

Supplementary Information

Reactivity in the Nucleophilic Aromatic Substitution Reactions of Pyridinium Ions

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Reference 34: GAUSSIAN 03, Revision B.04, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Pittsburgh PA, 2003.

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Characterization of *N*-methyl-2-piperidinopyridinium

¹H NMR δ (ppm, CD₃OD) 7.65 (d, 1 H, H-6, J_{5,6} = 6.5 Hz), 7.54 (dd, 1 H, H-4, J_{3,4} = 9.0, J_{4,5} = 6.5 Hz), 6.56 (d, 1 H, H-3, J_{3,4} = 9.0 Hz), 7.54 (t, 1 H, H-5, J_{5,6} = 9.0, J_{4,5} = 6.5 Hz), 3.58 (s, 3H, CH₃), 3.17 (t, 4H, CH₂NCH₂), 1.81 (m, 4H, N(CH₂CH₂)₂), 1.73 (m, 2 H N(CH₂CH₂)₂CH₂).

¹³C NMR δ (ppm, CD₃OD) 165.51, 142.31, 140.75, 120.45, 108.71, 45.99, 38.19, 24.99, 23.45.

Mass Spectrometry (Electrospray), *m/z* calcd for C₁₁H₁₇N₂ 177.1392, found 177.1386.

Table S1. Calculated electronic energies (hartrees) and zero-point vibrational energies (kcal/mol) for reactants in this study, using the MP2/6-31+G* basis set.

Compound	gas phase	MeOH ^a	ZPVE ^b
piperidine	-251.0170302	-251.0236619	98.05
2-fluoro- <i>N</i> -methyl pyridinium ⁺	-386.0467182	-386.1293724	75.28
4-fluoro- <i>N</i> -methyl pyridinium ⁺	-386.0489729	-386.1342622	75.16
2-chloro- <i>N</i> -methyl pyridinium ⁺	-746.0522295	-746.132799	74.43
4-chloro- <i>N</i> -methyl pyridinium ⁺	-746.0556179	-746.1385096	74.22
2-bromo- <i>N</i> -methyl pyridinium ⁺	-2856.4625888	-2856.5426627	74.35
4-bromo- <i>N</i> -methyl pyridinium ⁺	-2856.4662248	-2856.5488446	74.15
2-cyano- <i>N</i> -methyl pyridinium ⁺	-379.0232655	-379.1131532	79.29
4-cyano- <i>N</i> -methyl pyridinium ⁺	-379.0257207	-379.1200407	79.17

^aSolvent calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* structures. ^bFrequencies and zero-point vibrational energies were calculated at the HF/6-31+G* level and scaled according to the recommendations of Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502-16513.

Table S2. Calculated (MP2/6-31+G*) electronic energies (hartrees), zero-point vibrational energies (kcal/mol), and imaginary frequencies (cm⁻¹) for the transition states and adducts in the S_NAr addition step of piperidine with 2- and 4-substituted *N*-methylpyridinium cations^a

substrate	gas phase	MeOH	ZPVE ^b	iv (cm ⁻¹) ^c
2-fluoro ts	-637.0855269	-637.1606122	174.66	344
2-fluoro adduct	-637.0899547	-637.1651112	176.05	
4-fluoro ts	-637.0848989	-637.1619771	174.48	337
4-fluoro adduct	-637.0979399	-637.1778473		
2-chloro ts	-997.084363	-997.1592617	173.87	360
2-chloro adduct	-997.0853178	-997.1602783	175.14	
4-chloro ts	-997.0883589	-997.1635713	173.63	365
4-chloro adduct	-997.0956083	-997.1740098		
2-bromo ts	-3107.5017135	-3107.5761954	173.64	357
2-bromo adduct	-3107.506171	-3107.586517	174.94	
4-bromo ts	-3107.5051105	-3107.5749525	173.36	364
4-bromo adduct	-3107.5138451	-3107.5929581	175.00	
2-cyano ts ^d	NA	NA	178.73	339
2-cyano adduct ^e	-630.0681109	-630.1520134	179.75	
4-cyano adduct ^e	-630.0661272	-630.1532301	177.61	
4-cyano ts	-630.0627159	-630.1466735	178.65	354
4-cyano adduct	-630.063201	-630.1481339	180.07	

^aSolvent (MeOH) calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* geometries. ^bZero-point vibrational energies were calculated at the HF/6-31+G* level and scaled according to the recommendations of Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502. ^cImaginary frequencies were calculated at the HF/6-31+G* level. ^dA structure was not obtained at the MP2/6-31+G* level. ^eThis calculation did not converge. ^eThe more stable cyano adducts are ion-molecule complexes, not covalent adducts.

Table S3. Calculated enthalpies of isomerization, ΔH_{ISOM} , 2-substituted-*N*-methylpyridinium to 4-substituted *N*-methylpyridinium cations and the transition states (ts) formed by their $S_{\text{N}}\text{Ar}$ addition reactions with piperidine (MP2/6-31+G*), kcal/mol.^a

substituent	gas phase	MeOH ^a
fluoro		
substrate	-1.5	-3.2
ts	0.2	-1.0
chloro		
substrate	-2.3	-3.8
ts	-2.7	-2.9
bromo		
substrate	-2.5	-4.1
ts	-2.4	0.5
cyano		
substrate	-1.7	-4.4
ts ^b	NA	NA

^aSolvent (MeOH) calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* geometries. Zero-point vibrational energies were calculated at the HF/6-31+G* level and scaled according to the recommendations of Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502. ^bThe 2-cyano ts calculation did not converge.

Table S4. Enthalpies of solvation, ΔH_{SOLV} (kcal/mol, MP2/6-31+G*), gas phase to methanol, for substrates and transition states in the addition of piperidine to 2- and 4-substituted *N*-methylpyridinium cations.^a

substituent	substrate	transition state	$\Delta\Delta H_{\text{SOLV}}^b$
2-fluoro	-51.9	-47.1	4.8
4-fluoro	-53.5	-48.4	5.1
2-chloro	-50.6	-47.0	3.6
4-chloro	-52.0	-47.2	4.8
2-bromo	-50.2	-46.7	3.5
4-bromo	-51.8	-43.8	8.0
2-cyano	-56.4	NA ^b	NA ^b
4-cyano	-59.2	-52.7	6.5

^aSolvent (MeOH) calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* geometries. Zero-point vibrational energies were calculated at the HF/6-31+G* level and scaled according to the recommendations of Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502. ^b $\Delta\Delta H_{\text{SOLV}} = \Delta H_{\text{SOLV}}(\text{ts}) - \Delta H_{\text{SOLV}}(\text{substrate})$. Thus, a positive value indicates more favorable solvation of the reactant than of the transition state. ^bA structure was not obtained at the MP2/6-31+G* level.

Table S5. Carbon-leaving group (C-L) and carbon-nucleophile (C-N) bond distances (Å) in substrates and transition states (ts) for the reactions of piperidine with 2- and 4-substituted *N*-methylpyridinium cations.^a

substituent	substrate (C-L)	ts (C-L, C-N)	% elongation (C-L)
2-fluoro	1.294	1.358, 2.104	4.9
4-fluoro	1.296	1.348, 2.296	4.0
2-chloro	1.706	1.780, 1.885	4.3
4-chloro	1.704	1.740, 2.192	2.1
2-bromo	1.857	1.949, 1.965	5.0
4-bromo	1.854	1.905, 2.245	2.8
2-cyano	1.442	NA ^b	
4-cyano	1.442	1.458, 1.854	1.1

^aStructures were optimized at the MP2/6-31+G* level. ^bA transition state structure was not found for the 2-cyano reaction.

Table S6. Activation enthalpies (kcal/mol, MP2/6-31+G*) calculated for the addition of piperidine to 2- and 4-substituted *N*-methylpyridinium cations.^a

substrate	ΔH^\ddagger (gas)	ΔH^\ddagger (MeOH)	$\Delta\Delta H^\ddagger$ ^b
2-fluoro	-12.3	-3.4	8.9
4-fluoro	-10.6	-1.2	9.4
2-chloro	-8.1	-0.4	7.7
4-chloro	-8.5	0.5	9.0
2-bromo	-12.6	-5.0	7.6
4-bromo	-12.6	-0.4	12.2
2-cyano	NA ^c	NA ^c	NA
4-cyano	-11.1	-0.4	10.7

^aSolvent (MeOH) calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* geometries. Zero-point vibrational energies were calculated at the HF/6-31+G* level and scaled according to the recommendations of Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502. ^bThe difference in activation enthalpies, (MeOH – gas). The average difference is 9.4 ± 1.2 kcal/mol. ^cA structure was not found at the MP2/6-31+G* level.

Table S7. Calculated npa charges on the reacting carbon (C) and the leaving group (X), gas phase and in methanol, for substrates and transition states (ts) in the S_NAr addition step of piperidine with 2- and 4-substituted *N*-methylpyridinium cations, and also for the 2- and 4-cyano-*N*-methylpyridinium⁺ adducts with piperidine.^a

substituent (X)	substrate (gas)	ts (gas)	substrate (MeOH)	ts (MeOH)
2-fluoro	C = 0.659 X = -0.288	C = 0.673 X = -0.328	C = 0.668 X = -0.306	C = 0.672 X = -0.338
4-fluoro	C = 0.482 X = -0.291	C = 0.486 X = -0.312	C = 0.471 X = -0.319	C = 0.479 X = -0.332
2-chloro	C = 0.161 X = 0.160	C = 0.236 X = 0.055	C = 0.167 X = 0.133	C = 0.239 X = 0.036
4-chloro	C = -0.032 X = 0.151	C = 0.008 X = 0.091	C = -0.036 X = 0.101	C = -0.008 X = 0.058
2-bromo	C = 0.084 X = 0.238	C = 0.171 X = 0.116	C = 0.090 X = 0.238	C = 0.175 X = 0.092
4-bromo	C = -0.112 X = 0.227	C = -0.076 X = 0.159	C = 0.114 X = 0.170	C = -0.055 X = 0.097
2-cyano	C = 0.129 X = 0.051	C = NA X = NA	C = 0.120 X = 0.013	C = NA X = NA
4-cyano	C = -0.082 X = 0.067	C = -0.057 X = 0.027	C = -0.106 X = 0.015	C = -0.068 X = -0.004
2-cyano adduct	C = 0.148 X = 0.025	NA ^b NA ^b	C = 0.132 C = 0.016	NA ^b NA ^b
4-cyano adduct	C = -0.029 X = 0.025	C = -0.057 X = 0.027	C = -0.036 X = -0.004	C = -0.068 X = -0.004

^aSolvent (MeOH) calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* geometries. The charges listed for the cyano group are for the entire group. ^bThe 2-cyano ts calculation did not converge.

