	92.93373725	C103	-179.99844107
C07	N06	1.4612096800	C02	114.41816334	H01	180.00033594
C08	C07	1.3932240000	N06	119.94083698	C02	-180.01141713
C09	C08	1.3836936400	C07	120.51778870	N06	180.00053627
C10	C09	1.3883900600	C08	120.22522691	C07	-0.00135498
C11	C07	1.3864648500	N06	120.89519799	C02	-0.01449201
C12	C10	1.3826497100	C09	119.38064761	C08	-0.00152018
C13	N06	1.4727415800	C02	104.21639453	H01	58.17333973
C14	N06	1.4727427800	C02	104.21915528	H01	-58.16877978
H15	C14	1.0809704900	N06	109.32691507	C02	-67.12781971
H16	C14	1.0820850500	N06	109.20475142	C02	52.04025435
H17	C14	1.0837987400	N06	111.78625255	C02	-187.81868586
H18	C13	1.0809712500	N06	109.32681438	C02	67.11108038
H19	C13	1.0837988100	N06	111.78596827	C02	187.80100666
H20	C13	1.0820854300	N06	109.20469618	C02	-52.05720029
H21	C11	1.0713127000	C07	121.38913569	N06	0.00119893
H22	C12	1.0748109800	C10	120.28886444	C09	-179.99905184
H23	C10	1.0748519600	C09	120.26949569	C08	180.00016015
H24	C09	1.0750944900	C08	119.54207172	C07	179.99844464
H25	C08	1.0743552900	C07	120.57994082	N06	-0.00112730

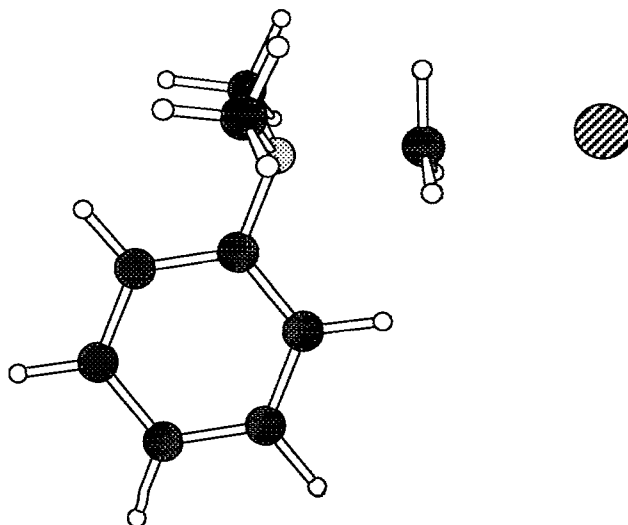
Version=SGI-G92RevG.2

HF=-862.8239037

MP2=-864.2970646

RMSD=9.701e-09

PG=C01 [X(C9H14Cl1N1)]



4a (H+)

MP2=MAXDISK=600000000/6-31+G* GEOM=CHECK

optimization of nme2php+

1 1

C01	2.2368917260	0.1328064047	1.2427178772
N02	1.5665425038	-0.3750008145	0.0001145210
C03	2.2370742331	0.1321986823	-1.2426740631
H04	1.7387058083	-0.2937692599	-2.0990914243
H05	2.1623253797	1.2070465993	-1.2662027125
H06	3.2745706582	-0.1666133325	-1.2180588372
H07	1.7381622185	-0.2924412628	2.0992895502
H08	3.2743051418	-0.1663443191	1.2186025366
H09	2.1624927821	1.2076954891	1.2655013209
C10	0.1030500954	-0.1599857444	-0.0000989673
C11	-0.7177642953	-1.2710391503	0.0001129304
C12	-2.0942500814	-1.0903622849	0.0001160290
C13	-0.4081894526	1.1265015630	-0.0002341066
C14	-1.7833160342	1.2935709658	-0.0001531776
C15	-2.6252899935	0.1888665741	0.0000000000
H16	-0.3090790141	-2.2674723050	0.0003144622
H17	-2.7410446644	-1.9476524333	0.0002682469
H18	0.2317117373	1.9898563130	-0.0003572404
H19	-2.1945034916	2.2857535260	-0.0002102010
H20	-3.6903369827	0.3277398063	0.0000561758
H21	1.6976557148	-1.3741351822	0.0003655763

