

Molecule 3

Singlet

UHF/STO-3G

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1 | 1 | UNPC-UNK | FOpt | UHF | STO-3G | C11H9N1 | PCUSER | 18-Oct-2002 | 0 | | #UHF STO-3G
OPT GUESS=(ALWAYS,MIX) | | molecule 7 | | 0,1 | C,1.5190246997,0.,0.579798236
6 | C,1.5130749495,0.,1.9972648708 | H,2.465347361,0.,2.5148212848 | C,0.305
8933798,0.,2.7592901194 | H,0.3640187854,0.,3.8401679138 | C,-0.902816084,
0.,2.1207829304 | H,-1.8343977817,0.,2.6722364755 | C,-0.9809820852,0.,0.6
178802668 | C,-2.2775360915,0.,0.0209985637 | H,-3.1510053598,0.,0.6599568
492 | C,-2.4159271657,0.,-1.3756949167 | H,-3.3991067888,0.,-1.8284673549 |
C,-1.2657959477,0.,-2.1785485489 | H,-1.3626831351,0.,-3.2564964547 | C,0.
0582100826,0.,-1.6161436821 | C,1.1531766695,0.,-2.5255239531 | H,0.953251
1644,0.,-3.5878689833 | H,2.1772311078,0.,-2.1929748939 | C,0.1780653355,0
.,-0.159013584 | N,2.7154501823,0.,-0.1247517178 | H,3.4728669162,0.,0.605
3453704 | | Version=x86-Win32-G98RevA.11.4 | State=1-A' | HF=-470.3808365 | S2=
2.379957 | S2-1=0. | S2A=8.821057 | RMSD=2.997e-009 | RMSF=7.498e-005 | Dipole=-
0.1752937,0.,0.7037035 | PG=CS [SG(C11H9N1)] | | @
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UCCSD(T)/STO-3G

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1 | 1 | UNPC-UNK | SP | UCCSD(T)-FC | STO-3G | C11H9N1 | PCUSER | 18-Oct-2002 | 0 | | #UCCS
D-T/STO-3G GUESS=(ALWAYS,MIX) | | molecule 7 | | 0,1 | C,C,1,1.41747912 | H,2,1.
08382996,1,118.28341605 | C,2,1.4275748,1,122.50238876,3,180.,0 | H,4,1.08
243955,2,119.18371448,1,180.,0 | C,4,1.36699305,2,119.89261445,1,0.,0 | H,
6,1.0825643,4,121.53092571,2,180.,0 | C,6,1.504934,4,120.82276391,2,0.,0
| C,8,1.42734721,6,117.6967279,4,180.,0 | H,9,1.08222745,8,119.0944111,6,
0.,0 | C,9,1.40353296,8,120.37812546,6,180.,0 | H,11,1.08242554,9,120.3856
1624,8,180.,0 | C,11,1.40263173,9,119.25844927,8,0.,0 | H,13,1.08229331,11
,119.78110992,9,180.,0 | C,13,1.43850311,11,122.06830162,9,0.,0 | C,15,1.4
2334968,13,117.27546338,11,180.,0 | H,16,1.0809936,15,119.05196978,13,0.
,0 | H,16,1.07669697,15,122.29947634,13,180.,0 | C,15,1.4620511,13,117.716
81937,11,0.,0 | N,1,1.38846123,19,120.65415542,8,180.,0 | H,20,1.05200849,
1,105.55923301,19,180.,0 | | Version=x86-Win32-G98RevA.11.4 | State=1-A' | HF
=-470.3808365 | MP2=-470.9225035 | MP3=-471.0199467 | MP4D=-471.0526751 | MP4D
Q=-471.0462344 | PUHF=-469.726073 | PMP2-0=-470.2624258 | PMP3-0=-470.351242
5 | MP4SDQ=-471.0606849 | CCSD=-471.1340038 | CCSD(T)=-471.1536202 | S2=2.3799
57 | S2-1=2.054427 | S2A=8.821057 | RMSD=2.997e-009 | PG=CS [SG(C11H9N1)] | | @
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UB3LYP/STO-3G

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1 | 1 | UNPC-UNK | SP | UB3LYP | STO-3G | C11H9N1 | PCUSER | 30-Jan-2003 | 0 | | #UB3LYP/ST
O-3G GUESS=(ALWAYS,MIX) | | molecule 7 | | 0,1 | C,C,1,1.41747912 | H,2,1.083829
96,1,118.28341605 | C,2,1.4275748,1,122.50238876,3,180.,0 | H,4,1.08243955
,2,119.18371448,1,180.,0 | C,4,1.36699305,2,119.89261445,1,0.,0 | H,6,1.08
25643,4,121.53092571,2,180.,0 | C,6,1.504934,4,120.82276391,2,0.,0 | C,8,1
.42734721,6,117.6967279,4,180.,0 | H,9,1.08222745,8,119.0944111,6,0.,0 | C
,9,1.40353296,8,120.37812546,6,180.,0 | H,11,1.08242554,9,120.38561624,8
,180.,0 | C,11,1.40263173,9,119.25844927,8,0.,0 | H,13,1.08229331,11,119.7
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8110992,9,180.,0|C,13,1.43850311,11,122.06830162,9,0.,0|C,15,1.4233496
8,13,117.27546338,11,180.,0|H,16,1.0809936,15,119.05196978,13,0.,0|H,1
6,1.07669697,15,122.29947634,13,180.,0|C,15,1.4620511,13,117.71681937,
11,0.,0|N,1,1.38846123,19,120.65415542,8,180.,0|H,20,1.05200849,1,105.
55923301,19,180.,0|Version=x86-Win32-G98RevA.11.4|State=1-A'|HF=-473.
3239269|S2=1.064986|S2-1=0.|S2A=0.590061|RMSD=7.006e-005|Dipole=-0.274
8799,0.,0.6158344|PG=CS [SG(C11H9N1)]|@

