Supplementary information for

Prediction of the standard potentials for one-electron oxidation of *N*,*N*,*N*',*N*' tetrasubstituted *p*-phenylenediamines by calculation

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Contents

1. Chemicals

NMR spectra were recorded on a Bruker 500 MHz apparatus equipped with a cryoprobe and carried out under an N_2-atmosphere to avoid air-oxidation of the substrates.

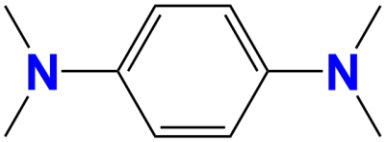

Figure S1. TMePD: Commercially available (Aldrich).

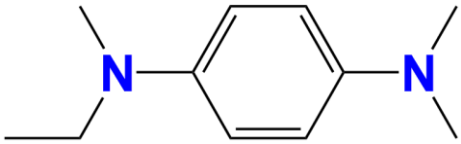

Figure S2. TrMeEtPD: A mixture of 10.0 g (60 mmol) *N*-ethyl-4-nitroaniline, 30 mL 30% HCHO in water and 200 mL EtOH was added to 700 mg 10% Pd on C and the mixture was hydrogenated on a Parr-shaker at 3.5 atm H2 overnight. The catalyst was removed by filtration, the solvent removed in vacuum and the residual liquid distilled in vacuum. Bp. 90 °C/2 mmHg. Yield: 5.2 g (49%). Pale yellow liquid. ^{1}H NMR (500 MHz in CS_2 with DMSO-d6 as lock signal) δ ppm: 0.80 (broad singlet, 3H); 2.52 (broad singlet overlapping with the DMSO signal, 9 H); 2.95 (broad singlet, 2 H); 6.28 (s, 4 H). ^{13}C NMR (125 MHz in CS_2 with DMSO-d6 as lock signal) δ ppm: 11.11; 37.59; 41.04; 114.53; 141.25; 141.44. GC-MS: 178 (M^+).

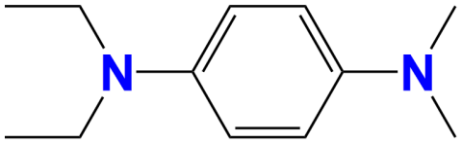

Figure S3. DMeDEtPD: A mixture of 12.0 g (73 mmol) of *N*,*N*-diethyl-p-phenylenediamine, 25 mL 30% HCHO in water and 150 mL EtOH was added to 800 mg 10% Pd on C and the mixture was hydrogenated on a Parr-shaker at 3.5 atm H_2 overnight. The catalyst was removed by filtration, the solvent removed in vacuum and the residual liquid distilled in vacuum. Bp. 100 °C/0.1 mmHg. Yield: 70%. Colorless liquid. ^{1}H NMR (500 MHz in CS2 with CDCl3 as lock signal) δ ppm: 1.39 (t of doublets, 6H); 3.10 (d, 6H); 3.48 (quartet of doublets, 4 H); 6.85 (d, 4 H). ^{13}C NMR (125 MHz in CS2 with CDCl3 as lock signal) δ ppm: 13.64; 42.17; 46.25; 42.17; 46.26; 115.66; 116.63; 140.92; 143.62. GC-MS: 192.3 (M^+).

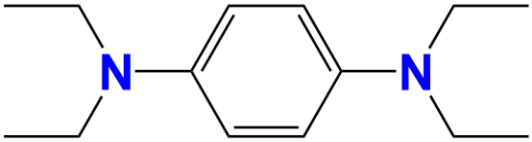

Figure S4. TEtPD: Prepared as described by G. Grampp, A.-M. Kelterer, S. Landgraf, M. Sacher, D. Niethammer, J.P. Telo, R.M.B. Dias, A.J.S.C. Vieira, *Monatshefte für Chemie* **2005**,*136*, 519–536.