Table S8. Calculated electronic energies (hartrees) and zero-point vibrational energies (kcal/mol) for H-bonded complexes between piperidine and the addition products (I-1) from 2-substituted-*N*-methylpyridinium ions and for 4-cyano-*N*-methylpyridinium ion. Electronic energies for the subsequent proton transfer transition states, MP2/6-31+G*.

Compound	$E_{CX, \text{ gas}}$	$E_{CX, \text{ MeOH}}^a$	$E_{ts, \text{ gas}}$	ZPVE ^{b, c}
2-fluoro	-888.1403284	-888.2076163	-888.1373313	275.30
2-chloro	-1248.1360087	-1248.2018047	-1248.1335027	274.39
2-bromo	-3358.5561394	-3358.6242215	-3358.5547237	274.22
2-cyano	-881.107446	-881.1777844	-881.1043014	279.06
4-cyano	-881.1216773	-881.1927856	-881.1177383	279.24

^aSolvent calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* structures. ^bFrequencies and zero-point vibrational energies were calculated at the HF/6-31+G* level and scaled according to the recommendations of Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502. ^cZPVE values are for the complexes.

Table S9. Enthalpies of hydrogen-bonded complex formation, ΔH_{CX} , for the association of the addition intermediate (I-1) with piperidine and activation enthalpies for proton transfer from this complex, (kcal/mol, MP2/6-31+G*)^a

substrate	$\Delta H_{CX}(\text{ gas})$	$\Delta H_{CX}(\text{ MeOH})$	$\Delta H^\ddagger(\text{ gas})$
2-fluoro	-19.7	-10.6	-0.5
2-chloro	-19.9	-0.8	-0.8
2-bromo	-19.4	-7.6	-1.5
2-cyano	-12.7	-0.1	-0.4
4-cyano	-20.6	-6.4	-0.1

^aSolvent (MeOH) calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* geometries. Zero-point vibrational energies were calculated at the HF/6-31+G* level and scaled according to the recommendations of Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502.

Table 10. Enthalpies of hydrogen-bonded complex formation, ΔH_{CX}° , from substrates and two piperidines (kcal/mol, MP2/6-31+G*^a).

substrate	ΔH_{CX}° (gas)	ΔH_{CX}° (MeOH)
2-fluoro	-31.9	-12.3
2.chloro	-27.1	-6.2
2-bromo	-33.6	-17.7
2-cyano	-27.8	-7.2
4-cyano	-34.9	-12.0

^aSolvent (MeOH) calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* geometries. Zero-point vibrational energies were calculated at the HF/6-31+G* level and scaled according to the recommendations of Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502.

* * *

Table S11. Cartesian coordinates for compounds in this study, MP2/6-31+G*.

piperidine			
H	-0.794935	-2.235383	0.000000
N	-0.707819	-1.218801	0.000000
C	-0.012981	-0.776452	1.211503
C	-0.012981	-0.776452	-1.211503
C	-0.012981	0.747593	1.258144
H	1.033718	-1.139057	1.247233
H	-0.537179	-1.190399	2.079975
H	-0.537179	-1.190399	-2.079975
H	1.033718	-1.139057	-1.247233
C	-0.012981	0.747593	-1.258144
H	-1.052123	1.093589	1.326120
H	0.511689	1.093208	2.158118
C	0.642386	1.320161	0.000000
H	0.511689	1.093208	-2.158118
H	-1.052123	1.093589	-1.326120
H	0.582917	2.415582	0.000000
H	1.711760	1.062070	0.000000
piperidinium+			
C	0.696859	-1.262969	0.245935
C	0.696868	1.262965	0.245935

C -0.745673 -1.258461 -0.231092
H 0.768074 -1.256933 1.337648
H 1.272324 -2.107476 -0.141940
H 1.272338 2.107468 -0.141940
H 0.768082 1.256928 1.337648
C -0.745664 1.258466 -0.231091
H -0.772205 -1.337455 -1.326699
H -1.230211 -2.161351 0.155012
C -1.481852 0.000005 0.229854
H -1.230196 2.161359 0.155012
H -0.772195 1.337461 -1.326699
H -2.501566 0.000009 -0.166262
H -1.569398 0.000005 1.324306
N 1.384739 -0.000005 -0.227212
H 2.365580 -0.000008 0.084081
H 1.412973 -0.000005 -1.256931

2-fluoro-N-methylpyridinium+

H -2.985935 0.814329 0.000072
C -1.982316 0.431461 0.000030
C -0.914056 1.306584 -0.000033
C -1.755700 -0.946933 0.000048
C -0.468505 -1.400563 -0.000019
H -1.025417 2.373190 -0.000013
H -2.566112 -1.649051 0.000111
H -0.223206 -2.443396 -0.000034
N 0.577011 -0.545846 -0.000124
C 1.977956 -1.047558 0.000057
C 0.347441 0.762931 -0.000083
F 1.403104 1.511020 0.000056
H 2.480765 -0.693979 0.886183
H 2.481983 -0.691274 -0.884258
H 1.941993 -2.123608 -0.001693

2-chloro-N-methylpyridinium+

H 2.576201 -2.031371 -0.000023
C 1.879615 -1.213641 -0.000007
C 0.520272 -1.466982 -0.000016
C 2.332929 0.100775 0.000013
C 1.408367 1.108595 0.000007
H 0.131094 -2.465815 -0.000044
H 3.378327 0.340008 0.000024
H 1.693643 2.140829 -0.000004
N 0.084697 0.862050 0.000007
C -0.858338 2.011719 -0.000015
C -0.359215 -0.404802 0.000011
Cl -2.040734 -0.687622 0.000007
H -1.472655 1.970304 0.885222

H -1.472711 1.970220 -0.885211
H -0.276076 2.917076 -0.000086

2-bromo-N-methylpyridinium+

H -2.690057 -2.380200 -0.000083
C -2.150836 -1.450971 -0.000064
C -0.767817 -1.459758 0.000011
C -2.831164 -0.239862 -0.000112
C -2.094760 0.912742 -0.000107
H -0.214713 -2.377585 0.000037
H -3.902238 -0.187680 -0.000167
H -2.558254 1.878186 -0.000161
N -0.749240 0.905498 -0.000027
C -0.035913 2.209587 -0.000041
C -0.084482 -0.261860 0.000048
Br 1.772148 -0.259681 0.000065
H 0.574951 2.283146 -0.885523
H 0.574783 2.283261 0.885547
H -0.775151 2.991956 -0.000164

2-cyano-N-methylpyridinium+

H -2.558825 -2.024974 0.000773
C -1.848880 -1.219073 0.000185
C -0.482222 -1.494360 0.000117
C -2.273362 0.094388 -0.000104
C -1.326612 1.099865 -0.000369
H -0.109641 -2.500288 0.000667
H -3.314199 0.353582 0.000099
H -1.603396 2.134988 -0.000462
N -0.022377 0.833728 -0.000214
C 0.962095 1.950942 0.000397
C 0.405188 -0.448634 -0.000220
H 1.574802 1.882606 -0.885102
H 1.573413 1.882405 0.886825
H 0.416574 2.879164 0.000271
C 1.826813 -0.687470 -0.000150
N 2.942827 -0.888218 -0.000101

4-fluoro-N-methylpyridinium+

C 0.629621 -1.180894 -0.012261
N 1.297407 0.000271 -0.020155
C 0.629391 1.181229 -0.012219
C 2.782614 -0.000195 0.022607
C -0.755274 -1.214848 -0.001838
H 1.233914 -2.082385 -0.016103
C -0.755568 1.214842 -0.001865
H 1.233327 2.082930 -0.016017
C -1.437033 -0.000053 0.003767

H -1.289357 -2.160348 -0.000072
H -1.289845 2.160231 -0.000119
F -2.770073 -0.000238 0.011015
H 3.145320 0.894703 -0.481133
H 3.145232 -0.885447 -0.498037
H 3.107714 -0.009928 1.064290

4-chloro-N-methylpyridinium+

C -1.063515 1.178872 -0.012800
N -1.733995 0.000001 -0.020397
C -1.063510 -1.178877 -0.012805
C -3.217704 -0.000004 0.025691
C 0.321569 1.207241 -0.004499
H -1.665236 2.082362 -0.016823
C 0.321570 -1.207229 -0.004493
H -1.665244 -2.082358 -0.016829
C 1.031684 0.000008 0.001942
H 0.837710 2.162983 -0.002775
H 0.837728 -2.162962 -0.002772
Cl 2.736294 -0.000004 0.007412
H -3.582003 -0.890328 -0.485199
H -3.582011 0.890247 -0.485313
H -3.540529 0.000058 1.068268

4-bromo-N-methylpyridinium+

C 1.709800 -1.173136 -0.000015
N 2.377530 0.008297 -0.000034
C 1.706123 1.184767 -0.000013
C 3.861928 -0.010707 0.000009
C 0.325234 -1.204641 0.000028
H 2.316572 -2.074129 -0.000043
C 0.319293 1.209987 0.000026
H 2.303174 2.091139 -0.000038
C -0.387272 0.002196 0.000066
H -0.187021 -2.162464 0.000012
H -0.195711 2.166301 0.000008
Br -2.249392 -0.002616 -0.000010
H 4.224174 1.015946 -0.000585
H 4.207111 -0.527565 -0.896205
H 4.207085 -0.526538 0.896828

4-cyano-N-methylpyridinium+

C -0.969749 -1.176026 -0.000004
N -1.633253 0.008577 -0.000006
C -0.965003 1.187752 -0.000003
C -3.120028 -0.009872 0.000006
C 0.415944 -1.208968 0.000001
H -1.580793 -2.073944 -0.000006

C	0.422995	1.212202	0.000000
C	1.130603	0.000651	0.000002
H	0.930528	-2.166072	0.000002
H	0.941926	2.166934	0.000001
H	-3.482017	1.016727	-0.000087
H	-3.462050	-0.527176	0.897166
H	-3.462062	-0.527339	-0.897054
C	2.563393	-0.003608	0.000004
H	-1.565601	2.091547	-0.000005
N	3.749130	-0.007643	-0.000002

