Quantum chemical calculations of hydration electrostatics and electrochemical oxidation potential of cyclic nitroxide radicals

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Table S1 Correlations between the experimental and calculated data for the considered computational schemes.[a]

PCM SMD method	multiple−conformations				single–conformation[c]			
	R	a	MUE/V	SD/V[b]	R	a	MUE/V	SD/V
gas-phase calculations B3LYP/6−31G(d)//B3LYP/aug−cc−pVTZ								
B3LYP/6−31G(d)	0.96	1.014	0.182	0.019	0.96	0.981	0.182	0.018
B3LYP/aug−cc−pVTZ	0.97	0.962	0.192	0.016	0.97	0.925	0.193	0.015
PBE/6−31G(d)	0.96	0.986	0.152	0.019	0.96	0.954	0.151	0.018
M05−2X/midi	0.94	0.970	0.158	0.022	0.94	0.944	0.157	0.021
M05−2X/6−31+G(d,p)	0.96	0.906	0.136	0.016	0.97	0.876	0.136	0.015
M05−2X/cc−pVTZ	0.96	0.922	0.134	0.017	0.96	0.890	0.134	0.016
M05−2X/aug−cc−pVTZ	0.96	0.901	0.127	0.017	0.96	0.860	0.127	0.016
M06−2X/aug−cc−pVTZ	0.97	0.923	0.144	0.015	0.97	0.886	0.144	0.014
gas-phase calculations B3LYP/6−31G(d)//M05−2X/aug−cc−pVTZ								
B3LYP/6−31G(d)	0.97	1.018	0.060	0.017	0.96	0.979	0.060	0.016
B3LYP/aug−cc−pVTZ	0.98	0.964	0.071	0.012	0.98	0.924	0.071	0.011
PBE/6−31G(d)	0.96	0.991	0.034	0.017	0.96	0.954	0.032	0.017
M05−2X/midi	0.93	0.975	0.041	0.024	0.93	0.942	0.039	0.024
M05−2X/6−31+G(d,p)	0.98	0.909	0.018	0.011	0.98	0.874	0.017	0.010
M05−2X/cc−pVTZ	0.98	0.926	0.016	0.012	0.98	0.889	0.016	0.011
M05−2X/aug−cc−pVTZ	0.98	0.903	0.010	0.011	0.98	0.861	0.011	0.010
M06−2X/aug−cc−pVTZ	0.98	0.925	0.024	0.011	0.98	0.885	0.023	0.010
gas-phase calculations B3LYP/6−31G(d)//M06−2X/aug−cc−pVTZ								
B3LYP/6−31G(d)	0.96	1.013	0.156	0.018	0.96	0.978	0.154	0.017
B3LYP/aug−cc−pVTZ	0.98	0.959	0.165	0.013	0.98	0.950	0.168	0.011
PBE/6−31G(d)	0.96	0.984	0.125	0.018	0.96	0.951	0.124	0.017

M05−2X/midi	0.93	0.971	0.131	0.024	0.93	0.941	0.129	0.023
M05−2X/6−31+G(d,p)	0.98	0.903	0.109	0.013	0.98	0.873	0.109	0.012
M05−2X/cc−pVTZ	0.97	0.920	0.107	0.014	0.98	0.886	0.107	0.012
M05−2X/aug−cc−pVTZ	0.98	0.898	0.100	0.013	0.98	0.857	0.100	0.012
M06−2X/aug−cc−pVTZ	0.98	0.920	0.117	0.012	0.98	0.884	0.116	0.011

[a] The free-energy quantum mechanical calculations employed low-energy structures determined for the isolated radical and cation. The quantum mechanical part was performed with the Gaussian-09 program.[S1] The total electronic energies were calculated using the hybrid B3LYP and two hybrid meta exchange-correlation M05–2X and M06–2X functionals, along with the correlation consistent aug–cc–pVTZ basis set.[S1] In the calculations of $\Delta G^\circ_s(X)$, we have also included the DFT schemes (B3LYP/6−31G(d), PBE/6−31G(d), M05−2X/midi, M05−2X/6−31+G(d,p), M05−2X/cc−pVTZ) that had been employed in the development of SMD.