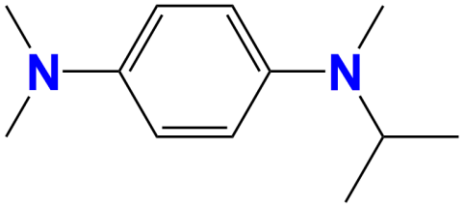

Figure S5. TrMeiPrPD: A mixture of 7.7 g *N*-isopropyl-4-nitroaniline (40 mmol), 50 mL 30 % HCHO in water, 150 mL EtOH was added to 700 mg 10 % Pd on C and the mixture was hydrogenated on a Parr-shaker for 48 hours. After removal of the catalyst by filtration, the solvent was removed in vacuum and the crude product purified by column chromatography on aluminum oxide 90 with heptane as eluent. Yield 2.4 g (31 %). Pale yellow oil. ^{1}H NMR (500 MHz in CS2 with CDCl3 as lock signal) δ ppm: 1.36 (d, 6H); 2.89 (s, 3 H); 3.04 (s, 6 H); 6.82 (d, 2 H); 6.90 (d, 2H). ^{13}C NMR (125 MHz in CS2 with CDCl3 as lock signal) δ ppm: 19.63; 31.46; 41.96; 51.53; 115.21; 117.54; 143.12; 143.97. GC-MS: 190 (M^+).

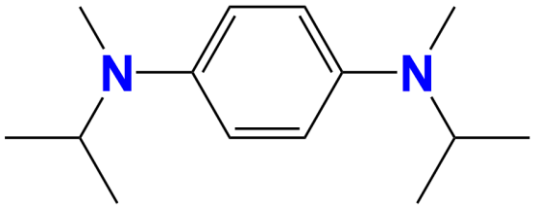

Figure S6. DMeDiPrPD: A mixture of 8.1 g (40 mmol) *N*,*N*'-diisopropyl-*p*-phenylenediamine, 40 mL 30% HCHO in water, 40 mL glacial acetic acid and 100 mL MeOH was added to 800 mg 10% Pd on carbon and hydrogenated on a Parr-shaker at 3.5 atm H_2 overnight. The catalyst was removed by filtration; the filtrate was made alkaline with NaOH (aq) and extracted with diethyl ether. The organic phase was dried over Na_2SO_4, filtered and concentrated in vacuum. The residual yellow oil was purified by column chromatography on aluminum oxide S using heptane as eluent to give 3.97 g (45%) of product. Pale yellow oil. ^{1}H NMR (500 MHz in CS2 with CDCl3 as lock signal) δ ppm: 1.36 (broad singlet,12 H); 2.87 (broad singlet , 6 H); 4.05 (m, 2 H); 6.89 (s, 4 H). ^{13}C NMR (125 MHz in CS2 with CDCl3 as lock signal): δ ppm 19.66; 31.36; 51.05; 117.04; 143.36. GC-MS: 192 (M^+).

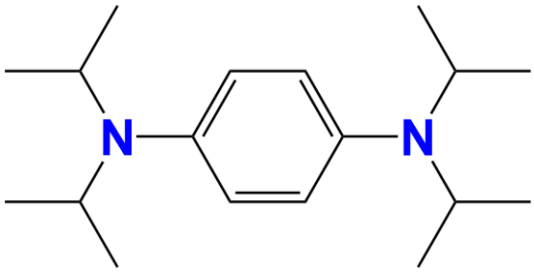

Figure S7. TiPrPD: A mixture of 33.5 g (170 mmol) *N*,*N*'-diisopropyl-*p*-phenylenediamine, 50 g K_2CO_3, 122 g (990 mmol) 2-bromopropane and 250 mL 2-propanol was refluxed for 2 weeks and concentrated in vacuum. The residue was dissolved in a mixture of water and diethyl ether. The organic phase was separated, dried over Na_2SO_4, filtered and concentrated in vacuum to give 33.5 g of a dark yellow oil. This material was purified in 5 g batches by column chromatography on aluminum oxide 90 with heptane as eluent. Yield: 27.3 g (58 %). Pale yellow oil, that solidifies upon standing in the refrigerator. ^{1}H NMR (500 MHz in CS2 with CDCl3 as lock signal) δ ppm: 1.38 (d, 24 H); 3.89 (septet, 4 H); 7.01 (s, 4 H). ^{13}C NMR (125 MHz in CS2 with CDCl3 as lock signal): δ ppm: 22.34; 48.36; 124.35; 141.57;. GC-MS: 276 (M^+).