2-piperidino-2-fluoro-N-methylpyridinim+, step 1, ts

C	-2.370901	1.764495	0.562964
C	-1.808832	1.936849	-0.721156
C	-2.409045	0.502222	1.105890
N	-1.885391	-0.571300	0.430890
H	-2.889883	0.274088	2.051459
H	-1.855499	2.904850	-1.214014
C	-1.264250	0.857078	-1.384062
H	-0.875972	0.926258	-2.395234
C	-1.176171	-0.385731	-0.715808
N	0.834823	-0.553931	-0.121686
F	-1.051907	-1.507593	-1.470692
C	1.078161	0.162471	1.147801
C	1.699787	-0.052819	-1.211713
H	1.018364	-1.557365	0.001534
H	0.420988	-0.263019	1.915703
H	0.772062	1.205071	0.983755
C	2.543022	0.100161	1.574712
C	3.180640	-0.121761	-0.845540
H	1.407448	0.990268	-1.394565
H	1.478622	-0.635015	-2.113309
H	2.674849	0.680484	2.495716
C	3.450273	0.623507	0.461283
H	2.805822	-0.939925	1.814378
H	3.772346	0.299372	-1.666879
H	3.480339	-1.174442	-0.746825
H	4.501808	0.517828	0.748531
H	3.270078	1.697926	0.315709
H	-2.814095	2.591461	1.107664
C	-1.978763	-1.934041	0.989498
H	-2.547695	-1.882222	1.916549
H	-0.976516	-2.319625	1.190974
H	-2.485445	-2.585625	0.277439

2-piperidino-2-chloro-N-methylpyridinium+, step 1, ts

C	2.174646	-2.024458	-0.778566
C	1.654033	-1.235105	-1.835314

C	2.198572	-1.481621	0.475996
N	1.691076	-0.224900	0.737822
H	2.654800	-1.980164	1.325219
H	1.729870	-1.577868	-2.864733
C	1.130376	0.005713	-1.576056
H	0.809208	0.659950	-2.380397
C	0.996179	0.487174	-0.223452
N	-0.827985	0.354764	0.233879
Cl	1.143283	2.254555	-0.074517
C	-1.141651	-1.022566	0.689542
C	-1.694797	0.767966	-0.900366
H	-0.961623	1.020580	1.008452
H	-0.474555	-1.268795	1.521227
H	-0.905304	-1.688780	-0.150339
C	-2.607644	-1.146738	1.096448
C	-3.169919	0.685826	-0.518971
H	-1.473628	0.081769	-1.726651
H	-1.406441	1.781179	-1.196489
H	-2.800045	-2.183789	1.394947
C	-3.530358	-0.719953	-0.043436
H	-2.791652	-0.524002	1.983501
H	-3.769583	0.974234	-1.389974
H	-3.385592	1.420827	0.269146
H	-4.574950	-0.754187	0.283023
H	-3.436734	-1.427417	-0.878751
H	2.604336	-3.005574	-0.948398
C	1.837421	0.327390	2.097283
H	2.182995	-0.470137	2.754467
H	0.878117	0.700400	2.465199
H	2.562180	1.143520	2.096783

2-piperidino-2-bromo-N-methylpyridinium+, step 1, ts,

C	-1.417980	2.762434	-0.822347
C	-1.106207	1.851876	-1.859392
C	-1.568407	2.268795	0.447052
N	-1.375881	0.935257	0.735396
H	-1.884087	2.882256	1.284938
H	-1.092435	2.182441	-2.895551
C	-0.896273	0.524685	-1.569360
H	-0.733851	-0.203245	-2.357700
C	-0.887077	0.064819	-0.212583
N	0.994381	-0.249825	0.261639
Br	-1.469242	-1.785657	-0.021993
C	1.616204	1.014030	0.717221
C	1.718398	-0.836373	-0.889721
H	0.970952	-0.937536	1.027142
H	1.037053	1.398194	1.563555
H	1.521042	1.725078	-0.114438

C	3.082705	0.808592	1.092078
C	3.184702	-1.089114	-0.548782
H	1.637603	-0.113862	-1.711829
H	1.204723	-1.758080	-1.181245
H	3.509474	1.774228	1.387642
C	3.860342	0.195161	-0.071399
H	3.142609	0.153397	1.972611
H	3.686650	-1.491686	-1.436294
H	3.249117	-1.863264	0.228577
H	4.892857	-0.009137	0.230825
H	3.910682	0.914681	-0.900328
H	-1.601307	3.814321	-1.013483
C	-1.632115	0.464430	2.109790
H	-1.710858	1.334155	2.761902
H	-0.810624	-0.169930	2.449620
H	-2.561385	-0.108055	2.139240

2-piperidino-2-cyano-N-methylpyridinium+, step 1, ts
NA

4-piperidino-4-fluoro-N-methylpyridinium+, step 1, ts

N	-2.584962	-0.752139	0.226752
C	-2.014020	-0.129104	1.293092
C	-2.390869	-0.268297	-1.030984
C	-1.588566	0.829082	-1.259056
H	-2.927300	-0.770514	-1.830232
H	-2.264816	-0.522225	2.273661
C	-1.204478	0.975392	1.127797
H	-0.788853	1.485683	1.990736
C	-0.896988	1.398296	-0.176482
N	1.205153	0.520318	-0.465848
F	-0.348747	2.619277	-0.335859
C	1.129260	-0.916540	-0.759511
C	2.012789	0.799608	0.733041
H	1.600341	1.023785	-1.267630
H	0.549592	-1.048833	-1.681805
H	0.560168	-1.377364	0.063993
C	2.500696	-1.581988	-0.871686
C	3.412044	0.188706	0.661973
H	1.470381	0.372982	1.590569
H	2.055253	1.886241	0.868228
H	2.373892	-2.659327	-1.035148
C	3.330595	-1.312158	0.383780
H	3.020156	-1.184272	-1.754557
H	3.943613	0.384625	1.601046
H	3.980703	0.686220	-0.135758
H	4.335284	-1.734446	0.272853
H	2.869779	-1.819608	1.243727

H -1.461766 1.216809 -2.265311
C -3.511934 -1.884527 0.443872
H -3.463801 -2.547657 -0.419429
H -4.527897 -1.505151 0.572014
H -3.198519 -2.428519 1.334433

4-piperidino-4-chloro-N-methylpyridinium+, step 1, ts

N -2.502159 -1.079644 0.201747
C -1.955350 -0.485910 1.298620
C -2.307652 -0.527107 -1.027980
C -1.529482 0.596623 -1.193952
H -2.835374 -0.992090 -1.855566
H -2.215899 -0.916937 2.260968
C -1.174249 0.643618 1.188904
H -0.812094 1.124781 2.092252
C -0.829390 1.148019 -0.091066
N 1.200901 0.372828 -0.375358
Cl -0.331563 2.812327 -0.197232
C 1.135908 -1.009468 -0.864587
C 1.957246 0.485814 0.881381
H 1.607079 0.990581 -1.087889
H 0.583775 -1.014606 -1.811780
H 0.547937 -1.576496 -0.125678
C 2.518330 -1.642032 -1.026162
C 3.364370 -0.101320 0.768475
H 1.386769 -0.064448 1.644273
H 1.984534 1.541980 1.171475
H 2.404658 -2.685551 -1.344206
C 3.306676 -1.548060 0.279949
H 3.059064 -1.121222 -1.828415
H 3.861194 -0.035325 1.743828
H 3.953173 0.507921 0.069084
H 4.318765 -1.943394 0.141232
H 2.826072 -2.174859 1.044796
H -1.433849 1.031893 -2.184706
C -3.417683 -2.227842 0.360418
H -3.362060 -2.847929 -0.534092
H -4.438839 -1.867547 0.504484
H -3.101870 -2.812618 1.224162

4-piperidino-4-bromo-N-methylpyridinium+, step 1, ts

N -2.260207 -1.806592 0.188031
C -1.796723 -1.178241 1.303048
C -2.135010 -1.207865 -1.029384
C -1.514163 0.015307 -1.164635
H -2.590486 -1.723198 -1.870095
H -1.995723 -1.667309 2.252206
C -1.171205 0.048408 1.223333

H -0.869148 0.547915 2.138598
C -0.909736 0.625151 -0.040870
N 1.256925 0.129138 -0.354909
Br -0.591939 2.502844 -0.096588
C 1.374843 -1.218145 -0.922719
C 1.966906 0.259107 0.925030
H 1.593008 0.835942 -1.018642
H 0.847839 -1.235884 -1.884419
H 0.845083 -1.896711 -0.234910
C 2.827497 -1.669707 -1.079568
C 3.437735 -0.145566 0.823958
H 1.451978 -0.398543 1.641867
H 1.858824 1.292453 1.273591
H 2.850376 -2.699288 -1.457287
C 3.570109 -1.556541 0.251863
H 3.317302 -1.041226 -1.836052
H 3.900391 -0.079549 1.816084
H 3.963635 0.571341 0.178582
H 4.626128 -1.816200 0.119946
H 3.154914 -2.282200 0.966114
H -1.469937 0.481339 -2.144871
C -3.012751 -3.072415 0.308847
H -2.819380 -3.682791 -0.573188
H -4.080626 -2.858089 0.391308
H -2.668346 -3.602309 1.196473

4-piperidino-4-cyano-N-methylpyridinium+, step 1, ts

N -2.689643 -0.738726 0.166864
C -2.057723 -0.237415 1.270177
C -2.393096 -0.199620 -1.052829
C -1.397943 0.726921 -1.218597
H -3.021768 -0.512821 -1.881967
H -2.431594 -0.578024 2.232016
C -1.056523 0.693452 1.180284
H -0.663055 1.127314 2.094870
C -0.536500 1.105151 -0.111972
N 1.093659 0.258222 -0.365146
C 0.883849 -1.197968 -0.550379
C 2.053243 0.550602 0.734911
H 1.441601 0.673547 -1.243741
H 0.173132 -1.330871 -1.372111
H 0.422488 -1.561995 0.377049
C 2.205236 -1.912231 -0.822449
C 3.394497 -0.131584 0.480054
H 1.593822 0.169360 1.655164
H 2.159008 1.636731 0.814270
H 2.004376 -2.985647 -0.918132
C 3.215733 -1.635944 0.289037