[b] R is the correlation coefficient, a is the slope of linear plot of E°_{ox}(calculated) *vs.* E°_{ox} (experimental), MUE is the mean unsigned error between the experimental and calculated values, and SD is the standard deviation of calculated points from the linear plot.

[c] The single-conformation calculations employed the lowest energy structures of radicals and cations in water determined using the B3LYP/6−31G(d) for geometries and the M05–2X/aug–cc–pVTZ scheme for the $E_{tot}(X)$ and $\Delta G^\circ_s(X)$ calculations.

References

S1. Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S2 The conformational occupancies x_i of nitroxide **3** in gas phase and water.

Conformation	x_i (%) gas / water[a]	
	radical	cation
chair equatorial *gauche*($\pm$)	64.9 / 71.3	3.8 / 55.0
chair equatorial *trans*	31.2 / 26.7	0.2 / 27.0
chair axial *gauche*($\pm$)	2.0 / 0.2	62.1 / 0.6
twist *gauche*(+)	0.8 / 0.6	17.9 / 4.2
twist *gauche*(−)	0.8 / 0.4	16.0 / 3.3
twist *trans*	0.3 / 0.8	0.0 / 9.9

[a] The x_i values were determined from the Boltzmann probabilities, derived from the free energies in gas and water; the free-energy contributions E_{tot} and $\Delta G°_s(X)$ were calculated at the M05–2X/aug–cc–pVTZ level.

The B3LYP/6−31G(d) optimized structures of the employed conformers of nitroxide **3** and their statistical weights (*w*).

Radical 3.

Conformation 1, $w = 2$
```
1\1\GINC-NODE147\FOpt\UB3LYP\6-31G(d)\C9H18N1O2(2)\LUZHKOV\07-Dec-2016
\0\\#N UB3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH - chair, conf2:O29= +120 eq gauche\\0,2\C,-
0.0628417881,0.0179772096,-0.0566907605\C,-0.060810151,0.0543070267,1.
4656501519\C,1.3827963939,0.0546561715,-0.5534610004\C,0.6175229609,1.
3040861773,2.0579917951\C,2.1684519986,1.3036018181,-0.1065918749\N,1.
9139412881,1.5776301407,1.3482516115\O,2.6642780708,2.4732221709,1.883
4440376\C,-0.2868461863,2.5515058867,1.9553208284\C,0.9583102109,1.048
2015683,3.5355865623\C,3.676455934,1.0447395006,-0.2606462409\C,1.7811
421328,2.5505663871,-0.9311464443\H,-1.0889435734,-0.0043560663,1.8403
048505\H,0.4569786312,-0.8485694219,1.8141341488\H,1.879027956,-0.8496
477154,-0.1785574171\H,1.4148451852,0.0041473895,-1.6508659653\H,-0.64
46056888,2.7260797959,0.9359444018\H,-1.1632725927,2.432727444,2.60221
09345\H,0.2717457814,3.433360566,2.2812233697\H,1.6469599676,0.2022918
791,3.6319188677\H,1.4293928207,1.9269367807,3.97975155\H,0.0425045391
,0.8138538266,4.0892046901\H,3.9879501172,0.197522295,0.3592457644\H,3
.9063306247,0.8122575406,-1.3063862528\H,4.2497082498,1.9221495462,0.0
442616636\H,0.7013144503,2.7278603096,-0.9388968995\H,2.27190536,3.431
5677349,-0.5083394695\H,2.1103337976,2.4314148547,-1.969727638\H,-0.62
24529023,0.8798036732,-0.4529620378\O,-0.7175129436,-1.1924441581,-0.4
358432711\H,-0.7210957162,-1.2348767632,-1.4050545372\\Version=EM64L-G
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adrupole=-1.9605292,-3.246668,5.2071973,-4.2240255,-1.7654443,-0.26091
7\PG=C01 [X(C9H18N1O2)]\\@
```