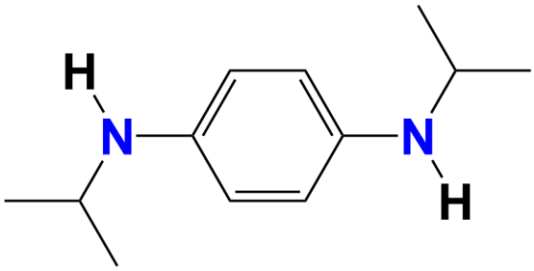

Figure S8. DHDiPrPD: Prepared as described by R.T. Major, *J. Am. Chem. Soc*., **1931**, *53*, 4373-4378.

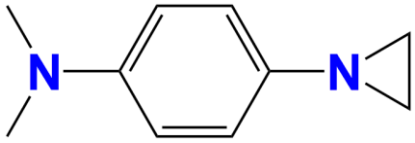

Figure S9. DMeAzirA: Prepared as described by K. Crimaldi, R.L. Lichter, A.D. Baker, *J. Org. Chem.*, **1982**, *47*, 3524-3528.

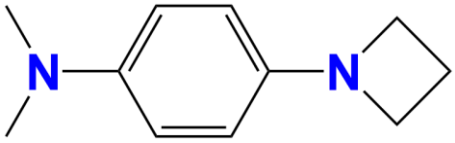

Figure S10. DMeAzetA: A mixture of 5.0 g (23.9 mmol) *N*,*N*-dimethyl-*p*-phenylenediamine dihydrochloride, 14 g K_2CO_3, 3.7 g (23.5 mmol) 1-bromo-3-chloropropane and 100 mL 2-propanol was refluxed for 5 days and concentrated in vacuum. The residue was dissolved in a mixture of water and diethyl ether. The organic phase was separated, dried over Na_2SO_4, filtered and concentrated in vacuum to give a dark oil. This material was purified by column chromatography on aluminum oxide 90 with heptane/toluene (1:1) as eluent. Yield: 70 mg (2 %). ^{1}H NMR (500 MHz in CS2 in CDCl3 as lock signal) δ ppm: 2.54 (s,2 H); 3.04 (s, 6 H); 3.96 (s, 4 H); 6.47 (s, 1 H); 6.80 (s, 1 H). ^{13}C NMR (125 MHz in CS2 with CDCl3 as lock signal): δ ppm: 12.97; 36.83; 48.09; 107.3; 109.98. GC-MS: 176 (M^+).

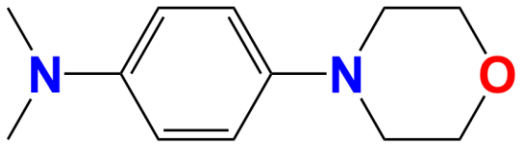

Figure S11. DMeMorphA: Prepared as described by J.B. Christensen, N.-C. Schiødt, K. Bechgaard, T. Buch-Rasmussen, *Acta Chem. Scand*., **1996**, *50*, 1013-1019.

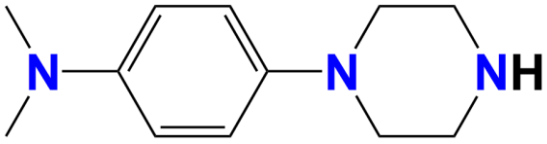

Figure S12. DMePiprzA: Prepared as described in US Patent 5,432,177 (1995).