UHF/4-31G

1|1|UNPC-UNK|FOpt|UHF|4-31G|C11H9N1|PCUSER|31-Jan-2003|0|#UHF/4-31G O
PT GUESS=(ALWAYS,MIX)|molecule 7|0,1|C,1.4903873429,0.,0.5645734277|
C,1.4881916337,0.,1.9734522232|H,2.435737038,0.,2.4782802518|C,0.30748
99307,0.,2.7223594806|H,0.352506445,0.,3.7928016856|C,-0.8901918215,0.
,2.0729796497|H,-1.8129799114,0.,2.6179826285|C,-0.9525062073,0.,0.622
5352483|C,-2.2480608265,0.,0.0265194262|H,-3.1099368885,0.,0.663927418
1|C,-2.3801688495,0.,-1.3382665579|H,-3.3514852182,0.,-1.7915950898|C,
-1.2411367197,0.,-2.1353054047|H,-1.3460588908,0.,-3.20228888|C,0.0641
285809,0.,-1.6002802888|C,1.1328185267,0.,-2.5195975231|H,0.9016591398
,0.,-3.5676361708|H,2.1512692371,0.,-2.2188468475|C,0.1949085103,0.,-0
.146638933|N,2.6477456599,0.,-0.1047649404|H,3.4499088256,0.,0.5067450
979|Version=x86-Win32-G98RevA.11.4|State=1-A'|HF=-475.5125203|S2=1.60
2743|S2-1=0.|S2A=4.614714|RMSD=7.782e-009|RMSF=1.136e-004|Dipole=-0.28
57529,0.,0.9200565|PG=CS [SG(C11H9N1)]|@

UCCSD(T)/4-31G

1|1|UNPC-UNK|SP|UCCSD(T)-RW|4-31G|C11H9N1|PCUSER|01-Apr-2003|0|#UCCSD
(T,WINDOW=(13,110))/4-31G GUESS=(ALWAYS,MIX)|molecule 7|0,1|C|C,1,1.
40888051|H,2,1.07363571,1,117.95825876|C,2,1.39818403,1,122.475841,3,1
80.,0|H,4,1.07138835,2,119.97844162,1,180.,0|C,4,1.36240073,2,119.1470
229,1,0.,0|H,6,1.07171176,4,120.96727136,2,180.,0|C,6,1.45178237,4,120
.92647436,2,0.,0|C,8,1.42607736,6,117.16468974,4,180.,0|H,9,1.07196982
,8,118.81025234,6,0.,0|C,9,1.37116495,8,120.23351515,6,180.,0|H,11,1.0
7189656,9,120.54806661,8,180.,0|C,11,1.39020326,9,119.45357387,8,0.,0|
H,13,1.07212984,11,119.36629992,9,180.,0|C,13,1.41066274,11,122.728950
42,9,0.,0|C,15,1.40969585,13,117.00834731,11,180.,0|H,16,1.07322862,15
,118.26481946,13,0.,0|H,16,1.06192882,15,122.84497017,13,180.,0|C,15,1
.45951245,13,117.42950221,11,0.,0|N,1,1.33697125,19,121.19119485,8,180
,0|H,20,1.00866757,1,112.63856855,19,180.,0|Version=x86-Win32-G98Rev
A.11.4|State=1-A'|HF=-475.5125202|MP2=-476.376085|MP3=-476.4293382|MP4
D=-476.4551262|MP4DQ=-476.4429336|PUHF=-475.8286457|PMP2-0=-476.688945
9|PMP3-0=-476.7371721|MP4SDQ=-476.458218|CCSD=-476.4831405|CCSD(T)=-47
6.5210574|S2=1.602746|S2-1=1.414962|S2A=4.61473|RMSD=6.164e-009|PG=CS
[SG(C11H9N1)]|@

UB3LYP/4-31G

1|1|UNPC-UNK|SP|UB3LYP|4-31G|C11H9N1|PCUSER|31-Jan-2003|0|#UB3LYP/4-3
1G GUESS=(ALWAYS,MIX)|molecule 7|0,1|C|C,1,1.40888051|H,2,1.07363571
,1,117.95825876|C,2,1.39818403,1,122.475841,3,180.,0|H,4,1.07138835,2,
119.97844162,1,180.,0|C,4,1.36240073,2,119.1470229,1,0.,0|H,6,1.071711
76,4,120.96727136,2,180.,0|C,6,1.45178237,4,120.92647436,2,0.,0|C,8,1.