Conformation 2, *w* = 1

1\1\GINC-CLI20-X\FOpt\UB3LYP\6-31G(d)\C9H18N1O2(2)\LUZHKOV\29-Sep-2015
\0\\#N UB3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH - chair, conf2:O29= +120\\0,2\C,-0.05672887
18,-0.0039437666,-0.0453667423\C,-0.0559494322,0.0493993543,1.48230197
47\C,1.3871681751,0.0419332314,-0.5450430458\C,0.6235583293,1.30318549
82,2.0682578387\C,2.1676668072,1.2951956595,-0.1009593786\N,1.92014932
35,1.5686497768,1.3560363163\O,2.6738431969,2.4626570963,1.8892441639\
C,-0.2833602231,2.5474256469,1.952464673\C,0.9629489625,1.0616038255,3
.5484666138\C,3.6765589206,1.04756185,-0.2637068484\C,1.7656515815,2.5
368246004,-0.9260568929\H,-1.0840370131,-0.0076594442,1.8575619674\H,0
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.1653368308\H,1.4049316823,-0.0205337995,-1.639036452\H,-0.6440199719,
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47464582,3.4339446678,2.2663105946\H,1.6541662387,0.2186655499,3.65399
05648\H,1.4317599096,1.9452725372,3.9850693697\H,0.0469566995,0.830678
7646,4.1032842573\H,3.9996441299,0.206527991,0.358980606\H,3.900082289
,0.8107401444,-1.3097200366\H,4.2456645877,1.9307111172,0.0319996669\H
,0.6840976464,2.7024637221,-0.9335928484\H,2.2480139284,3.4237349786,-
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,0.8394781033,-0.4524419972\O,-0.7485112142,-1.1513214433,-0.533573971
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\PG=C01 [X(C9H18N1O2)]\\@

Conformation 3, *w* = 2

1\1\GINC-CLI20-X\FOpt\UB3LYP\6-31G(d)\C9H18N1O2(2)\LUZHKOV\30-Sep-2015
\0\\#N UB3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH - chair, O29= -120\\0,2\C,-0.0436282038,0.0
330686818,-0.0659243457\C,-0.0583877334,0.1267777516,1.463237818\C,1.3
932032185,0.1150965557,-0.5747483486\C,0.6598990127,1.3514666858,2.068
5542661\C,2.2143127604,1.3301834064,-0.0908259974\N,1.9680290678,1.575
6257555,1.3699022798\O,2.7625643968,2.412675792,1.9359951767\C,-0.1931
728979,2.6356793742,1.981087301\C,0.981936807,1.0618906172,3.545504251
7\C,3.7121860506,1.0089922335,-0.24224837\C,1.8903213562,2.6115067878,
-0.8888217371\H,-1.092621512,0.1111570246,1.8350671209\H,0.4161340852,
-0.7868898644,1.845925404\H,1.8986302412,-0.8034813307,-0.249750993\H,
1.3916452809,0.107354357,-1.6705328004\H,-0.5237224867,2.8321684948,0.
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085803\H,3.9903502174,0.147128011,0.3740800059\H,3.932780645,0.7725814
628,-1.2891634027\H,4.3211948808,1.860574409,0.0658137387\H,0.81912892
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18N1O2)]\\@