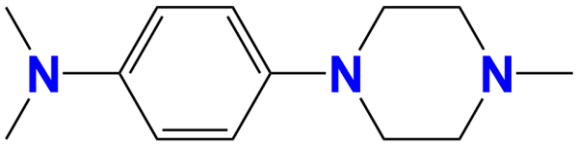

Figure S13. DMeMePiprzA: 750 mg (20 mmol) Lithium aluminum hydride was added to a stirred solution of 3.89 g (12.7 mmol) *tert*-butyl 4-(4-(dimethylamino)phenyl)piperazine-1-carboxylate (also described in US Patent 5,432,177 (1995)) in 100 mL THF. The reaction mixture was refluxed overnight, cooled to room temperature and hydrolyzed by addition of 25% NaOH in water until the gas evolution ceased. The mixture was filtered through a bed of anhydrous Na_2SO_4, concentrated and dried in vacuum. Yield: 2.88 g (74 %). An analytical sample was crystallized from 96 % EtOH. Mp. 80-82 ^{o}C. ^{1}H NMR (500 MHz in CS2 with CDCl3 as lock signal) δ ppm: 2.54 (s,3 H); 2.79 (m, 4 H); 3.14 (m, 6 H); 3.99 (m, 2 H); 6.84 (m, 2 H); 6.98 (m, 2 H). ^{13}C NMR (125 MHz in CS2 with CDCl3 as lock signal) δ ppm: 41.72; 46.77; 51.11 55.86; 114.72; 118.57; 143.69; 145.24. GC-MS: 219.3 (M^{+}).

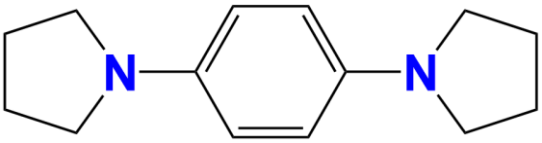

Figure S14. BPyrB: Prepared as described by J. B. Christensen, N.-C. Schiødt, K. Bechgaard, T. Buch-Rasmussen, *Acta Chem. Scand*., **1996**, *50*, 1013-1019.

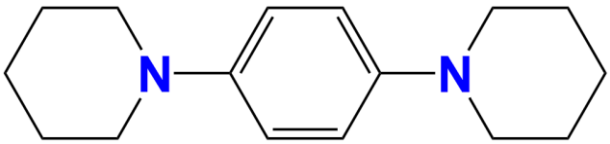

Figure S15. BPipB: Prepared as described by J. B. Christensen, N.-C. Schiødt, K. Bechgaard, T. Buch-Rasmussen, *Acta Chem. Scand*., **1996**, *50*, 1013-1019.

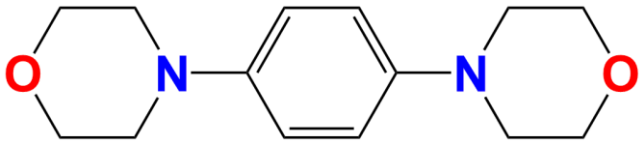

Figure S16. BMorphB: Prepared as described by J. B. Christensen, N.-C. Schiødt, K. Bechgaard, T. Buch-Rasmussen, *Acta Chem. Scand*., **1996**, *50*, 1013-1019.