H	2.606468	-1.579519	-1.789914
H	4.056971	0.084611	1.326065
H	3.864855	0.311947	-0.408415
H	4.176369	-2.104474	0.051259
H	2.866618	-2.089099	1.227087
H	-1.258249	1.176505	-2.198507
C	-3.848669	-1.636467	0.320597
H	-3.943963	-2.245473	-0.578559
H	-4.760586	-1.053767	0.474506
H	-3.676808	-2.290906	1.175436
C	-0.026318	2.468935	-0.175622
N	0.421068	3.564731	-0.243953

2-piperidino-2-fluoro-N-methylpyridinium+, step 1, addition product

C	-2.823554	-1.122463	-0.939066
C	-2.121630	-1.896758	0.031405
C	-2.586342	0.218006	-0.969982
N	-1.648734	0.819831	-0.148577
H	-3.131475	0.903157	-1.612240
H	-2.368318	-2.946810	0.170314
C	-1.173804	-1.327537	0.831542
H	-0.694366	-1.883633	1.631305
C	-0.819516	0.082387	0.698423
N	0.712822	0.275497	0.253605
F	-0.722845	0.716597	1.967004
C	0.918015	-0.130413	-1.177607
C	1.700402	-0.417197	1.158484
H	0.889723	1.289525	0.338145
H	0.156969	0.373826	-1.778857
H	0.729600	-1.209227	-1.216945
C	2.331424	0.219403	-1.623172
C	3.118829	-0.054430	0.740627
H	1.520372	-1.490922	1.047523
H	1.473717	-0.114851	2.182633
H	2.450358	-0.107617	-2.662096
C	3.377327	-0.427841	-0.717430
H	2.455375	1.312171	-1.624919
H	3.811848	-0.574699	1.411192
H	3.285251	1.021126	0.896629
H	4.382048	-0.113393	-1.016963
H	3.339948	-1.519530	-0.831271
H	-3.578015	-1.555871	-1.585356
C	-1.474210	2.280850	-0.215732
H	-2.429849	2.730304	-0.487481
H	-0.728679	2.562114	-0.969509
H	-1.189161	2.663628	0.764722

4-piperidino-4-chloro-N-methylpyridinium+, addition product, MP2/6-31+G*

N	-2.838738	-0.767680	0.182012
C	-2.144420	-0.304978	1.265765
C	-2.376090	-0.430802	-1.062060
C	-1.217715	0.259955	-1.256598
H	-2.989889	-0.744397	-1.902085
H	-2.578993	-0.521099	2.238020
C	-0.977898	0.395409	1.161178
H	-0.535088	0.788865	2.070893
C	-0.398249	0.740014	-0.138770
N	1.081922	0.181450	-0.276630
Cl	-0.112814	2.555977	-0.316221
C	1.101513	-1.310710	-0.478349
C	2.001251	0.556537	0.859652
H	1.453284	0.627246	-1.132771
H	0.401887	-1.540969	-1.284521
H	0.716958	-1.747364	0.450480
C	2.515121	-1.779685	-0.796930
C	3.425712	0.128543	0.537154
H	1.624080	0.031671	1.742386
H	1.918221	1.633225	1.014396
H	2.486164	-2.867910	-0.923035
C	3.504933	-1.375787	0.292522
H	2.826965	-1.363517	-1.765637
H	4.064059	0.428232	1.375870
H	3.786828	0.682086	-0.341314
H	4.521582	-1.662954	0.005695
H	3.273319	-1.913270	1.221815
H	-0.940131	0.533983	-2.272160
C	-4.160954	-1.388002	0.346109
H	-4.334303	-2.075879	-0.482412
H	-4.945867	-0.626943	0.364911
H	-4.172757	-1.951961	1.279527

2-chloro-N-methylpyridinium+, step 1, addition product

C	2.801325	-1.486481	-0.858284
C	2.064118	-0.792578	-1.860862
C	2.519779	-1.199964	0.441112
N	1.503714	-0.331824	0.812225
H	3.057157	-1.644737	1.272898
H	2.290132	-0.949423	-2.913087
C	1.089787	0.099679	-1.521913
H	0.605680	0.700573	-2.284924
C	0.769062	0.404802	-0.127469
N	-0.788792	0.188846	0.156202
Cl	0.908964	2.251938	0.187420
C	-1.115010	-1.270816	0.334771
C	-1.699501	0.795778	-0.884829
H	-0.990521	0.683820	1.039613

H	-0.412907	-1.683718	1.061733
H	-0.925077	-1.744919	-0.635147
C	-2.561356	-1.427227	0.786029
C	-3.145200	0.683987	-0.422414
H	-1.538392	0.226738	-1.804698
H	-1.390385	1.831698	-1.035290
H	-2.765262	-2.498623	0.892737
C	-3.534314	-0.773813	-0.192068
H	-2.678784	-0.988121	1.787656
H	-3.777707	1.147022	-1.188089
H	-3.287531	1.272756	0.495263
H	-4.557191	-0.839599	0.192079
H	-3.518642	-1.314926	-1.147522
H	3.590044	-2.188734	-1.102454
C	1.419628	0.030085	2.237977
H	1.809887	-0.802902	2.823671
H	0.383623	0.196655	2.545018
H	1.999127	0.933629	2.443115

4-piperidino-4-chloro-N-methylpyridinium+, addition product, MP2/6-31+G*

N	-2.838738	-0.767680	0.182012
C	-2.144420	-0.304978	1.265765
C	-2.376090	-0.430802	-1.062060
C	-1.217715	0.259955	-1.256598
H	-2.989889	-0.744397	-1.902085
H	-2.578993	-0.521099	2.238020
C	-0.977898	0.395409	1.161178
H	-0.535088	0.788865	2.070893
C	-0.398249	0.740014	-0.138770
N	1.081922	0.181450	-0.276630
Cl	-0.112814	2.555977	-0.316221
C	1.101513	-1.310710	-0.478349
C	2.001251	0.556537	0.859652
H	1.453284	0.627246	-1.132771
H	0.401887	-1.540969	-1.284521
H	0.716958	-1.747364	0.450480
C	2.515121	-1.779685	-0.796930
C	3.425712	0.128543	0.537154
H	1.624080	0.031671	1.742386
H	1.918221	1.633225	1.014396
H	2.486164	-2.867910	-0.923035
C	3.504933	-1.375787	0.292522
H	2.826965	-1.363517	-1.765637
H	4.064059	0.428232	1.375870
H	3.786828	0.682086	-0.341314
H	4.521582	-1.662954	0.005695
H	3.273319	-1.913270	1.221815
H	-0.940131	0.533983	-2.272160

C -4.160954 -1.388002 0.346109
H -4.334303 -2.075879 -0.482412
H -4.945867 -0.626943 0.364911
H -4.172757 -1.951961 1.279527

2-bromo-N-methylpyridinium+, step 1, addition product

C 2.826149 -1.829771 -0.761922
C 2.056108 -1.294061 -1.821861
C 2.383720 -1.646592 0.520173
N 1.199606 -0.992201 0.796474
H 2.907316 -2.039713 1.385371
H 2.349750 -1.457538 -2.855616
C 0.947033 -0.538476 -1.541877
H 0.404352 -0.057140 -2.347738
C 0.567289 -0.254529 -0.189731
N -0.934486 -0.159493 0.049012
Br 1.022883 1.949144 0.186880
C -1.584118 -1.518598 0.221696
C -1.701528 0.614942 -1.007898
H -1.045772 0.391990 0.916156
H -0.969579 -2.108675 0.903910
H -1.551430 -1.996284 -0.763339
C -3.005569 -1.325350 0.730640
C -3.114865 0.856613 -0.502599
H -1.708817 -0.006851 -1.907347
H -1.154024 1.539304 -1.194849
H -3.455825 -2.316305 0.857944
C -3.832742 -0.461770 -0.220308
H -2.973708 -0.868249 1.730926
H -3.644525 1.439619 -1.264167
H -3.081739 1.485903 0.398457
H -4.822395 -0.273425 0.207552
H -3.992580 -1.002616 -1.162484
H 3.740166 -2.386740 -0.937867
C 0.920358 -0.700013 2.216661
H 1.447485 -1.435715 2.823715
H -0.144550 -0.790794 2.441896
H 1.268098 0.310673 2.450431

2-cyano-N-methylpyridinium+, step 1, addition product

C 2.230876 -2.107505 -0.541285
C 1.844734 -1.448875 -1.711823
C 2.265852 -1.405797 0.657225
N 1.946147 -0.090625 0.703253
H 2.564235 -1.860357 1.596340
H 1.822298 -1.976644 -2.661932
C 1.513179 -0.096861 -1.652555
H 1.225816 0.462905 -2.538362

C	1.540946	0.567073	-0.421265
N	-1.076368	0.561670	0.577521
C	-1.328062	-0.858786	0.886758
C	-1.782063	0.969118	-0.654705
H	-1.449045	1.131688	1.345130
H	-0.822859	-1.100258	1.832153
H	-0.844372	-1.449546	0.092786
C	-2.809509	-1.226735	0.956318
C	-3.277634	0.659361	-0.635255
H	-1.309945	0.428887	-1.490499
H	-1.602312	2.039163	-0.809283
H	-2.916627	-2.303007	1.141318
C	-3.520034	-0.819730	-0.334764
H	-3.267266	-0.709158	1.811155
H	-3.725288	0.942105	-1.595955
H	-3.760723	1.278330	0.133987
H	-4.593658	-1.025002	-0.260645
H	-3.140979	-1.429595	-1.168170
H	2.504594	-3.158434	-0.543415
C	1.951946	0.633634	1.995471
H	2.290001	-0.050801	2.772012
H	0.931780	0.971691	2.186454
H	2.629585	1.485983	1.924266
C	1.286413	1.969880	-0.323783
N	1.125207	3.145154	-0.293539

2-piperidino-2-cyano-N-methylpyridinium+, C2-Npip bond constrained to 1.63 Å

C	2.253238	-1.923228	-0.671454
C	1.723317	-1.192607	-1.778614
C	2.270496	-1.305779	0.543293
N	1.713205	-0.055350	0.746541
H	2.765748	-1.731070	1.411408
H	1.876065	-1.556823	-2.792436
C	1.104854	0.008283	-1.594272
H	0.811935	0.632670	-2.433413
C	0.863674	0.531902	-0.226160
N	-0.693974	0.295501	0.191866
C	-0.988454	-1.141435	0.523816
C	-1.651769	0.812844	-0.850957
H	-0.846874	0.853563	1.048702
H	-0.264358	-1.461210	1.276254
H	-0.814545	-1.708924	-0.397088
C	-2.420954	-1.282367	1.023396
C	-3.085015	0.700394	-0.350418
H	-1.493187	0.196771	-1.741666
H	-1.375484	1.847621	-1.074586
H	-2.599415	-2.342920	1.233941
C	-3.426288	-0.743335	0.009091