42607736,6,117.16468974,4,180.,0|H,9,1.07196982,8,118.81025234,6,0.,0|C,9,1.37116495,8,120.23351515,6,180.,0|H,11,1.07189656,9,120.54806661,8,180.,0|C,11,1.39020326,9,119.45357387,8,0.,0|H,13,1.07212984,11,119.36629992,9,180.,0|C,13,1.41066274,11,122.72895042,9,0.,0|C,15,1.40969585,13,117.00834731,11,180.,0|H,16,1.07322862,15,118.26481946,13,0.,0|H,16,1.06192882,15,122.84497017,13,180.,0|C,15,1.45951245,13,117.42950221,11,0.,0|N,1,1.33697125,19,121.19119485,8,180.,0|H,20,1.00866757,1,12.63856855,19,180.,0|Version=x86-Win32-G98RevA.11.4|State=1-A'|HF=-478.6318343|S2=0.959544|S2-1=0.|S2A=0.287885|RMSD=2.110e-005|Dipole=-0.5968095,0.,0.7546176|PG=CS [SG(C11H9N1)]|@

UHF/6-311G(d)

1|1|UNPC-UNK|FOpt|UHF|6-311G(d)|C11H9N1|PCUSER|16-Dec-2003|0||#P UHF/6-311G(D) OPT SCF (CONVER=5) GEOM=CHECKPOINT GUESS=READ||mol 4||0,1|C,-1.2957168098,0.8762171826,0.|C,-2.415302795,0.0674326362,0.|H,-3.3841629955,0.5365070261,0.|C,-2.3368458511,-1.3280140454,0.|H,-3.246023734,-1.9026788136,0.|C,-1.1283191569,-1.9483722164,0.|H,-1.049050912,-3.020027435,0.|C,0.0457773635,-1.1618223593,0.|C,1.3047466197,-1.8232496711,0.|H,1.3042262361,-2.8991194331,0.|C,2.4846612834,-1.1507834972,0.|H,3.4220956102,-1.6755215093,0.|C,2.4506470491,0.2492681631,0.|H,3.3782349603,0.7916163075,0.|C,1.2674897552,0.9723699787,0.|C,1.3517614531,2.4077168218,0.|H,2.407342926,2.677852348,0.|H,-0.6664575799,2.8288596111,0.|C,0.0028312081,0.2512359887,0.|N,-1.4553484476,2.2266268966,0.|H,-2.3691460943,2.6041297318,0.||Version=x86-Win32-G98RevA.11.4|State=1-A'|HF=-476.2123887|S2=0.|S2-1=0.|S2A=0.|RMSD=3.829e-006|RMSF=4.762e-005|Dipole=0.4159024,-0.718673,0.|PG=CS [SG(C11H9N1)]|@

UB3LYP/6-311G(d)

1|1|UNPC-UNK|SP|UB3LYP|6-311G(d)|C11H9N1|PCUSER|16-Dec-2003|0||#P UB3LYP/6-311G(D) SCF (CONVER=5) GEOM=CHECKPOINT GUESS=READ||mol 4||0,1|C,-1.2957168098,0.8762171826,0.|C,-2.415302795,0.0674326362,0.|H,-3.3841629955,0.5365070261,0.|C,-2.3368458511,-1.3280140454,0.|H,-3.246023734,-1.9026788136,0.|C,-1.1283191569,-1.9483722164,0.|H,-1.049050912,-3.020027435,0.|C,0.0457773635,-1.1618223593,0.|C,1.3047466197,-1.8232496711,0.|H,1.3042262361,-2.8991194331,0.|C,2.4846612834,-1.1507834972,0.|H,3.4220956102,-1.6755215093,0.|C,2.4506470491,0.2492681631,0.|H,3.3782349603,0.7916163075,0.|C,1.2674897552,0.9723699787,0.|C,1.3517614531,2.4077168218,0.|H,2.407342926,2.677852348,0.|H,-0.6664575799,2.8288596111,0.|C,0.0028312081,0.2512359887,0.|N,-1.4553484476,2.2266268966,0.|H,-2.3691460943,2.6041297318,0.||Version=x86-Win32-G98RevA.11.4|State=1-A'|HF=-479.3249451|S2=0.|S2-1=0.|S2A=0.|RMSD=4.781e-006|Dipole=0.0877187,-0.9042944,0.|PG=CS [SG(C11H9N1)]|@

RHF/STO-3G

1|1|UNPC-UNK|FOpt|ROHF|STO-3G|C11H9N1|PCUSER|14-Dec-2003|0||#P ROHF/STO-3G OPT SCF (CONVER=5)||molecule 4||0,1|C,1.4676071699,0.,0.5311683624|C,1.5096856703,0.,1.9048136889|H,2.4713278601,0.,2.3962719645|C,0.3328184235,0.,2.6803419681|H,0.4172454111,0.,3.7604286451|C,-0.8836142492,0.,2.0850630872|H,-1.7946886558,0.,2.6653116387|C,-0.9776305027,0.,0.6619792865|C,-2.2684335463,0.,0.0395523739|H,-3.1415739113,0.,0.6826788607|C,-2.4112525516,0.,-1.3077721355|H,-3.3904803075,0.,-1.766899140

3|C,-1.2527797016,0.,-2.119007843|H,-1.3758210254,0.,-3.1972406418|C,0.0186331619,0.,-1.5916406384|C,1.1869348819,0.,-2.5094915232|H,0.7547140918,0.,-3.5362469916|H,2.5801497974,0.,-1.2234324449|C,0.1793715657,0.,-0.1448569592|N,2.647822882,0.,-0.2058904206|H,3.5363246349,0.,0.2794630468||Version=x86-Win32-G98RevA.11.4|State=1-A'|HF=-470.2585031|RM SD=1.999e-006|RMSF=4.996e-005|Dipole=-0.5529849,0.,-0.2870239|PG=CS [SG(C11H9N1)]||@