2. Electrochemistry – CV and DPV curves

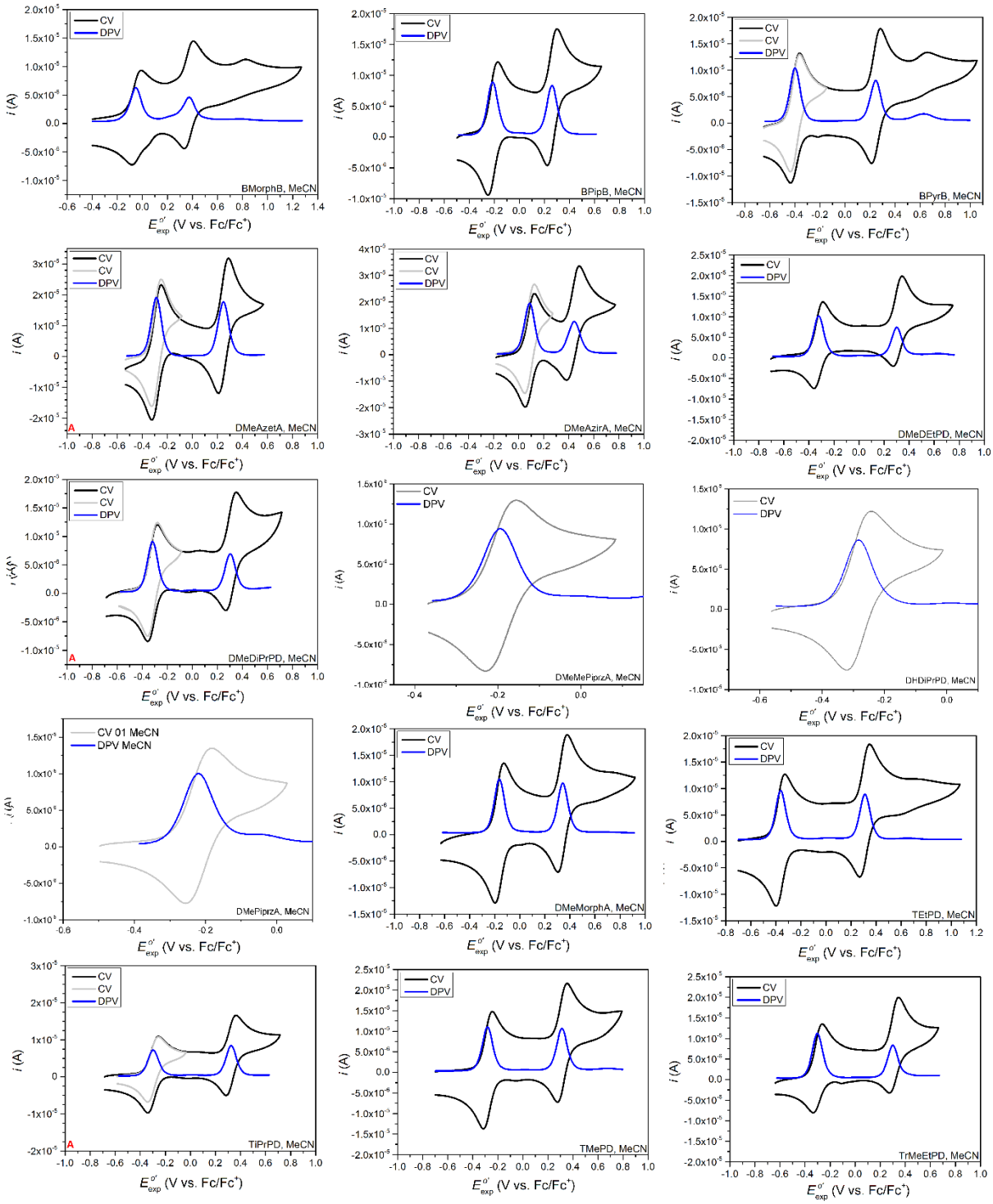

Figure S17. Voltammograms recorded by CV (black and grey) and DPV (blue).

3. Computational output

a) Neutral substrates in the gas phase – lowest free energy conformers B3LYP/6-31G(d,p)

BMorphB


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BPipB


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BPyrB

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-5.2064757559,-0.6402590269,-1.4164375359\H,-5.8129727633,-1.384721039
4,0.070389823\H,5.8005860779,1.4072925596,0.0197500136\H,5.8191661226,
-1.3113831525,0.1857026237\H,5.1940745236,0.6628349571,1.5065740488\H,
5.1979198517,-0.5716995352,-1.2953332685\\Version=EM64L-G09RevB.01\Sta
te=1-A\HF=-655.0581211\RMSD=4.447e-09\RMSF=2.172e-06\Dipole=-0.0000018
,0.0000002,0.00001\Quadrupole=9.0041279,-1.7063418,-7.2977861,0.064791
3,-0.0229075,-0.0891286\PG=C01 [X(C14H20N2)]\\@