Conformation 4, *w* = 2

1\1\GINC-NODE145\FOpt\UB3LYP\6-31G(d)\C9H18N1O2(2)\LUZHKOV\08-Dec-2016
\0\\#N UB3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH - twist equatorial gauche\\0,2\C,-0.1164597
112,-0.1898988122,0.0593916763\C,-0.3209277969,0.2098719029,1.52981229
7\C,1.3343418963,0.0275196281,-0.4173959847\C,0.6469372795,1.274578611
4,2.0759104373\C,2.4204305744,-0.0770687063,0.6702588716\N,2.049461301
4,0.843547217,1.7899794856\O,2.9884811369,1.3123962148,2.5284836114\C,
0.4117510628,2.6674753079,1.4519172866\C,0.4790216625,1.3706677903,3.6
01364616\C,2.5708663279,-1.5119073208,1.2195428114\C,3.7661349845,0.39
25627758,0.0940730516\H,-1.350118308,0.5517624917,1.6859781874\H,-0.20
66947406,-0.7020640781,2.125542173\H,1.5618903556,-0.6938737821,-1.213
4429706\H,1.4104681942,1.0205833512,-0.8775128454\H,0.4563775673,2.647
9885926,0.3583430849\H,-0.5718191402,3.0541218268,1.7431365818\H,1.177
7256745,3.361252837,1.8119415887\H,0.6892095084,0.4069092278,4.0762780
134\H,1.1630310372,2.1111227629,4.0189953767\H,-0.5507039132,1.6586444
853,3.8402472371\H,1.6151222949,-1.9367593384,1.5340678216\H,2.9870980
46,-2.1683007956,0.4460734768\H,3.2583606635,-1.5040307925,2.071271283
8\H,3.7040268291,1.4300196605,-0.250843023\H,4.5513857522,0.3347174284
,0.8494873538\H,4.0411136793,-0.2416650276,-0.7560859672\H,-0.77452926
29,0.4138623666,-0.5843425666\O,-0.521950943,-1.5614699799,-0.01519042
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Conformation 5, $w = 2$

1\1\GINC-NODE153\FOpt\UB3LYP\6-31G(d)\C9H18N1O2(2)\LUZHKOV\09-Dec-2016
\0\\#N UB3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH - twist equatorial gauche\\0,2\C,-0.1221946
105,-0.1880456112,0.0686349647\C,-0.3134120939,0.2005306043,1.54949874
\C,1.3273189252,-0.0063652156,-0.4071888689\C,0.6458333507,1.280836903
3,2.0825342806\C,2.4122346529,-0.0877737574,0.6840848018\N,2.047625015
2,0.8553152458,1.7885114976\O,2.9890375123,1.3468228747,2.5091103173\C
,0.3953877403,2.663288764,1.4422853807\C,0.4886295493,1.3923758844,3.6
078551609\C,2.5651792199,-1.5123036098,1.2589186069\C,3.7566008204,0.3
690606725,0.094827795\H,-1.3450694545,0.5322548119,1.7258693231\H,-0.1
691650445,-0.7070347899,2.1465575198\H,1.5272691401,-0.7645473018,-1.1
71991637\H,1.4171067721,0.9683028772,-0.900865682\H,0.4403236034,2.629
4219375,0.3491673339\H,-0.5911558071,3.0453474865,1.7298943737\H,1.155
8600338,3.3678598201,1.7926878525\H,0.7023948425,0.4336454767,4.091610
9593\H,1.1771342975,2.1363341317,4.0116630759\H,-0.538680419,1.6845839
423,3.8524831122\H,1.6099980889,-1.935512551,1.5781442153\H,2.98137486
21,-2.1804929859,0.4963362163\H,3.2506124485,-1.4896083244,2.112162094
7\H,3.6962231523,1.4020053663,-0.2634841376\H,4.5467079646,0.318097806
9,0.8456765227\H,4.0226774771,-0.2774737206,-0.7486294108\H,-0.7660776
186,0.4427265923,-0.56291309\O,-0.4720862513,-1.5619164302,-0.13957833
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Conformation 6, $w = 2$