RHF/6-311G(d)

1|1|UNPC-UNK|FOpt|ROHF|6-311G(d)|C11H9N1|PCUSER|14-Dec-2003|0||#P ROHF /6-311G(D) OPT SCF (CONVER=5) GEOM=CHECKPOINT GUESS=READ|molecule 4||0,1|C,1.4775198909,0.,0.5132903639|C,1.4996551044,0.,1.894456016|H,2.4554042385,0.,2.3897738635|C,0.3349694553,0.,2.6668339335|H,0.4187638755,0.,3.7391358949|C,-0.8854947039,0.,2.0701046718|H,-1.7913665433,0.,2.6481537866|C,-0.9581570054,0.,0.6589209071|C,-2.2414023278,0.,0.0460872673|H,-3.1030580814,0.,0.6903575521|C,-2.4091743473,0.,-1.3017067464|H,-3.3908741913,0.,-1.7380479024|C,-1.2675249874,0.,-2.1126135027|H,-1.387804595,0.,-3.1803942223|C,0.0199287879,0.,-1.5974456027|C,1.1201250121,0.,-2.5222956417|H,0.7085167614,0.,-3.5312297654|H,2.6633139853,0.,-1.160225703|C,0.1995724067,0.,-0.1526865088|N,2.6546358431,0.,-0.167553575|H,3.5045499352,0.,0.3376805767||Version=x86-Win32-G98RevA.11.4|State=1-A'|HF=-476.212388|RMSD=6.153e-006|RMSF=4.365e-005|Dipole=-0.8242628,0.,0.0955398|PG=CS [SG(C11H9N1)]||@

RHF/6-311G(d,p)

1|1|UNPC-UNK|FOpt|ROHF|6-311G(d,p)|C11H9N1|PCUSER|15-Dec-2003|0||#P RO HF/6-311** OPT SCF (CONVER=5) GEOM=CHECKPOINT GUESS=READ|molecule 4||0,1|C,1.4773627041,0.,0.5138718602|C,1.49999185,0.,1.8946583849|H,2.456037027,0.,2.3890342489|C,0.3347679049,0.,2.6668566421|H,0.4187022624,0.,3.739233399|C,-0.8855723605,0.,2.0705634961|H,-1.7919918664,0.,2.6474928976|C,-0.9584667506,0.,0.6590018317|C,-2.2413864235,0.,0.0457303698|H,-3.1028383806,0.,0.6906724529|C,-2.4081386015,0.,-1.3021935607|H,-3.389485041,0.,-1.7393676566|C,-1.2661469551,0.,-2.1124801544|H,-1.3841028562,0.,-3.1808133142|C,0.0207272044,0.,-1.5961605256|C,1.1218897204,0.,-2.5201622814|H,0.7108040247,0.,-3.5298696358|H,2.6500803061,0.,-1.1665471536|C,0.1991417563,0.,-0.1518289194|N,2.6522271761,0.,-0.1705100621|H,3.5021839979,0.,0.3365923361||Version=x86-Win32-G98RevA.11.4|State=1-A'|HF=-476.2320665|RMSD=4.044e-006|RMSF=3.804e-005|Dipole=-0.8334434,0.,0.0808256|PG=CS [SG(C11H9N1)]||@

RB3LYP/6-311G(d,p)

1|1|UNPC-UNK|FOpt|ROB3LYP|6-311G(d,p)|C11H9N1|PCUSER|15-Dec-2003|0||#P ROB3LYP/6-311** OPT SCF (CONVER=5) GEOM=CHECKPOINT GUESS=READ|molecule 4||0,1|C,-1.2942774894,0.8826886404,0.|C,-2.4324547017,0.0616378658,0.|H,-3.4074072833,0.5390221725,0.|C,-2.3540954843,-1.3345354606,0.|H,-3.271140915,-1.913342313,0.|C,-1.1330238583,-1.9674675786,0.|H,-1.055519747,-3.0479064597,0.|C,0.048813577,-1.1833417277,0.|C,1.3073203675,-1.8302470425,0.|H,1.3176375402,-2.9159134016,0.|C,2.5022236025,-1.1353187464,0.|H,3.4474118987,-1.6653747765,0.|C,2.4659535885,0.256517029

8,0. |H,3.392449608,0.8204579789,0. |C,1.255995417,0.9883768407,0. |C,1.2
922603997,2.4130570789,0. |H,2.3487674714,2.7296689286,0. |H,-0.52929843
83,2.7775850753,0. |C,0.0011370306,0.248591664,0. |N,-1.4109137557,2.232
210915,0. |H,-2.3256185394,2.6505750074,0. | |Version=x86-Win32-G98RevA.1
1.4 |State=1-A' |HF=-479.3480641 |RMSD=3.149e-006 |RMSF=8.378e-005 |Dipole=
0.1456251,-0.916475,0. |PG=CS [SG(C11H9N1)] | |@