H	-2.528453	-0.753189	1.981441
H	-3.746476	1.080871	-1.136834
H	-3.226115	1.357509	0.519552
H	-4.441087	-0.803642	0.414897
H	-3.409273	-1.364345	-0.896542
H	2.735178	-2.886297	-0.795490
C	1.845179	0.594120	2.058952
H	2.603283	0.059704	2.631721
H	0.903678	0.569750	2.622451
H	2.169387	1.630583	1.937545
C	0.959076	2.004629	-0.195987
N	1.008752	3.188258	-0.188974

4-piperidino-4-cyano-N-methylpyridinium+, ion-dipole addition product MP2/6-31+G*

N	-2.626110	-0.954521	0.194050
C	-2.069185	-0.399171	1.300400
C	-2.458126	-0.384150	-1.028348
C	-1.709814	0.769455	-1.175052
H	-2.957716	-0.868545	-1.861885
H	-2.272460	-0.892328	2.246186
C	-1.313730	0.757473	1.209417
H	-0.898794	1.195869	2.112316
C	-1.075005	1.333022	-0.052386
N	1.354644	0.472105	-0.479028
C	1.204828	-0.914289	-0.934544
C	2.076067	0.557066	0.799545
H	1.856668	1.019024	-1.186026
H	0.709329	-0.904131	-1.914351
H	0.524289	-1.412187	-0.222356
C	2.522071	-1.689209	-0.997435
C	3.422347	-0.167283	0.788577
H	1.427671	0.102186	1.566123
H	2.197010	1.617156	1.051815
H	2.327421	-2.729852	-1.286373
C	3.246011	-1.620279	0.347513
H	3.154500	-1.252453	-1.782651
H	3.878602	-0.112980	1.784640
H	4.101069	0.351768	0.097830
H	4.218264	-2.121174	0.282363
H	2.663116	-2.164558	1.105447
H	-1.597018	1.211156	-2.161149
C	-3.484489	-2.156072	0.326112
H	-3.376495	-2.763032	-0.572237
H	-4.522711	-1.841448	0.449528
H	-3.156613	-2.726201	1.194504
C	-0.400274	2.592917	-0.151711
N	0.122847	3.655968	-0.214486

4-cyano-N-methylpyridinium+ + piperidine, step 1, covalent addition product

N	-2.684272	-0.725924	0.145819
C	-2.057542	-0.221070	1.256392
C	-2.360273	-0.181306	-1.069376
C	-1.320647	0.685902	-1.234598
H	-3.005150	-0.450961	-1.901751
H	-2.473725	-0.520273	2.214937
C	-1.009920	0.649492	1.184896
H	-0.631727	1.091594	2.101967
C	-0.419305	1.025484	-0.114559
N	1.029651	0.226913	-0.330617
C	0.834747	-1.256432	-0.403939
C	2.065401	0.585336	0.697645
H	1.362187	0.554321	-1.253809
H	0.061682	-1.445964	-1.153090
H	0.461250	-1.562873	0.579541
C	2.148129	-1.948614	-0.747222
C	3.393017	-0.084427	0.365605
H	1.673933	0.237139	1.659660
H	2.153614	1.674683	0.719822
H	1.963427	-3.028571	-0.774166
C	3.238639	-1.599589	0.262770
H	2.461735	-1.660617	-1.760691
H	4.113426	0.189508	1.144608
H	3.783226	0.325299	-0.576719
H	4.188210	-2.058018	-0.031433
H	2.978323	-2.013244	1.246425
H	-1.169618	1.150056	-2.206188
C	-3.909047	-1.529132	0.292895
H	-4.040296	-2.138372	-0.601898
H	-4.780130	-0.882661	0.432416
H	-3.796725	-2.189513	1.153389
C	0.011336	2.428903	-0.168040
N	0.370212	3.556324	-0.233463

2-piperidino-2-fluoro-N-methyl-dihydropyridine

C	-3.237420	-0.223167	-0.916435
C	-2.441200	-1.409331	-0.960089
C	-2.713990	0.868221	-0.285220
N	-1.462101	0.868308	0.277423
H	-3.242987	1.815969	-0.228938
H	-2.796647	-2.282008	-1.505464
C	-1.224121	-1.449317	-0.349339
H	-0.611716	-2.346510	-0.377303
C	-0.695165	-0.316981	0.440322
N	0.713679	0.006319	0.259832
C	1.001947	0.372553	-1.135368

C	1.653286	-1.025671	0.721034
H	0.235452	1.075625	-1.479467
H	0.946054	-0.514784	-1.796546
C	2.391016	0.994572	-1.220366
C	3.067676	-0.454596	0.705685
H	1.618493	-1.922097	0.070185
H	1.368251	-1.327114	1.729826
H	2.601643	1.273930	-2.260924
C	3.446823	0.024058	-0.694127
H	2.401324	1.915670	-0.622213
H	3.770314	-1.220881	1.058125
H	3.111901	0.383662	1.413200
H	4.437668	0.494950	-0.688875
H	3.509778	-0.842100	-1.369156
H	-4.223564	-0.171226	-1.364286
C	-0.969854	2.074781	0.950917
H	-0.254689	2.617280	0.324986
H	-0.481509	1.795015	1.884458
H	-1.824337	2.720221	1.167648
F	-0.777830	-0.702080	1.860207

2-piperidino-2-chloro-N-methyl-dihydropyridine

C	3.255198	-0.875368	-0.538902
C	2.521237	-0.567501	-1.686978
C	2.599234	-0.954851	0.675980
N	1.261372	-0.761779	0.766801
H	3.117080	-1.149912	1.608180
H	3.011949	-0.489577	-2.653920
C	1.155559	-0.352693	-1.575120
H	0.559018	-0.092509	-2.443084
C	0.521429	-0.421108	-0.327948
N	-0.837354	-0.226280	-0.116226
C	-1.639442	-1.461506	-0.076733
C	-1.454613	0.819623	-0.946328
H	-1.096397	-2.226084	0.491601
H	-1.775862	-1.854313	-1.103303
C	-2.991380	-1.156701	0.555458
C	-2.794172	1.190847	-0.325620
H	-1.613952	0.460623	-1.982288
H	-0.766163	1.670021	-0.942571
H	-3.602512	-2.068463	0.566156
C	-3.699102	-0.035275	-0.206251
H	-2.829336	-0.851504	1.597669
H	-3.270803	1.965828	-0.938719
H	-2.601477	1.626400	0.662598
H	-4.640660	0.224875	0.292279
H	-3.961809	-0.393897	-1.212587
H	4.329409	-1.026493	-0.569046

C	0.657345	-0.579328	2.102983
H	-0.202253	-1.234601	2.231651
H	0.373087	0.476748	2.148908
H	1.419486	-0.812211	2.846624
Cl	1.282077	2.297332	0.526034

2-piperidino-2-chloro-N-methyldihydropyridine, constrained C2-Cl length to 1.900 Å

C	3.149197	-0.838742	-0.862345
C	2.315770	-0.199958	-1.834197
C	2.620428	-1.056773	0.376055
N	1.335769	-0.689580	0.710458
H	3.159088	-1.593678	1.152890
H	2.640126	-0.124695	-2.870505
C	1.101916	0.293639	-1.467143
H	0.467639	0.806216	-2.184899
C	0.635149	0.278233	-0.062280
N	-0.803136	0.083836	0.123175
C	-1.217357	-1.259069	-0.328780
C	-1.667870	1.095341	-0.500733
H	-0.520372	-1.998495	0.075743
H	-1.164602	-1.334106	-1.433270
C	-2.636672	-1.542906	0.150308
C	-3.100317	0.904911	-0.014397
H	-1.650979	1.012634	-1.605566
H	-1.302820	2.086693	-0.230618
H	-2.932999	-2.546914	-0.180676
C	-3.610852	-0.488813	-0.369046
H	-2.642062	-1.544163	1.248710
H	-3.736556	1.679154	-0.462453
H	-3.120819	1.049664	1.073535
H	-4.615522	-0.653523	0.039671
H	-3.693024	-0.578058	-1.462194
H	4.147316	-1.192287	-1.097317
C	0.957003	-0.843556	2.120597
H	1.214584	-1.856761	2.439705
H	-0.116270	-0.686349	2.217942
H	1.484199	-0.111422	2.742654
Cl	1.022134	1.986615	0.673705

2-piperidino-2-bromo-N-methyldihydropyridine, C2-Br length constrained to 2.100 Å

C	2.758032	-1.758582	-0.713044
C	1.970613	-1.256546	-1.794919
C	2.270181	-1.610495	0.553449
N	1.056723	-1.009559	0.810278
H	2.779667	-2.011750	1.425505
H	2.256914	-1.457312	-2.825339
C	0.872826	-0.497177	-1.525750
H	0.288470	-0.059678	-2.330326

C 0.458801 -0.168695 -0.153833
N -0.976842 -0.082879 0.088210
C -1.604566 -1.415359 -0.046421
C -1.708462 0.884436 -0.740166
H -1.007316 -2.145092 0.508296
H -1.607890 -1.738255 -1.106511
C -3.029659 -1.365838 0.492200
C -3.134642 1.023864 -0.221063
H -1.744180 0.562742 -1.800098
H -1.192449 1.843411 -0.695201
H -3.481987 -2.361953 0.399057
C -3.857871 -0.319542 -0.248920
H -2.992787 -1.120963 1.562345
H -3.665164 1.765896 -0.831594
H -3.095164 1.410309 0.805713
H -4.859284 -0.234522 0.190887
H -3.994314 -0.637901 -1.292826
H 3.692351 -2.286086 -0.873512
C 0.714900 -0.788227 2.221059
H 0.958068 -1.696047 2.778005
H -0.349383 -0.574931 2.305359
H 1.282729 0.061537 2.617154
Br 1.197475 1.770303 0.169660