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\0\\#N UB3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH - twist equatorial\\0,2\C,-0.1154755139,-0.
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688724\C,2.430518542,-0.0860859953,0.680964881\N,2.0514255351,0.851638
1964,1.7824106553\O,2.9854697712,1.3331176325,2.5191706622\C,0.3717845
469,2.6332562804,1.4296596381\C,0.4802814766,1.3693437552,3.5984424415
\C,2.6116484142,-1.5032686333,1.2688875641\C,3.771124578,0.3820804025,
0.0916597751\H,-1.3425289096,0.4680982418,1.7158561171\H,-0.1519623938
,-0.7404586813,2.143711803\H,1.5569822725,-0.7807655583,-1.1777685766\
H,1.4365555183,0.9478937959,-0.9121446995\H,0.4231303475,2.5984544781,
0.3368393309\H,-0.622826704,2.9982947926,1.7107899445\H,1.1178045311,3
.3518262949,1.7827956789\H,0.7078725805,0.4155268209,4.0858317835\H,1.
1553497024,2.1252241455,4.0027661652\H,-0.5522428177,1.6449228054,3.83
93891442\H,1.6839406838,-1.9075948401,1.6874175533\H,2.9690950663,-2.1
949866471,0.4973057433\H,3.3506000155,-1.4721078551,2.0756235173\H,3.6
929507371,1.407014913,-0.2850020256\H,4.557104163,0.3592667281,0.84820
94162\H,4.0541307253,-0.2729800285,-0.7397172948\H,-0.7475477064,0.434
1655841,-0.5640131182\O,-0.6260096866,-1.5175827056,-0.2061764745\H,-0
.1226384108,-2.1459109656,0.3355965483\\Version=EM64L-G09RevB.01\State
=2-A\HF=-558.921575\S2=0.753839\S2-1=0.\S2A=0.750011\RMSD=4.151e-09\RM
SF=2.311e-07\Dipole=-0.316293,-0.2534409,-0.2436034\Quadrupole=-2.5688
508,3.1093842,-0.5405335,-5.2279141,-5.6840043,-3.0615486\PG=C01 [X(C9
H18N1O2)]\\@

Cation 3.

Conformation 1, $w = 2$

1\1\GINC-NODE153\FOpt\RB3LYP\6-31G(d)\C9H18N1O2(1+)\LUZHKOV\07-Dec-201
6\0\\#N B3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH - chair, conf2:O29= +120 eq gauche\\1,1\C,-
0.0518605643,-0.0115882579,-0.0624412096\C,-0.0585038298,0.0440673751,
1.4644609272\C,1.3983729362,0.0497106049,-0.5645910437\C,0.5987716561,
1.2925111198,2.0807879997\C,2.1942622204,1.2989576773,-0.1350657199\N,
1.9339989008,1.5656364464,1.3606896134\O,2.8190634608,2.0536651211,1.9
985358982\C,-0.2510067902,2.5787694647,1.8910517305\C,0.9128198466,1.0
891798348,3.5677802956\C,3.7044539317,1.0980117495,-0.3085514779\C,1.7
429267439,2.5867113878,-0.8765996046\H,-1.0887488879,0.0014850465,1.83

15900436\H,0.4447476084,-0.8571556136,1.8348113923\H,1.9110460563,-0.8
518083891,-0.2088759327\H,1.4297885127,0.0192009056,-1.6600060587\H,-0
.5967026242,2.7225948663,0.8669715858\H,-1.1313499927,2.4637485212,2.5
305470481\H,0.295893663,3.4662959141,2.2212963767\H,1.6367905686,0.282
8790919,3.7191344238\H,1.2870527611,1.9982267728,4.0422467926\H,-0.019
9326209,0.8028302196,4.0618846122\H,4.0781317478,0.2893755138,0.326778
6554\H,3.8794559095,0.8172202447,-1.3510334934\H,4.2718517066,2.006814
4315,-0.0990286226\H,0.6616947844,2.7284015264,-0.8802260514\H,2.22613
66505,3.4738287843,-0.4577287179\H,2.0732260556,2.4786499898,-1.914170
8849\H,-0.6380068142,0.8223738836,-0.4765137645\O,-0.6452974773,-1.250
4025875,-0.3936194497\H,-0.8555611915,-1.2676180772,-1.3408399451\\Ver
sion=EM64L-G09RevB.01\State=1-A\HF=-558.675304\RMSD=8.074e-09\RMSF=8.2
57e-07\Dipole=0.1179374,0.7487829,-0.3909855\Quadrupole=-0.8294862,-5.
3467181,6.1762043,-1.0601212,-2.4218059,1.6325408\PG=C01 [X(C9H18N1O2)
]\\@