Triplet

UHF/STO-3G

1 | 1 | UNPC-UNK | FOpt | UHF | STO-3G | C11H9N1(3) | PCUSER | 18-Oct-2002 | 0 | | #UHF STO
-3G OPT GUESS=(ALWAYS,MIX) | | molecule 7 | | 0,3 | C | 1.4882463613,0.,0.587599
9706 | C | 1.4756962828,0.,2.0301199445 | H | 2.4270531971,0.,2.5484736152 | C | 0
.2739494021,0.,2.7638904734 | H | 0.2981911049,0.,3.8460910501 | C | -0.955594
7012,0.,2.0763829765 | H | -1.886193359,0.,2.6290752234 | C | -1.0073817199,0.
,0.6404802271 | C | -2.2897712053,0.,-0.0063975258 | H | -3.1808983379,0.,0.60
76808994 | C | -2.3923230568,0.,-1.4112814174 | H | -3.3647769304,0.,-1.886632
5753 | C | -1.2225717119,0.,-2.1942269811 | H | -1.3017743014,0.,-3.2734793515
| C | 0.1015527655,0.,-1.6133795135 | C | 1.1975392582,0.,-2.5143118114 | H | 1.0
025954941,0.,-3.5777991504 | H | 2.220858219,0.,-2.1806572238 | C | 0.21642636
35,0.,-0.1470555359 | N | 2.7168179192,0.,-0.0920893385 | H | 3.45261125,0.,0.
6609480402 | | Version=x86-Win32-G98RevA.11.4 | State=3-A' | HF=-470.437518 | S
2=3.797684 | S2-1=0. | S2A=5.356412 | RMSD=1.435e-009 | RMSF=1.025e-004 | Dipole
=-0.144855,0.,0.6523695 | PG=CS [SG(C11H9N1)] | | @

UCCSD(T)/STO-3G

1 | 1 | UNPC-UNK | SP | UCCSD(T)-FC | STO-3G | C11H9N1(3) | PCUSER | 18-Oct-2002 | 0 | | #U
CCSD-T/STO-3G GUESS=(ALWAYS,MIX) | | molecule 7 | | 0,3 | C | 1.44257457 | H | 2
,1.0834069,1,118.08560896 | C | 2,1.40805353,1,121.90614615,3,180.,0 | H | 4,1
.08247205,2,120.12444675,1,180.,0 | C | 4,1.4087034,2,119.3803017,1,0.,0 | H
,6,1.08235049,4,120.08146295,2,180.,0 | C | 6,1.43683632,4,121.27754335,2,
0.,0 | C | 8,1.43630555,6,118.83334386,4,180.,0 | H | 9,1.08221988,8,118.66133
523,6,0.,0 | C | 9,1.40862189,8,120.94281585,6,180.,0 | H | 11,1.0824164,9,120
.22512785,8,180.,0 | C | 11,1.40759439,9,119.62044714,8,0.,0 | H | 13,1.082154
67,11,119.5982289,9,180.,0 | C | 13,1.44592165,11,122.51916223,9,0.,0 | C | 15
,1.41875488,13,116.89342139,11,180.,0 | H | 16,1.08120691,15,119.03383365,
13,0.,0 | H | 16,1.07633967,15,122.5201848,13,180.,0 | C | 15,1.47081676,13,11
8.16486604,11,0.,0 | N | 1,1.40405329,19,121.03458122,8,180.,0 | H | 20,1.0528
329,1,105.38349146,19,180.,0 | | Version=x86-Win32-G98RevA.11.4 | State=3-A
' | HF=-470.437518 | MP2=-470.9411508 | MP3=-471.0366991 | MP4D=-471.0672798 | M
P4DQ=-471.0623637 | PUHF=-470.5759199 | PMP2-0=-471.0730622 | PMP3-0=-471.15
88565 | MP4SDQ=-471.0754343 | CCSD=-471.1429358 | CCSD(T)=-471.1602153 | S2=3.
797684 | S2-1=3.412986 | S2A=5.356412 | RMSD=1.435e-009 | PG=CS [SG(C11H9N1)] |
| @

UB3LYP/STO-3G

1 | 1 | UNPC-UNK | SP | UB3LYP | STO-3G | C11H9N1(3) | PCUSER | 30-Jan-2003 | 0 | | #UB3LYP
/STO-3G GUESS=(ALWAYS,MIX) | | molecule 7 | | 0,3 | C | 1.44257457 | H | 2,1.083
4069,1,118.08560896 | C | 2,1.40805353,1,121.90614615,3,180.,0 | H | 4,1.08247
205,2,120.12444675,1,180.,0 | C | 4,1.4087034,2,119.3803017,1,0.,0 | H | 6,1.0
8235049,4,120.08146295,2,180.,0 | C | 6,1.43683632,4,121.27754335,2,0.,0 | C

,8,1.43630555,6,118.83334386,4,180.,0|H,9,1.08221988,8,118.66133523,6,0.,0|C,9,1.40862189,8,120.94281585,6,180.,0|H,11,1.0824164,9,120.22512785,8,180.,0|C,11,1.40759439,9,119.62044714,8,0.,0|H,13,1.08215467,11,119.5982289,9,180.,0|C,13,1.44592165,11,122.51916223,9,0.,0|C,15,1.41875488,13,116.89342139,11,180.,0|H,16,1.08120691,15,119.03383365,13,0.,0|H,16,1.07633967,15,122.5201848,13,180.,0|C,15,1.47081676,13,118.16486604,11,0.,0|N,1,1.40405329,19,121.03458122,8,180.,0|H,20,1.0528329,1,105.38349146,19,180.,0|Version=x86-Win32-G98RevA.11.4|State=3-A'|HF=-473.336213|S2=2.158545|S2-1=0.|S2A=2.014318|RMSD=4.479e-005|Dipole=-0.2355193,-0.0000854,0.5388729|PG=CS [SG(C11H9N1)]|@