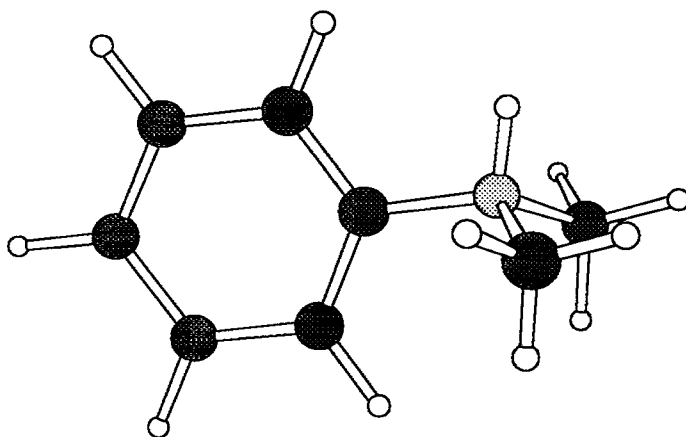
Version=SGI-G94RevC.2

HF=-364.1672993

MP2=-365.355905

RMSD=5.288e-09

PG=C01 [X(C8H12N1)]



4a (CH3+)

RHF/6-31+G* OPT OPTCYC=100

optimization CH3-4a+

1 1

C01	-2.1734418696	-1.1697858285	0.0001450186
C02	-0.7906640855	-1.1749583657	0.0001539034
C03	-0.0971095910	0.0298950426	-0.0000175082
C04	-0.7829161275	1.2315622802	-0.0001948203
C05	-2.1735456507	1.2236043771	-0.0002088493
C06	-2.8709005075	0.0307545243	-0.0000402419
N07	1.4002064018	-0.0148123917	0.0000212182
C08	1.8910780017	-0.7305400238	1.2287641810
C09	1.8911671344	-0.7303323516	-1.2288071948
C10	2.0257466546	1.3470066808	0.0001494271
H11	-2.7026214083	-2.1044770627	0.0002825574
H12	-0.2824534971	-2.1201806656	0.0003107867
H13	-0.2840155961	2.1784793096	-0.0003376218
H14	-2.6995031824	2.1600847389	-0.0003543404
H15	-3.9449346793	0.0313882841	-0.0000506623
H16	1.7278837344	1.8819685381	0.8871625566
H17	3.0966465156	1.2187033248	-0.0001382815
H18	1.7274399023	1.8823338780	-0.8864972081
H19	1.5301690915	-1.7444602427	1.2268983463
H20	2.9706428214	-0.7283960158	1.2196698662
H21	1.5208306951	-0.2114578134	2.0988412812
H22	1.5208566633	-0.2111917155	-2.0988222117
H23	2.9707321794	-0.7280456859	-1.2197076490
H24	1.5303981945	-1.7443001430	-1.2270694408

Version=DEC-AXP-OSF/1-G94RevD.2

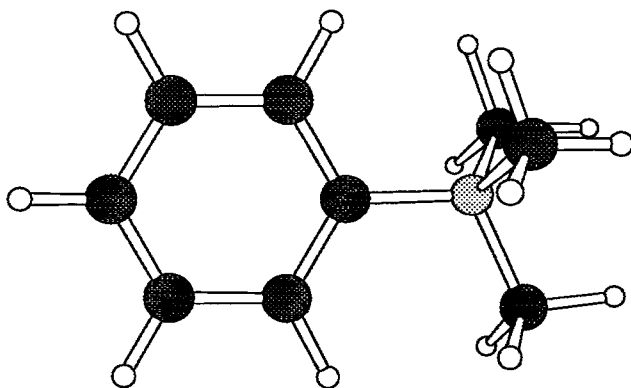
HF=-403.1924722

RMSD=7.896e-09

RMSF=1.382e-05

Dipole=1.7632376,-0.0233669,0.0000388

PG=C01 [X(C9H14N1)]