2-piperidino-2-bromo-N-methyl-dihydropyridine

C 2.960234 -1.581550 -0.417795
C 2.313060 -1.273287 -1.621037
C 2.241149 -1.530295 0.757331
N 0.918990 -1.208728 0.770297
H 2.690321 -1.712099 1.727377
H 2.855344 -1.289676 -2.562995
C 0.980558 -0.907073 -1.592770
H 0.455065 -0.660476 -2.508978
C 0.260080 -0.887294 -0.384193
N -1.062776 -0.542641 -0.293939
C -2.048078 -1.538016 0.145085
C -1.586431 0.406560 -1.281353
H -1.570030 -2.257276 0.816255
H -2.403215 -2.104480 -0.736067
C -3.217745 -0.829951 0.816608
C -2.728895 1.174328 -0.628445
H -1.943380 -0.127286 -2.182982
H -0.774258 1.089670 -1.543553
H -3.976634 -1.569657 1.103126
C -3.812231 0.221969 -0.122052
H -2.859670 -0.347855 1.735541
H -3.146509 1.882805 -1.354949
H -2.303908 1.759374 0.196380

H	-4.604676	0.779781	0.390981
H	-4.284219	-0.284208	-0.977441
H	4.015506	-1.831837	-0.380697
C	0.300405	-0.869247	2.066640
H	-0.299018	-1.700292	2.445179
H	-0.303726	0.023696	1.895258
H	1.103046	-0.629612	2.762505
Br	1.268109	1.912061	0.268927

2-piperidino-2-cyano-N-methylpyridine, deprotonated adduct, MP2/6-31+G*

C	2.547808	-1.697200	-0.570998
C	1.989664	-1.018113	-1.707531
C	2.334984	-1.146206	0.657378
N	1.597557	-0.001760	0.855226
H	2.782784	-1.555888	1.560169
H	2.240914	-1.349502	-2.713990
C	1.195761	0.072010	-1.547899
H	0.810203	0.619504	-2.404858
C	0.730326	0.538097	-0.189173
N	-0.687874	0.220756	0.129715
C	-0.937792	-1.228783	0.125216
C	-1.662610	0.907704	-0.733197
H	-0.164988	-1.719537	0.724725
H	-0.871026	-1.641953	-0.899634
C	-2.318019	-1.507895	0.711171
C	-3.067132	0.705918	-0.175106
H	-1.621883	0.521798	-1.770731
H	-1.420157	1.974813	-0.761228
H	-2.495645	-2.591172	0.713193
C	-3.400683	-0.781023	-0.082779
H	-2.332754	-1.169952	1.756113
H	-3.788903	1.229777	-0.815079
H	-3.115102	1.164148	0.821291
H	-4.385539	-0.930018	0.376903
H	-3.454448	-1.205467	-1.096022
H	3.179176	-2.572673	-0.673357
C	1.305971	0.418160	2.226187
H	0.387701	-0.042368	2.607081
H	1.192587	1.504800	2.260621
H	2.152593	0.138145	2.857650
C	0.857100	2.022988	-0.139723
N	1.012062	3.196948	-0.125530

4-piperidino-4-cyano-N-methylpyridine, deprotonated adduct, MP2/6-31+G*

N	-2.655421	-0.782285	0.123728
C	-2.056721	-0.222239	1.241920
C	-2.279285	-0.260623	-1.104597
C	-1.207188	0.550146	-1.267166

H	-2.898164	-0.556980	-1.948378
H	-2.506277	-0.492260	2.195071
C	-0.994593	0.616810	1.173551
H	-0.595206	1.030111	2.095986
C	-0.289734	0.908482	-0.128264
N	1.018315	0.202205	-0.299268
C	0.869104	-1.258102	-0.234982
C	2.049644	0.636227	0.656184
H	0.048073	-1.553134	-0.894908
H	0.610427	-1.587719	0.791351
C	2.168703	-1.923928	-0.674776
C	3.397350	0.046753	0.253107
H	1.802720	0.315264	1.688119
H	2.102172	1.729590	0.647118
H	2.046183	-3.014519	-0.636617
C	3.329486	-1.478026	0.211576
H	2.367781	-1.649399	-1.718771
H	4.166497	0.384236	0.960074
H	3.663791	0.437680	-0.737210
H	4.277106	-1.898931	-0.147234
H	3.175976	-1.862794	1.230578
H	-0.951263	0.911208	-2.259588
C	-3.990743	-1.356644	0.261259
H	-4.194532	-1.993475	-0.602243
H	-4.763933	-0.580073	0.329095
H	-4.021049	-1.974892	1.161018
C	-0.008359	2.360120	-0.215752
N	0.171923	3.528970	-0.279577

2-piperidino-2-fluoro-N-methyl-dihydropyridine, ts for loss of F-

C	3.375285	-0.690777	-0.021327
C	2.561321	-1.528090	-0.776964
C	2.774403	0.275337	0.732874
N	1.445275	0.413704	0.789431
H	3.343563	0.973836	1.310672
H	2.993895	-2.294387	-1.394175
C	1.198376	-1.358192	-0.738326
H	0.545595	-1.970264	-1.328440
C	0.642586	-0.346491	0.034552
N	-0.734969	-0.119409	0.121645
C	-1.473839	-1.195669	0.782018
C	-1.352935	0.327499	-1.142846
H	-0.952358	-1.474759	1.691961
H	-1.523743	-2.087154	0.150896
C	-2.885990	-0.719697	1.112090
C	-2.753005	0.851184	-0.850943
H	-1.420035	-0.511352	-1.842378

H	-0.702140	1.082779	-1.561006
H	-3.441343	-1.539215	1.561254
C	-3.603827	-0.199910	-0.135188
H	-2.822969	0.072222	1.854186
H	-3.221011	1.144373	-1.786578
H	-2.673926	1.745887	-0.239063
H	-4.572744	0.209743	0.136704
H	-3.795514	-1.031594	-0.812242
H	4.444676	-0.768709	-0.037738
C	0.891186	1.591433	1.488260
H	0.049076	1.295208	2.089249
H	0.615312	2.291009	0.714724
H	1.669226	1.994394	2.118836
F	1.138994	1.863127	-1.323288

Transition states for loss of Cl⁻ and Br⁻ from the dihydropyridines did not converge.

2-piperidino-2-cyano-N-methyldihydropyridine, ts for loss of CN⁻

C	-3.180877	-0.614430	0.841692
C	-2.377256	0.005787	1.818254
C	-2.598282	-1.024327	-0.337044
N	-1.272303	-0.825868	-0.580868
H	-3.150745	-1.548136	-1.109655
H	-2.789445	0.264771	2.790707
C	-1.064848	0.288270	1.516466
H	-0.429299	0.813068	2.223135
C	-0.543839	0.032390	0.214862
N	0.846707	0.033416	-0.056773
C	1.494767	-1.187022	0.468755
C	1.565779	1.233157	0.389733
H	0.893342	-2.059148	0.186505
H	1.524888	-1.158677	1.576270
C	2.906482	-1.292898	-0.094523
C	2.973265	1.210134	-0.191662
H	1.631942	1.273694	1.495400
H	0.992166	2.094981	0.039227
H	3.386456	-2.196889	0.302496
C	3.721421	-0.047026	0.248621
H	2.841261	-1.404951	-1.185062
H	3.509219	2.112757	0.128127
H	2.897616	1.243080	-1.286111
H	4.712063	-0.096443	-0.219658
H	3.885366	-0.010486	1.335702
H	-4.237241	-0.803377	1.002667
C	-0.768895	-1.070129	-1.940041
H	0.183680	-1.596142	-1.911945
H	-0.640956	-0.090223	-2.414446
H	-1.509169	-1.666715	-2.474542

C -1.200866 1.829800 -0.847542
N -2.326154 2.027680 -1.220108

2-piperidino-2-fluoro-N-methylpyridinium+ + piperidine, H-bonded complex

C -0.323595 -2.894382 -0.443985
C 0.244557 -2.398668 -1.660457
C 0.322283 -2.592579 0.716974
N 1.376158 -1.698331 0.780135
H 0.074785 -3.060285 1.666700
H -0.081925 -2.804457 -2.615708
C 1.254094 -1.486452 -1.634729
H 1.798886 -1.202783 -2.530172
C 1.724066 -0.917157 -0.355566
N 1.220860 0.555124 -0.172172
C 1.591731 1.416902 -1.347029
C 1.667089 1.174089 1.120044
N -1.581979 0.654755 -0.000603
H 1.194114 0.932331 -2.241679
H 2.685249 1.433613 -1.404122
C 1.026781 2.823265 -1.197468
C 1.101043 2.579772 1.281911
H 2.762328 1.196178 1.112207
H 1.319338 0.519964 1.923527
H 1.354881 3.406910 -2.065378
C 1.484277 3.471807 0.105207
H -0.069673 2.789010 -1.240690
H 1.483784 2.984749 2.226012
H 0.009102 2.532430 1.381796
H 1.037437 4.465320 0.216697
H 2.573431 3.613549 0.086467
H -1.147253 -3.599960 -0.439383
C 2.350146 -1.897824 1.874992
H 1.791182 -2.033910 2.803712
H 3.004154 -1.035037 1.972628
H 2.962612 -2.782674 1.680689
C -2.338968 0.131692 -1.165612
H -1.749073 1.668405 0.030735
C -2.105494 0.091129 1.268562
C -3.840127 0.377405 -1.050469
H -2.130573 -0.943292 -1.220337
H -1.926613 0.593273 -2.071512
C -3.600927 0.332587 1.450930
H -1.531038 0.526395 2.096574
H -1.892557 -0.984350 1.247404
H -4.350987 -0.058195 -1.917897
H -4.033859 1.459762 -1.080101
C -4.382879 -0.208660 0.253458
H -3.782887 1.412243 1.555986

H -3.938059 -0.136533 2.383448
H -5.449382 0.018389 0.359881
H -4.295312 -1.304324 0.225512
H 0.134086 0.498088 -0.135164
F 3.116010 -0.744800 -0.395548