UHF/4-31G

1|1|UNPC-UNK|FOpt|UHF|4-31G|C11H9N1(3)|PCUSER|05-Dec-2002|0|#UHF 4-31G OPT GUESS=(ALWAYS,MIX)|molecule 7||0,3|C,1.4818529211,0.,0.5754111865|C,1.4692469275,0.,2.0037993252|H,2.4142790004,0.,2.5133643208|C,0.2878011114,0.,2.7307951276|H,0.3128002227,0.,3.8020891101|C,-0.9274711642,0.,2.054523|H,-1.8485963067,0.,2.6036236641|C,-0.9853769969,0.,0.6357779442|C,-2.2569734744,0.,0.0081403019|H,-3.1348019415,0.,0.6243924933|C,-2.3685320012,0.,-1.3772316093|H,-3.3348048691,0.,-1.841419876|C,-1.2209703002,0.,-2.1578978712|H,-1.3076459945,0.,-3.2266231157|C,0.0967228763,0.,-1.6009720577|C,1.162632476,0.,-2.5120476462|H,0.9382747705,0.,-3.5616778668|H,2.1809722866,0.,-2.2103981477|C,0.2209066984,0.,-0.1497568733|N,2.6536906323,0.,-0.0741108772|H,3.4446539625,0.,0.5521805924|Version=x86-Win32-G98RevA.11.4|State=3-A'|HF=-475.550308|S2=3.205492|S2-1=0.|S2A=3.336164|RMSD=4.336e-009|RMSF=3.166e-005|Dipole=-0.1746714,0.,0.8337444|PG=CS [SG(C11H9N1)]|@

UCCSD(T)/4-31G

1|1|UNPC-UNK|SP|UCCSD(T)-RW|4-31G|C11H9N1(3)|PCUSER|01-Apr-2003|0|#UC CSD(T,WINDOW=(13,110))/4-31G GUESS=(ALWAYS,MIX)|molecule 7||0,3|C,1.42844376|H,2,1.07365828,1,117.82807915|C,2,1.38720478,1,122.11146256,3,180.,0|H,4,1.07158563,2,120.26904231,1,180.,0|C,4,1.39076623,2,119.29920871,1,0.,0|H,6,1.07237263,4,120.10503608,2,180.,0|C,6,1.41992627,4,121.43218967,2,0.,0|C,8,1.41805734,6,118.60735567,4,180.,0|H,9,1.07254351,8,118.66028319,6,0.,0|C,9,1.38985634,8,120.87400437,6,180.,0|H,11,1.07198601,9,120.26305422,8,180.,0|C,11,1.38792567,9,119.62290415,8,0.,0|H,13,1.07223427,11,119.59012194,9,180.,0|C,13,1.43055292,11,122.86177409,9,0.,0|C,15,1.40222038,13,116.56671085,11,180.,0|H,16,1.07334057,15,118.45646825,13,0.,0|H,16,1.06207739,15,122.97798262,13,180.,0|C,15,1.45651884,13,117.80246957,11,0.,0|N,1,1.3398069,19,121.09829283,8,180.,0|H,20,1.00889246,1,112.62894849,19,180.,0|Version=x86-Win32-G98RevA.11.4|State=3-A'|HF=-475.550308|MP2=-476.3619673|MP3=-476.424364|MP4D=-476.4476554|MP4DQ=-476.4386469|PUHF=-475.6245292|PMP2-0=-476.4306423|PMP3-0=-476.4843582|MP4SDQ=-476.4556113|CCSD=-476.4914891|CCSD(T)=-476.5266623|S2=3.205492|S2-1=2.906017|S2A=3.336164|RMSD=6.536e-009|PG=CS [SG(C11H9N1)]|@

UB3LYP/4-31G

1|1|UNPC-UNK|SP|UB3LYP|4-31G|C11H9N1(3)|PCUSER|31-Jan-2003|0|#UB3LYP/

4-31G GUESS=(ALWAYS,MIX) | molecule 7 | |0,3|C|C,1,1.42844376|H,2,1.07365
828,1,117.82807915|C,2,1.38720478,1,122.11146256,3,180.,0|H,4,1.071585
63,2,120.26904231,1,180.,0|C,4,1.39076623,2,119.29920871,1,0.,0|H,6,1.
07237263,4,120.10503608,2,180.,0|C,6,1.41992627,4,121.43218967,2,0.,0|
C,8,1.41805734,6,118.60735567,4,180.,0|H,9,1.07254351,8,118.66028319,6
,0.,0|C,9,1.38985634,8,120.87400437,6,180.,0|H,11,1.07198601,9,120.263
05422,8,180.,0|C,11,1.38792567,9,119.62290415,8,0.,0|H,13,1.07223427,1
1,119.59012194,9,180.,0|C,13,1.43055292,11,122.86177409,9,0.,0|C,15,1.
40222038,13,116.56671085,11,180.,0|H,16,1.07334057,15,118.45646825,13,
0.,0|H,16,1.06207739,15,122.97798262,13,180.,0|C,15,1.45651884,13,117.
80246957,11,0.,0|N,1,1.3398069,19,121.09829283,8,180.,0|H,20,1.0088924
6,1,112.62894849,19,180.,0| |Version=x86-Win32-G98RevA.11.4|HF=-478.637
906|S2=2.096181|S2-1=0.|S2A=2.005165|RMSD=6.505e-005|Dipole=-0.3595235
,0.0008265,0.7171236|PG=CS [SG(C11H9N1)]| |@