Conformation 2, $w = 1$

1\1\GINC-CLI19-X\FOpt\RB3LYP\6-31G(d)\C9H18N1O2(1+)\LUZHKOV\29-Sep-201
5\0\\#N B3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH - chair, conf2:O29= +120\\1,1\C,-0.05175731
23,-0.0223777278,-0.0413368651\C,-0.0562321778,0.0359355814,1.49139331
81\C,1.3951325743,0.0279679423,-0.5479433354\C,0.601768973,1.292321399
7,2.0975020822\C,2.1879979842,1.2835970059,-0.1313096801\N,1.932060033
6,1.5645624043,1.3643407765\O,2.8170483318,2.0654468424,1.9922252989\C
,-0.2562396409,2.5716340371,1.9001466847\C,0.927676745,1.1056214917,3.
5839450471\C,3.6984887149,1.0903664536,-0.3092559135\C,1.7252529212,2.
5607590897,-0.8839512047\H,-1.085951809,-0.0035870329,1.8608135871\H,0
.4561508275,-0.8546158482,1.881261372\H,1.9280470293,-0.8627016992,-0.
186938179\H,1.4066943471,-0.0172574345,-1.6416426624\H,-0.6086252028,2
.7044913026,0.8769313248\H,-1.1323430531,2.4587726971,2.5458666957\H,0
.2884403099,3.4647926019,2.2185554271\H,1.656352124,0.3041678798,3.739
2709639\H,1.3021807096,2.0209606923,4.0460099437\H,-0.0004101263,0.821
899909,4.0883586084\H,4.0809432081,0.2907711168,0.3324845744\H,3.87004
10876,0.8006329892,-1.3498809428\H,4.2611195764,2.004659423,-0.1114705
356\H,0.6435587568,2.6976242562,-0.8825088596\H,2.2077771635,3.4542462
384,-0.4781860176\H,2.0480208739,2.4413622718,-1.9226111728\H,-0.61914
38166,0.8206903195,-0.4484305944\O,-0.7347223552,-1.1572150006,-0.5229
682961\H,-0.2932942512,-1.9629834641,-0.205731696\\Version=AM64L-G03Re
vD.01\State=1-A\HF=-558.6736237\RMSD=5.925e-09\RMSF=1.209e-06\Thermal=
0.\Dipole=0.5519969,0.3371752,0.3914933\PG=C01 [X(C9H18N1O2)]\\@

Conformation 3, $w = 2$

1\1\GINC-CLI14-X\FOpt\RB3LYP\6-31G(d)\C9H18N1O2(1+)\LUZHKOV\29-Sep-201
5\0\\#N B3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH - chair, axial O29\\1,1\C,-0.0842383209,-0.
033982276,-0.0237930561\C,-0.0828075268,0.0634756597,1.50120788\C,1.35
35341032,0.0479048137,-0.5560974153\C,0.6037220409,1.3107706822,2.1035
940047\C,2.1627931755,1.2945787774,-0.1296489017\N,1.9243991201,1.5647
468451,1.3642148618\O,2.8248279551,2.0460188594,1.9881376118\C,-0.2325
665732,2.6117156407,1.938375243\C,0.9420219569,1.095143007,3.584554440
9\C,3.6686991759,1.0717183867,-0.3197952043\C,1.7228796278,2.590394411
5,-0.8670132135\H,-1.1134603453,0.0588380195,1.8686242711\H,0.40631895
96,-0.8319337907,1.9025236115\H,1.8940812798,-0.8500287311,-0.23130812
74\H,1.3567527395,0.0310479931,-1.6517652235\H,-0.6007275742,2.7494388
952,0.9241676002\H,-1.0979448792,2.5012316624,2.5991818919\H,0.3397921
861,3.4832523137,2.2684996141\H,1.6656286382,0.2855772023,3.721960401\
H,1.327805162,2.0000762679,4.0573298693\H,0.0157237336,0.812462289,4.0
928434212\H,4.0432429987,0.2648472349,0.3177528457\H,3.8272760669,0.78
1492654,-1.362379824\H,4.2489981968,1.9756176746,-0.1258102183\H,0.643
9576092,2.7300835133,-0.8543399992\H,2.2323905771,3.4650082103,-0.4527
68928\H,2.0425242645,2.4735574487,-1.9074213632\H,-0.4809865182,-1.024
1060881,-0.2858524776\O,-0.9331863081,0.9855537529,-0.5417706322\H,-1.
2180085609,0.7400277827,-1.4363974559\\Version=AM64L-G03RevD.01\State=
1-A\HF=-558.6804765\RMSD=5.592e-09\RMSF=7.953e-07\Thermal=0.\Dipole=0.
0320153,-0.4440949,-0.3795433\PG=C01 [X(C9H18N1O2)]\\@