4b

MP2=MAXDISK=390000000/6-31+G* GEOM=CHECK GUESS=READ

MP2/6-31+G*//rhf/6-31+G*

0 1

N01	0.1064223872	0.0000008824	-2.2778176046
C02	0.0699213240	0.0000003665	-0.9085278198
C03	1.2315477110	0.0000006921	-0.1090140763
C04	1.1515563135	0.0000001511	1.2661289498
C05	-1.1672934877	-0.0000005345	-0.2316448385
C06	-1.2327023201	-0.0000010685	1.1452806619
C07	-0.0775414252	-0.0000007370	1.9190851705
H08	2.2075963678	-0.0000005912	-0.5474627754
H09	2.0593681950	-0.0000009890	1.8418054273
H10	-2.0872993529	-0.0000008236	-0.7789914200
H11	-2.1951205104	-0.0000017521	1.6240389616
C12	-0.1502303123	-0.0000012968	3.3566297933
N13	-0.2076728054	-0.0000017396	4.4937131837
C14	1.3199503605	0.0000018118	-3.0673492176
H15	2.2013022728	0.0000061367	-2.4519643264
H16	1.3601759697	-0.8807332840	-3.7019736430
H17	1.3601709539	0.8807366274	-3.7019763014
C18	-1.1236828671	0.0000005072	-3.0407368209
H19	-0.8769976413	-0.0000006845	-4.0930737577
H20	-1.7247970065	-0.8822614143	-2.8403906878
H21	-1.7247981015	0.8822600351	-2.8403913461

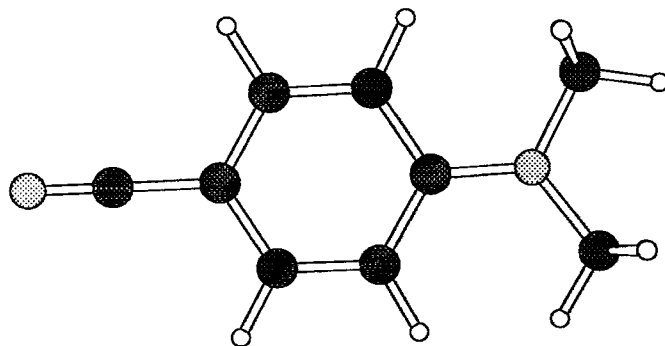
Version=SGI-G94RevC.2

HF=-455.5277257

MP2=-456.998943

RMSD=8.202e-09

PG=C01 [X(C9H10N2)]



4b (TS)

MP2=MAXDISK=590000000/6-31+G* GEOM=CHECK GUESS=READ

mp2/6-31+G* calculation

0 1

H01	1.8527238432	0.0000427143	-2.7222140468
C02	1.8356643589	-0.0000050108	-1.6583125687
C103	4.2556892219	-0.0000480252	-1.8168818805
H04	1.9692424177	-0.9218299793	-1.1454056080
H05	1.9692807573	0.9217668975	-1.1453231580
N06	-0.1073072619	0.0000282746	-1.5616618619
C07	-0.6399430359	0.0000172058	-0.2033416763
C08	-2.0188273398	0.0000351105	0.0006357248
C09	-2.5410407006	0.0000218633	1.2784283433
C10	-1.6852376799	-0.0000097998	2.3759721975
C11	0.2082368478	-0.0000163374	0.8937046205
C12	-0.3135246367	-0.0000292921	2.1801520243
C13	-0.5112429296	-1.2153450315	-2.2939041156
C14	-0.5111912604	1.2154437925	-2.2938642218
H15	-0.1849479468	2.0882578025	-1.7461365046
H16	-0.0395440442	1.2137403539	-3.2670927329
H17	-1.5849205201	1.2636731641	-2.4296892157
H18	-0.1851048025	-2.0881913904	-1.7461657453
H19	-1.5849678391	-1.2634855513	-2.4297975396
H20	-0.0395339819	-1.2136690986	-3.2671028430
H21	1.2729263180	-0.0000344523	0.7794390970
H22	0.3515922606	-0.0000549905	3.0232921783
H23	-3.6048805395	0.0000357901	1.4260681797
H24	-2.6965374907	0.0000585320	-0.8319175140
C25	-2.2301522726	-0.0000225942	3.7147896591
N26	-2.6639060682	-0.0000325174	4.7650157901

Version=SGI-G94RevC.2

HF=-954.5554508

MP2=-956.3061445

RMSD=5.215e-09

PG=C01 [X(C10H13C11N2)]