UHF/6-311G(d)

1|1|UNPC-UNK|FOpt|UHF|6-311G(d)|C11H9N1(3)|PCUSER|16-Dec-2003|0| |#P UH
F/6-311G(D) OPT SCF (CONVER=5) GUESS=READ GEOM=CHECKPOINT| |molecule 4|
|0,3|C,1.4968188342,0.,0.5617253272|C,1.4907935143,0.,1.997138645|H,2.
4413259608,0.,2.5017171514|C,0.3142076556,0.,2.7319571257|H,0.34635782
88,0.,3.8063432067|C,-0.907330154,0.,2.0629899232|H,-1.8258878025,0.,2
.6214375541|C,-0.9761526281,0.,0.6423893671|C,-2.2565591711,0.,0.02846
11384|H,-3.1306274707,0.,0.6544708715|C,-2.3828561035,0.,-1.3571685672
|H,-3.3565975626,0.,-1.8129984573|C,-1.2429110802,0.,-2.1496133736|H,-
1.3435560845,0.,-3.2197977574|C,0.0825999213,0.,-1.6062792719|C,1.1335
254784,0.,-2.5339801176|H,0.8887812588,0.,-3.5812947034|H,2.16148858,0
,-2.257535657|C,0.2214147559,0.,-0.1540071154|N,2.6523027295,0.,-0.08
88117587|H,3.4112900485,0.,0.5676616162| |Version=x86-Win32-G98RevA.11.
4|State=3-A'|HF=-476.3133111|S2=3.135908|S2-1=0.|S2A=3.16137|RMSD=8.14
3e-006|RMSF=9.042e-005|Dipole=-0.2034838,0.,0.7462465|PG=CS [SG(C11H9N
1)]| |@

UB3LYP/6-311G(d)

1|1|UNPC-UNK|SP|UB3LYP|6-311G(d)|C11H9N1(3)|PCUSER|16-Dec-2003|0| |#P U
B3LYP/6-311G(D) SP SCF (CONVER=5) GUESS=READ GEOM=CHECKPOINT| |molecule
4| |0,3|C,1.4968188342,0.,0.5617253272|C,1.4907935143,0.,1.997138645|H
,2.4413259608,0.,2.5017171514|C,0.3142076556,0.,2.7319571257|H,0.34635
78288,0.,3.8063432067|C,-0.907330154,0.,2.0629899232|H,-1.8258878025,0
,2.6214375541|C,-0.9761526281,0.,0.6423893671|C,-2.2565591711,0.,0.02
84611384|H,-3.1306274707,0.,0.6544708715|C,-2.3828561035,0.,-1.3571685
672|H,-3.3565975626,0.,-1.8129984573|C,-1.2429110802,0.,-2.1496133736|
H,-1.3435560845,0.,-3.2197977574|C,0.0825999213,0.,-1.6062792719|C,1.1
335254784,0.,-2.5339801176|H,0.8887812588,0.,-3.5812947034|H,2.1614885
8,0.,-2.257535657|C,0.2214147559,0.,-0.1540071154|N,2.6523027295,0.,-0
.0888117587|H,3.4112900485,0.,0.5676616162| |Version=x86-Win32-G98RevA.
11.4|State=3-A'|HF=-479.3636018|S2=2.093052|S2-1=0.|S2A=2.00491|RMSD=7
.437e-006|Dipole=-0.4050741,0.,0.6680714|PG=CS [SG(C11H9N1)]| |@

ROHF/STO-3G

1|1|UNPC-UNK|FOpt|ROHF|STO-3G|C11H9N1(3)|PCUSER|15-Dec-2003|0||#P ROHF /STO-3G OPT SCF (CONVER=5)|molecule 4||0,3|C,1.4566648459,0.,0.5762682577|C,1.4795653765,0.,1.941254587|H,2.4335817628,0.,2.4545353616|C,0.290033861,0.,2.7102910607|H,0.353375819,0.,3.7905628138|C,-0.9031543084,0.,2.0774038926|H,-1.8286306364,0.,2.6391663619|C,-0.9828020733,0.,0.6481470974|C,-2.2710512906,0.,0.0284306021|H,-3.1461287441,0.,0.6646416272|C,-2.3854907304,0.,-1.3176431868|H,-3.3571781113,0.,-1.7949112427|C,-1.218474697,0.,-2.117995353|H,-1.3297231906,0.,-3.1941559463|C,0.0433558859,0.,-1.5837519094|C,1.1675986884,0.,-2.5363835711|H,0.940827067,0.,-3.5917562732|H,2.1932631126,0.,-2.2152474883|C,0.1922214972,0.,-0.1367265887|N,2.7249758799,0.,-0.1561444153|H,3.4549794302,0.,0.6044063609|Version=x86-Win32-G98RevA.11.4|State=3-A'|HF=-470.3330458|RMSD=4.745e-006|RMSF=1.788e-005|Dipole=-0.1255509,0.,0.5863305|PG=CS [SG(C11H9N1)]||@