Conformation 4, $w = 2$

1\1\GINC-NODE168\FOpt\RB3LYP\6-31G(d)\C9H18N1O2(1+)\LUZHKOV\08-Dec-201
6\0\\#N B3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH cat - twist equatorial gauche\\1,1\C,-0.111
0775071,-0.219727535,0.0577503252\C,-0.3270788173,0.1966412185,1.52929
48904\C,1.3249067028,0.0665436992,-0.4391770848\C,0.6242028981,1.25762
69808,2.1024623023\C,2.4330755034,-0.0553777513,0.6185081972\N,2.06267

43789,0.8395717559,1.7994811162\O,2.9354051434,1.2318082474,2.51733893
86\C,0.4688786835,2.6530077242,1.4350843464\C,0.480713233,1.3822721667
,3.6256650319\C,2.5445234127,-1.4843136046,1.2243109039\C,3.7969461313
,0.4096347382,0.0891775513\H,-1.3448470528,0.5726381116,1.670276803\H,
-0.2560764473,-0.710145931,2.1377484677\H,1.5685757076,-0.6433138057,-
1.2365706899\H,1.3802116589,1.0616370042,-0.8945938671\H,0.5556167376,
2.6282379782,0.3472763283\H,-0.5344682606,3.0102648273,1.686429954\H,1
.1987652566,3.35924286,1.8399087653\H,0.709618793,0.4362909822,4.12573
53617\H,1.1193270626,2.166708624,4.035439295\H,-0.5599906104,1.6376363
86,3.8432004679\H,1.5888033142,-1.8834977062,1.5634098512\H,2.90349533
42,-2.1326514416,0.4191876097\H,3.2768845027,-1.5001905121,2.035992920
6\H,3.7678855474,1.4563154763,-0.2297246615\H,4.587881804,0.2845366906
,0.83083711\H,4.0431163154,-0.2045357497,-0.7812802046\H,-0.8009827746
,0.3354882027,-0.5903880297\O,-0.4199447624,-1.6066024102,0.0320351302
\H,-0.6412561697,-1.8708329471,-0.8753181981\\Version=EM64L-G09RevB.01
\State=1-A\HF=-558.6764957\RMSD=5.330e-09\RMSF=3.885e-07\Dipole=-0.008
4493,0.4661918,-0.4876324\Quadrupole=0.0019248,-2.0197514,2.0178266,-3
.528432,-0.815656,4.5400705\PG=C01 [X(C9H18N1O2)]\\@

