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

^{1}H NMR δ (ppm, CD_3OD) 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, CH_3), 3.17 (t, 4H, CH_2NCH_2), 1.81 (m, 4H, $N(CH_2\underline{CH_2})_2$), 1.73 (m, 2 H $N(CH_2CH_2)_2\underline{CH_2}$).

^{13}C NMR δ (ppm, CD_3OD) 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 $C_{11}H_{17}N_2$ 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-*N*-methyl pyridinium$^+$	-386.0467182	-386.1293724	75.28
4-fluoro-*N*-methyl pyridinium$^+$	-386.0489729	-386.1342622	75.16
2-chloro-*N*-methyl pyridinium$^+$	-746.0522295	-746.132799	74.43
4-chloro-*N*-methyl pyridinium$^+$	-746.0556179	-746.1385096	74.22
2-bromo-*N*-methyl pyridinium$^+$	-2856.4625888	-2856.5426627	74.35
4-bromo-*N*-methyl pyridinium$^+$	-2856.4662248	-2856.5488446	74.15
2-cyano-*N*-methyl pyridinium$^+$	-379.0232655	-379.1131532	79.29
4-cyano-*N*-methyl pyridinium$^+$	-379.0257207	-379.1200407	79.17

[a]Solvent calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* structures. [b]Frequencies 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]	iν (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	

[a]Solvent (MeOH) calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* geometries. [b]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. [c]Imaginary frequencies were calculated at the HF/6-31+G* level. [d]A structure was not obtained at the MP2/6-31+G* level. [d]This calculation did not converge. [e]The 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_NAr 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

[a]Solvent (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]The 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	$\Delta\Delta H_{SOLV}$[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

[a]Solvent (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]$\Delta\Delta H_{SOLV} = \Delta H_{SOLV}$ (ts) - ΔH_{SOLV} (substrate). Thus, a positive value indicates more favorable solvation of the reactant than of the transition state. [b]A 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

[a]Structures were optimized at the MP2/6-31+G* level. [b]A 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	$\Delta H^{\ddagger}$ (gas)	$\Delta H^{\ddagger}$ (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

[a]Solvent (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]The difference in activation enthalpies, (MeOH – gas). The average difference is 9.4 ± 1.2 kcal/mol. [c]A 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

[a]Solvent (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. [b]The 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}, gas	E_{CX}, MeOH[a]	E_{ts}, 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

[a]Solvent calculations used the polarizable continuum model (PCM) applied to the gas phase MP2/6-31+G* structures. [b]Frequencies 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. [c]ZPVE 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	ΔH_{CX} (gas)	ΔH_{CX} (MeOH)	$\Delta H^{\ddagger}$(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

[a]Solvent (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}^{o}, from substrates and two piperidines (kcal/mol, MP2/6-31+G*).[a]

substrate	ΔH_{CX}^{o} (gas)	ΔH_{CX}^{o} (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

[a]Solvent (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-methyllpyridinium+, 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
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