2-piperidino-2-chloro-N-methylpyridinium+ + piperidine, H-bonded complex

C -0.292211 -2.868490 -0.427730
C 0.264610 -2.324392 -1.627287
C 0.289339 -2.512300 0.749221
N 1.280896 -1.547693 0.854794
H 0.029246 -2.986417 1.691896
H -0.017225 -2.735116 -2.594754
C 1.214308 -1.353191 -1.573248
H 1.740615 -1.035749 -2.468023
C 1.652867 -0.763205 -0.283044
N 1.016012 0.677456 -0.127106
C 1.310756 1.578906 -1.292099
C 1.329972 1.348275 1.176683
N -1.786012 0.506772 -0.027513
H 1.012455 1.045642 -2.197343
H 2.392556 1.743180 -1.314855
C 0.570810 2.904806 -1.171340
C 0.604722 2.683098 1.309389
H 2.415113 1.493416 1.222176
H 1.017690 0.662905 1.967618
H 0.852663 3.518335 -2.034993
C 0.913430 3.608871 0.137413
H -0.511667 2.740126 -1.246353
H 0.915871 3.131840 2.260135
H -0.476949 2.514985 1.384292
H 0.351692 4.544359 0.230460
H 1.978975 3.876028 0.145528
H -1.063847 -3.630615 -0.442175
C 2.172870 -1.686895 2.026122
H 1.557896 -2.002638 2.871271
H 2.654125 -0.744556 2.278013
H 2.942921 -2.439578 1.833213
C -2.486664 -0.063527 -1.205609
H -2.014321 1.508811 -0.008674
C -2.311456 -0.073912 1.233278
C -4.000453 0.109100 -1.128979
H -2.223710 -1.126792 -1.245080
H -2.075413 0.410318 -2.105772
C -3.820634 0.096916 1.377963
H -1.778378 0.393150 2.071656
H -2.046976 -1.137628 1.224813
H -4.468044 -0.358445 -2.004168

H	-4.246131	1.180447	-1.173938
C	-4.546132	-0.491352	0.167180
H	-4.056800	1.167479	1.468405
H	-4.157580	-0.380140	2.306535
H	-5.624673	-0.315412	0.245647
H	-4.405171	-1.581684	0.151924
H	-0.059837	0.495651	-0.123462
Cl	3.446578	-0.503759	-0.358982

2-piperidino-2-bromo-N-methylpyridinium+ + piperidine, H-bonded complex

C	-0.498646	-2.987187	-0.391593
C	0.010821	-2.354137	-1.567364
C	-0.042960	-2.535151	0.806274
N	0.772095	-1.417641	0.953315
H	-0.286098	-3.026360	1.744865
H	-0.201347	-2.771249	-2.549638
C	0.812881	-1.259797	-1.474944
H	1.296139	-0.863989	-2.361539
C	1.182948	-0.658512	-0.176638
N	0.608993	0.793324	-0.079640
C	0.982095	1.667216	-1.244523
C	0.868811	1.491862	1.222248
N	-2.159432	0.580974	-0.086480
H	0.723793	1.126362	-2.156148
H	2.065796	1.812710	-1.211648
C	0.254783	3.003956	-1.193094
C	0.162054	2.841400	1.286498
H	1.953601	1.613532	1.322723
H	0.496135	0.837445	2.011902
H	0.586481	3.590243	-2.057852
C	0.542739	3.736034	0.112550
H	-0.825600	2.850128	-1.315225
H	0.431702	3.304835	2.242826
H	-0.925239	2.691805	1.308617
H	-0.008368	4.681396	0.156448
H	1.610767	3.987169	0.167414
H	-1.143403	-3.858255	-0.435064
C	1.569869	-1.435916	2.203090
H	0.886412	-1.600821	3.039638
H	2.097782	-0.499198	2.349326
H	2.306900	-2.243522	2.157448
C	-2.780942	-0.080316	-1.262166
H	-2.471406	1.560348	-0.095866
C	-2.646213	-0.019969	1.180873
C	-4.305087	-0.054388	-1.210311
H	-2.415648	-1.113740	-1.272646
H	-2.401846	0.412288	-2.166098

C	-4.167043	0.001880	1.298246
H	-2.178076	0.518814	2.014789
H	-2.276019	-1.052091	1.202371
H	-4.710115	-0.582753	-2.082015
H	-4.653428	0.986489	-1.281677
C	-4.809814	-0.680524	0.090215
H	-4.509851	1.045021	1.361965
H	-4.469994	-0.487393	2.232140
H	-5.901586	-0.611202	0.149292
H	-4.560704	-1.751373	0.100477
H	-0.481271	0.639081	-0.123946
Br	3.217004	-0.427172	-0.229697

2-piperidino-2-cyano-N-methylpyridinium⁺ + piperidine, H-bonded complex

C	-0.191212	-2.723857	-0.362946
C	0.352650	-2.270719	-1.605517
C	0.511352	-2.449322	0.775831
N	1.595006	-1.595418	0.790116
H	0.288515	-2.922461	1.729054
H	0.008737	-2.710799	-2.539720
C	1.377831	-1.374225	-1.626005
H	1.920694	-1.135201	-2.536342
C	1.820433	-0.748772	-0.345541
N	1.018826	0.631180	-0.121281
C	1.217591	1.561540	-1.281141
C	1.381198	1.282659	1.177457
N	-1.786258	0.389147	0.043618
H	0.893181	1.029745	-2.179770
H	2.292753	1.766387	-1.357187
C	0.445046	2.861283	-1.092777
C	0.606942	2.579094	1.385843
H	2.459815	1.485947	1.154913
H	1.165708	0.558581	1.968161
H	0.671737	3.507828	-1.948530
C	0.820636	3.541932	0.220846
H	-0.633808	2.665128	-1.128887
H	0.947379	3.021687	2.329302
H	-0.460801	2.360451	1.511438
H	0.227784	4.451590	0.363534
H	1.873820	3.852546	0.187234
H	-1.030187	-3.410620	-0.322547
C	2.634686	-1.792558	1.818056
H	2.161479	-2.268319	2.679182
H	3.061860	-0.840138	2.134786
H	3.433019	-2.441648	1.445070
C	3.234746	-0.357450	-0.436471
N	4.369323	-0.035538	-0.545212
C	-2.475215	-0.091216	-1.180003

H	-1.991869	1.393428	0.117560
C	-2.359342	-0.246445	1.256391
C	-3.985133	0.121879	-1.128862
H	-2.242538	-1.158099	-1.276307
H	-2.030317	0.420056	-2.043340
C	-3.865440	-0.034071	1.377108
H	-1.830472	0.152840	2.131576
H	-2.129149	-1.315975	1.192698
H	-4.444540	-0.282693	-2.039026
H	-4.198012	1.201109	-1.120251
C	-4.579825	-0.530835	0.119607
H	-4.069995	1.037016	1.521944
H	-4.239471	-0.550127	2.269862
H	-5.653915	-0.324730	0.183589
H	-4.472989	-1.622735	0.046781
H	-0.038362	0.380120	-0.076720

4-piperidino-4-cyano-N-methylpyridinium+ + piperidine, H-bonded complex, MP2/6-31+G*

N	3.718216	-1.155562	-0.412188
C	3.647936	-0.445858	0.763156
C	2.569249	-1.778382	-0.836054
C	1.347974	-1.527083	-0.291137
H	2.690422	-2.514587	-1.626745
H	4.600235	-0.161370	1.203799
C	2.472351	-0.151360	1.383078
H	2.501853	0.314775	2.363382
C	1.161766	-0.492500	0.763906
N	0.456869	0.805649	0.150748
C	1.191809	1.306981	-1.050310
C	0.297580	1.890491	1.173302
H	-0.540909	0.484749	-0.142620
H	1.263956	0.476786	-1.757100
H	2.202831	1.575754	-0.717775
C	0.475085	2.503186	-1.663827
C	-0.434661	3.087859	0.580128
H	1.302954	2.179265	1.500735
H	-0.245775	1.467215	2.024337
H	1.059507	2.839578	-2.528158
C	0.296961	3.625288	-0.645870
H	-0.503453	2.186675	-2.050037
H	-0.518167	3.853151	1.360609
H	-1.457989	2.798728	0.309275
H	-0.258455	4.459148	-1.088024
H	1.279497	4.018471	-0.350698
H	0.494118	-2.109563	-0.622884
C	5.023230	-1.596668	-0.923632
H	4.930787	-1.810253	-1.989257
H	5.368433	-2.491471	-0.396423

H	5.745527	-0.790107	-0.791368
C	0.190617	-0.959724	1.769319
N	-0.597834	-1.358172	2.559391
N	-2.169137	-0.001970	-0.491433
C	-2.269403	-1.402424	-0.975284
H	-2.476478	0.604458	-1.262701
C	-3.103477	0.224217	0.643948
C	-4.548039	-0.123814	0.297607
H	-3.017465	1.272634	0.952390
H	-2.750945	-0.395898	1.476561
C	-3.691136	-1.797960	-1.363834
H	-1.912794	-2.047613	-0.161162
H	-1.585055	-1.516449	-1.825356
C	-4.651683	-1.566182	-0.197652
H	-4.911667	0.564093	-0.479900
H	-5.180511	0.032672	1.179832
H	-3.704314	-2.848316	-1.679873
H	-4.007266	-1.201332	-2.232043
H	-5.680006	-1.794405	-0.499024
H	-4.402613	-2.252801	0.623536

2-fluoro-N-methylpyridinium+ + pip, proton transfer ts

C	-0.326686	-2.929902	-0.449421
C	0.230723	-2.414813	-1.665912
C	0.310053	-2.610653	0.712588
N	1.321784	-1.671531	0.789987
H	0.082491	-3.100601	1.656666
H	-0.069405	-2.841435	-2.621018
C	1.200572	-1.462746	-1.637082
H	1.748043	-1.173971	-2.529477
C	1.651317	-0.867206	-0.353774
N	1.136545	0.552735	-0.169423
C	1.496259	1.410954	-1.344823
C	1.614524	1.173298	1.105396
N	-1.483818	0.647101	0.019754
H	1.082309	0.935534	-2.237846
H	2.589696	1.432706	-1.433668
C	0.947563	2.824682	-1.194025
C	1.064718	2.584592	1.282470
H	2.711636	1.199238	1.090056
H	1.282495	0.527736	1.923295
H	1.268733	3.402808	-2.068321
C	1.430486	3.473937	0.098646
H	-0.150955	2.810814	-1.224088
H	1.471950	2.986575	2.217671
H	-0.026055	2.556854	1.411359
H	0.995756	4.472382	0.216375