Conformation 5, $w = 2$

1\1\GINC-NODE146\FOpt\RB3LYP\6-31G(d)\C9H18N1O2(1+)\LUZHKOV\09-Dec-201
6\0\\#N B3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH cat - twist equatorial gauche\\1,1\C,-0.133
3996968,-0.2317133016,0.091729155\C,-0.3352498544,0.2046308646,1.56941
02682\C,1.2924572978,0.0394967706,-0.4159876818\C,0.6251928185,1.27184
39317,2.1196395364\C,2.4108410906,-0.0687300826,0.6314238831\N,2.05973
52691,0.847758324,1.8010316893\O,2.9427269326,1.2556799778,2.497338048
9\C,0.462306103,2.6580232449,1.436028389\C,0.5048650549,1.4156963076,3
.6431577472\C,2.5229207217,-1.4878585122,1.2594352298\C,3.7693677312,0
.379600394,0.0753117687\H,-1.3480750755,0.5929509753,1.7214322049\H,-0
.2536357042,-0.6915189398,2.1924861103\H,1.5087556921,-0.6927416643,-1
.1994783688\H,1.3467943622,1.0248754879,-0.8896589238\H,0.5338722312,2
.6175132536,0.3475393488\H,-0.536218733,3.0221107957,1.6966544989\H,1.
1997609423,3.3678643166,1.8203327777\H,0.737953999,0.4752509115,4.1517
574884\H,1.1531143502,2.2023310978,4.0332913245\H,-0.5311021225,1.6788
935894,3.8737249846\H,1.5692012237,-1.8744120763,1.6184779344\H,2.8619
442943,-2.1515887443,0.4584004153\H,3.2670194077,-1.4958754747,2.06045
02979\H,3.7413971441,1.421042085,-0.2604327087\H,4.5703540908,0.262204
7218,0.8072668689\H,3.9985328694,-0.2503339312,-0.7884523217\H,-0.8246
848322,0.3225567789,-0.5554539959\O,-0.3567669233,-1.6294009031,-0.037
4119187\H,-1.3080432076,-1.8112359191,0.0291821659\\Version=EM64L-G09R
evB.01\State=1-A\HF=-558.6763971\RMSD=7.881e-09\RMSF=5.103e-07\Dipole=
-0.4382103,0.5127917,0.0890129\Quadrupole=4.4426432,-2.3178609,-2.1247
823,-1.5905831,-2.2077931,1.4593093\PG=C01 [X(C9H18N1O2)]\\@

Conformation 6, $w = 2$

1\1\GINC-NODE172\FOpt\RB3LYP\6-31G(d)\C9H18N1O2(1+)\LUZHKOV\08-Dec-201
6\0\\#N B3LYP/6-31G(d) Int(Grid=UltraFine) SCF(Tight) Opt=(Redun,GDIIS
,Tight)\\nitroxypiridin-OH cat - twist equatorial\\1,1\C,-0.123211185,
-0.197945849,0.0524199793\C,-0.2977357848,0.1238796977,1.5537707036\C,
1.343706081,-0.0203282189,-0.4271718303\C,0.6137610717,1.2288484403,2.
1074614237\C,2.4510233369,-0.073266218,0.6407695618\N,2.0659160853,0.8
672001531,1.7847241306\O,2.9356874504,1.3437780052,2.4527702305\C,0.39
45343887,2.601697915,1.4124476213\C,0.4916105287,1.3735250091,3.630624
3051\C,2.6018997301,-1.4668395273,1.3133007366\C,3.8046518453,0.388528
4573,0.0847146211\H,-1.3314499076,0.4275950873,1.7452404509\H,-0.14585
86539,-0.7867654847,2.1451278608\H,1.5580893328,-0.805969634,-1.158585
2091\H,1.444131297,0.9267421744,-0.9688202696\H,0.5055686618,2.5600212
55,0.3267984702\H,-0.6313029487,2.9096801371,1.6367622938\H,1.07965500
39,3.3515618944,1.8166032935\H,0.7439204891,0.4392191743,4.1417341463\
H,1.1231862052,2.1748313161,4.0181512028\H,-0.5497104337,1.6152497536,
3.8603572979\H,1.6780659594,-1.8426607354,1.7571280543\H,2.9131059424,
-2.163094091,0.5284927206\H,3.3789043717,-1.4433872682,2.0822335384\H,
3.7550903044,1.4188516077,-0.2805928547\H,4.6029086341,0.3110949208,0.
8251025053\H,4.0554218539,-0.2586965416,-0.7603125017\H,-0.7335078084,
0.4957722965,-0.5312314475\O,-0.6708412514,-1.4618975348,-0.2605226482
\H,-0.248917263,-2.1523607423,0.2756648759\\Version=EM64L-G09RevB.01\S
tate=1-A\HF=-558.6697163\RMSD=7.159e-09\RMSF=4.804e-07\Dipole=0.582173
5,0.278541,0.5156953\Quadrupole=-0.8712677,2.5151087,-1.643841,-5.3421
82,-5.6408686,0.2837125\PG=C01 [X(C9H18N1O2)]\\@