ROHF/6-311G(d)

1|1|UNPC-UNK|FOpt|ROHF|6-311G(d)|C11H9N1(3)|PCUSER|15-Dec-2003|0||#P ROHF/6-311G(D) OPT SCF (CONVER=5) GEOM=CHECKPOINT GUESS=READ|molecule 4||0,3|C,1.4621093152,0.,0.5748323876|C,1.4704296028,0.,1.9477283399|H,2.417874686,0.,2.4583480432|C,0.2871460438,0.,2.7040844373|H,0.3349730688,0.,3.777758201|C,-0.9024619999,0.,2.0583533786|H,-1.8231246662,0.,2.6140092467|C,-0.9724617784,0.,0.6394677933|C,-2.251847533,0.,0.0290396604|H,-3.1248340986,0.,0.6566449464|C,-2.3656511394,0.,-1.3203659498|H,-3.3323159861,0.,-1.7912260511|C,-1.2078404125,0.,-2.112348808|H,-1.3164975889,0.,-3.1818888795|C,0.0649834414,0.,-1.5841767259|C,1.151378217,0.,-2.5420871483|H,0.8950273747,0.,-3.5842883515|H,2.177177405,0.,-2.2652441807|C,0.2080923327,0.,-0.1431231762|N,2.6704472782,0.,-0.1080708451|H,3.4153323197,0.,0.5639578077|Version=x86-Win32-G98RevA.11.4|State=3-A'|HF=-476.2455011|RMSD=7.168e-006|RMSF=4.042e-005|Dipole=-0.1554674,0.,0.6787356|PG=CS [SG(C11H9N1)]||@

ROHF/6-311G(d,p)

1|1|UNPC-UNK|FOpt|ROHF|6-311G(d,p)|C11H9N1(3)|PCUSER|15-Dec-2003|0||#P ROHF/6-311** OPT SCF (CONVER=5) GEOM=CHECKPOINT GUESS=READ|molecule 4||0,3|C,1.4620948858,0.,0.5748651849|C,1.4706096888,0.,1.9475857126|H,2.4188100004,0.,2.4566588801|C,0.287355492,0.,2.7036567749|H,0.3352339711,0.,3.7772920466|C,-0.9021756261,0.,2.0581867751|H,-1.8234306037,0.,2.6128470889|C,-0.9722188364,0.,0.6393470564|C,-2.2515839725,0.,0.0290702976|H,-3.1237033396,0.,0.6577412762|C,-2.3655967906,0.,-1.3201810521|H,-3.3324462018,0.,-1.7907236184|C,-1.2082627326,0.,-2.1124892591|H,-1.3156474384,0.,-3.1821952032|C,0.064520809,0.,-1.5843836356|C,1.1513786666,0.,-2.5420407575|H,0.8919010195,0.,-3.5838338635|H,2.1767529989,0.,-2.2603299185|C,0.2080927636,0.,-0.1434533341|N,2.670333667,0.,-0.1079664276|H,3.4149078391,0.,0.5673257259|Version=x86-Win32-G98RevA.11.4|State=3-A'|HF=-476.2638172|RMSD=6.248e-006|RMSF=1.159e-004|Dipole=-0.1530886,0.,0.6660057|PG=CS [SG(C11H9N1)]||@

ROB3LYP/6-311G(d,p)

1|1|UNPC-UNK|FOpt|ROB3LYP|6-311G(d,p)|C11H9N1(3)|PCUSER|16-Dec-2003|0|


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|#P ROB3LYP/6-311** OPT SCF (CONVER=5) GEOM=CHECKPOINT GUESS=READ| |mol  
ecule 4| |0,3|C,1.5050916283,0.,0.5542363701|C,1.4886592267,0.,1.994440  
022|H,2.4494026443,0.,2.499044324|C,0.3177066,0.,2.7222303666|H,0.3475  
260507,0.,3.8060295785|C,-0.9000617585,0.,2.0581895279|H,-1.8270545193  
,0.,2.6204348565|C,-0.9758080855,0.,0.6378242208|C,-2.2557960995,0.,0.  
0284850425|H,-3.1340579485,0.,0.6636714935|C,-2.3802303925,0.,-1.34949  
63936|H,-3.3621799265,0.,-1.8094104857|C,-1.2459764484,0.,-2.141961469  
6|H,-1.3442459713,0.,-3.2217948805|C,0.0751166505,0.,-1.6024558933|C,1  
.1341919279,0.,-2.5165699864|H,0.9009148976,0.,-3.5752354879|H,2.16178  
00347,0.,-2.1980845505|C,0.2145216499,0.,-0.1557651004|N,2.6464146799,  
0.,-0.1036211679|H,3.4185225858,0.,0.5657530874| |Version=x86-Win32-G98  
RevA.11.4|State=3-A'|HF=-479.3741446|RMSD=2.840e-006|RMSF=9.789e-005|D  
ipole=-0.4353652,0.,0.6580324|PG=CS [SG(C11H9N1)]| |@
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