H	2.520436	3.604202	0.059764
H	-1.117909	-3.672045	-0.448108
C	2.336202	-1.893175	1.843029
H	1.807584	-2.146251	2.765021
H	2.930385	-0.997379	2.006256
H	3.004550	-2.713532	1.566381
C	-2.228671	0.135899	-1.166075
H	-1.648099	1.661368	0.068164
C	-1.995019	0.053571	1.287586
C	-3.724016	0.396184	-1.038836
H	-2.019422	-0.936929	-1.226356
H	-1.803718	0.612052	-2.057279
C	-3.486985	0.307062	1.462672
H	-1.412364	0.476407	2.114488
H	-1.781293	-1.019029	1.236490
H	-4.237161	-0.020075	-1.913641
H	-3.909136	1.480341	-1.051783
C	-4.269950	-0.209369	0.254890
H	-3.661180	1.385858	1.587583
H	-3.828023	-0.174821	2.386524
H	-5.334186	0.025088	0.364496
H	-4.190792	-1.304567	0.208233
H	-0.146888	0.518304	-0.096734
F	3.056932	-0.724406	-0.404077

2-chloro-N-methylpyridinium+ + piperidine, proton transfer ts

C	-0.311207	-2.963725	-0.445222
C	0.224922	-2.375913	-1.636339
C	0.227649	-2.570125	0.739562
N	1.140546	-1.533666	0.873149
H	-0.015807	-3.065440	1.676430
H	-0.023041	-2.793864	-2.610130
C	1.107113	-1.345905	-1.566570
H	1.620612	-1.000112	-2.458104
C	1.530558	-0.743936	-0.269852
N	0.949257	0.667754	-0.126301
C	1.274631	1.547129	-1.294625
C	1.304538	1.339557	1.160998
N	-1.677648	0.567557	-0.020104
H	0.942056	1.031334	-2.198263
H	2.363107	1.671053	-1.343264
C	0.599719	2.909224	-1.184179
C	0.643248	2.708199	1.292982
H	2.396020	1.446028	1.211048
H	0.969389	0.684100	1.968115
H	0.903221	3.499399	-2.056790
C	0.983866	3.611199	0.113153
H	-0.491919	2.803590	-1.251923

H	0.983417	3.147718	2.238142
H	-0.446360	2.600324	1.382359
H	0.469316	4.574078	0.201881
H	2.061306	3.824857	0.110565
H	-1.024581	-3.780436	-0.472747
C	2.025674	-1.663881	2.052775
H	1.400795	-1.940792	2.905032
H	2.531108	-0.728871	2.279489
H	2.778461	-2.439461	1.882300
C	-2.362432	-0.006360	-1.213185
H	-1.909823	1.569259	0.007436
C	-2.182992	-0.036523	1.244849
C	-3.873322	0.166508	-1.124990
H	-2.089010	-1.065512	-1.250311
H	-1.945630	0.479446	-2.103114
C	-3.691142	0.130208	1.382309
H	-1.646827	0.431886	2.078648
H	-1.905816	-1.095244	1.216090
H	-4.339943	-0.293075	-2.004208
H	-4.121873	1.237470	-1.160467
C	-4.413434	-0.450282	0.165854
H	-3.931647	1.198604	1.485119
H	-4.024841	-0.356867	2.306186
H	-5.492012	-0.277954	0.247153
H	-4.268461	-1.539425	0.139413
H	-0.318497	0.534777	-0.100344
Cl	3.362815	-0.576507	-0.348122

2-bromo-N-methylpyridinium+ + pip, proton transfer ts

C	-0.427525	-3.051154	-0.379149
C	0.035298	-2.385193	-1.557374
C	0.007169	-2.572433	0.816556
N	0.742987	-1.401961	0.965281
H	-0.197037	-3.082491	1.754800
H	-0.156735	-2.812819	-2.539390
C	0.765909	-1.242230	-1.466416
H	1.218623	-0.819993	-2.356688
C	1.117990	-0.620494	-0.169692
N	0.539243	0.788465	-0.067590
C	0.891720	1.659509	-1.235302
C	0.825855	1.490429	1.221250
N	-2.085594	0.570061	-0.053868
H	0.609206	1.127009	-2.145104
H	1.977813	1.804952	-1.237771
C	0.176986	3.003568	-1.175848
C	0.128196	2.844408	1.302286
H	1.912976	1.615673	1.311895
H	0.467119	0.845039	2.025188

H	0.498968	3.585247	-2.047425
C	0.491151	3.737356	0.122153
H	-0.908252	2.865475	-1.282087
H	0.419560	3.305795	2.253255
H	-0.961188	2.708345	1.349493
H	-0.051489	4.687366	0.174679
H	1.562024	3.979286	0.157574
H	-1.010848	-3.964732	-0.420016
C	1.555108	-1.393842	2.207232
H	0.884051	-1.552897	3.055475
H	2.078509	-0.452060	2.331231
H	2.299594	-2.194650	2.163161
C	-2.682097	-0.057235	-1.266755
H	-2.401841	1.548494	-0.029707
C	-2.568096	-0.086365	1.193298
C	-4.204617	-0.030128	-1.220859
H	-2.309493	-1.086229	-1.301826
H	-2.289930	0.471057	-2.143711
C	-4.088633	-0.067542	1.289824
H	-2.104215	0.426685	2.044182
H	-2.189443	-1.114143	1.170399
H	-4.600666	-0.525589	-2.115134
H	-4.553179	1.012397	-1.258023
C	-4.718198	-0.705762	0.051107
H	-4.433736	0.971812	1.391155
H	-4.398551	-0.591575	2.201755
H	-5.810177	-0.638517	0.103101
H	-4.468143	-1.775689	0.023338
H	-0.702768	0.628200	-0.088920
Br	3.183014	-0.394422	-0.252729

2-cyano-N-methylpyridinium+ + pip, proton transfer ts

C	-0.194844	-2.783160	-0.399466
C	0.361504	-2.300113	-1.628888
C	0.469947	-2.483191	0.755326
N	1.505339	-1.574980	0.809442
H	0.250170	-2.979675	1.698087
H	0.068350	-2.759614	-2.571323
C	1.341425	-1.357163	-1.622518
H	1.902693	-1.105452	-2.518512
C	1.733943	-0.705414	-0.327868
N	0.935025	0.618601	-0.123200
C	1.152144	1.538905	-1.284619
C	1.317944	1.284991	1.158840
N	-1.679988	0.402555	0.031910
H	0.822245	1.012865	-2.185288
H	2.229404	1.740083	-1.374288
C	0.403120	2.856040	-1.114717

C	0.565997	2.596017	1.364111
H	2.399466	1.485893	1.140984
H	1.102800	0.578847	1.966609
H	0.644168	3.488545	-1.977127
C	0.788097	3.546110	0.190765
H	-0.681974	2.690244	-1.155182
H	0.920669	3.041074	2.301246
H	-0.506721	2.406489	1.504780
H	0.211127	4.467420	0.325467
H	1.846371	3.837689	0.151778
H	-0.994976	-3.516278	-0.382477
C	2.548537	-1.777615	1.832037
H	2.082437	-2.275884	2.684763
H	2.961251	-0.824913	2.166785
H	3.358124	-2.407851	1.449883
C	3.161622	-0.337090	-0.400351
N	4.299471	-0.023081	-0.499689
C	-2.365446	-0.103692	-1.190882
H	-1.897945	1.405589	0.099392
C	-2.216712	-0.237000	1.266601
C	-3.871480	0.112340	-1.112325
H	-2.122211	-1.167853	-1.267487
H	-1.924240	0.404078	-2.056649
C	-3.719334	-0.020619	1.395185
H	-1.670856	0.176224	2.123183
H	-1.977180	-1.302086	1.196277
H	-4.342100	-0.300948	-2.012083
H	-4.085750	1.191317	-1.112768
C	-4.446722	-0.530856	0.150356
H	-3.923454	1.051223	1.534875
H	-4.081172	-0.528852	2.296700
H	-5.519567	-0.324062	0.226336
H	-4.339903	-1.622848	0.086190
H	-0.328609	0.386146	-0.058917

4-piperidino-4-cyano-N-methylpyridinium+ + piperidine, proton transfer ts, MP2/6-31+G*

N	3.729948	-1.016218	-0.433740
C	3.625679	-0.338174	0.761174
C	2.619468	-1.712195	-0.849344
C	1.388825	-1.536243	-0.298229
H	2.782463	-2.440465	-1.640084
H	4.563507	-0.012996	1.204995
C	2.439129	-0.125336	1.390027
H	2.446926	0.321813	2.379516
C	1.138387	-0.503295	0.754969
N	0.377990	0.734324	0.166084
C	1.075364	1.254901	-1.042925
C	0.249028	1.816241	1.188360

H	-0.850103	0.353362	-0.127156
H	1.146004	0.436566	-1.764377
H	2.096311	1.547190	-0.752972
C	0.331604	2.444819	-1.638463
C	-0.521036	3.008761	0.631052
H	1.255520	2.138913	1.487329
H	-0.253190	1.393634	2.066710
H	0.890935	2.792210	-2.515195
C	0.163643	3.562393	-0.614426
H	-0.652910	2.123596	-2.008140
H	-0.588110	3.769860	1.417495
H	-1.552167	2.718238	0.389652
H	-0.413972	4.391692	-1.037115
H	1.149312	3.965800	-0.344990
H	0.576831	-2.179978	-0.621932
C	5.055749	-1.381367	-0.947927
H	4.973552	-1.599262	-2.013646
H	5.455655	-2.255115	-0.423091
H	5.731025	-0.534505	-0.817793
C	0.198415	-1.048271	1.754016
N	-0.584687	-1.507894	2.515606
N	-2.094773	0.019039	-0.406852
C	-2.163713	-1.336224	-1.025503
H	-2.401068	0.698738	-1.116671
C	-3.029184	0.129078	0.755149
C	-4.462365	-0.178894	0.341136
H	-2.936593	1.139231	1.166566
H	-2.675964	-0.577538	1.512730
C	-3.579760	-1.677020	-1.471816
H	-1.819505	-2.046457	-0.264032
H	-1.458072	-1.356100	-1.864050
C	-4.557616	-1.562382	-0.302274
H	-4.813637	0.588414	-0.364380
H	-5.108383	-0.113219	1.224190
H	-3.588172	-2.689087	-1.893070
H	-3.879749	-0.995821	-2.281439
H	-5.580581	-1.753048	-0.643804
H	-4.324898	-2.331163	0.447211