DHDiPrPD


```
1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C12H20N2\HAMMERICH\25-Mar-201
 9\0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\DHDiPrPD_syn_syn_02_B
 3LYP_6-31G_dp\\0,1\C,-0.716840871,1.1093878652,-0.37834406\C,0.6697951
 088,1.1087038115,-0.431492867\C,1.4087322537,-0.0868116524,-0.35807581
 62\C,0.6805947882,-1.2797769169,-0.2378012076\C,-0.7151350026,-1.27908
 91037,-0.1843063313\C,-1.4491675793,-0.0854024748,-0.2485371733\H,-1.2
 493572302,2.0566222967,-0.434085895\H,1.1974146451,2.0554155095,-0.527
 8698764\H,1.1966819455,-2.232014665,-0.1803226898\H,-1.2262456022,-2.2
 308206042,-0.0874589002\N,2.8123109446,-0.0341155852,-0.3446120558\N,-
 2.8475443706,-0.0313225917,-0.1276809794\H,3.1649746908,0.8475278363,-
 0.6991863665\H,-3.2254497315,0.8506714034,-0.4542745584\C,-3.707661948
 7,-1.1613145385,-0.4828531031\C,3.6416001421,-1.1649275425,-0.76458627
 4\C,3.4771863525,-1.5285853786,-2.250594542\H,4.0596257142,-2.42089782
 81,-2.5052831757\H,2.4290705542,-1.7235035497,-2.4936981891\H,3.824906
 823,-0.7061358801,-2.8870450809\C,5.0999352636,-0.8506819404,-0.419020
 0303\H,5.2071531661,-0.6279301156,0.6459726576\H,5.7495584593,-1.69455
 4136,-0.669652868\H,5.4558365341,0.0183213458,-0.9872363153\C,-5.13495
 23401,-0.8456347834,-0.026676559\H,-5.8026854889,-1.6888652445,-0.2267
 819558\H,-5.1601035711,-0.6227837984,1.043383377\H,-5.5324559051,0.023
 721973,-0.5660390238\C,-3.6578546675,-1.52512848,-1.9770615834\H,-4.05
 24737739,-0.7023348959,-2.585081686\H,-2.6316187268,-1.7210762997,-2.2
 996813034\H,-4.2589583926,-2.4168666224,-2.1863482865\H,-3.3593244464,
 -2.0242730075,0.0980752876\H,3.3379102827,-2.0275851561,-0.158691729\\
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 =2.533e-06\Dipole=-0.0209786,0.0106626,-0.5470584\Quadrupole=5.8519368
 ,1.4180917,-7.2700285,-0.0634294,-0.5045468,-1.598069\PG=C01 [X(C12H20
 N2)]\\@
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DMeAzetA


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1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C11H16N2\CECILIE\25-Apr-2014\
 0\\# freq=noraman opt=tight rb3lyp/6-31g(d,p)\\DMeAzetA\\0,1\C,-1.1994
 297798,0.6214328928,0.7589422\C,0.1693678121,0.871827884,0.7962766399\
 C,1.0905114713,-0.1501523863,1.0726849732\C,0.578319479,-1.4338781106,
 1.3157045361\C,-0.7902183301,-1.6857377805,1.2787000581\C,-1.721504766
 8,-0.6687859587,0.9844382508\H,-1.8621524544,1.4514421643,0.5467487635
 \H,0.5236557737,1.8831765606,0.619734523\H,1.2565496875,-2.2489447329,
 1.5506160298\H,-1.1266799379,-2.6952175211,1.4809054694\N,-3.098993641
 9,-0.93240643,0.8987575826\C,-3.59345336,-2.1788109277,1.4566741362\H,
 -3.1536709196,-3.0383808114,0.9399384166\H,-4.6739229705,-2.2316420103
 ,1.3084298334\C,-4.0144555354,0.1948369096,0.9219403473\H,-5.038479925
 4,-0.1762373636,0.8453896566\H,-3.9362641918,0.8063264398,1.837034369\
 H,-3.3869448915,-2.2907847999,2.5347495068\H,-3.8438363182,0.852833299
 7,0.0633283179\N,2.4606608016,0.1090295644,1.1444418527\C,3.144607116,
 1.1673663443,0.3841305323\H,3.2196780666,2.1317085906,0.9004929963\H,2
 .7082401502,1.3358555573,-0.6130366358\C,3.5078929873,-0.8808718194,0.
 8455562488\H,3.856565167,-1.4591177206,1.7094319334\H,3.2257567977,-1.
 5819494877,0.044284523\C,4.4136740307,0.2779061104,0.3564434531\H,4.88
 82544366,0.142853427,-0.6166891671\H,5.1667783691,0.5764141444,1.08857
 29587\\Version=EM64L-G09RevB.01\State=1-A'\HF=-538.2848978\RMSD=4.707e
 -09\RMSF=5.793e-07\Dipole=-0.0181761,-0.0390037,-0.1588246\Quadrupole=
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7.1349872,-0.5138279,-6.6211592,0.7973011,-2.2678898,-1.8396037\PG=CS
[SG(C3H2N2),X(C8H14)]\\@

DMeAzirA

1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C10H14N2\CECILIE\25-Apr-2014\
0\\# freq=noraman opt=tight rb3lyp/6-31g(d,p)\\DMeAzirA\\0,1\C,-1.3031
002589,1.1812923815,-0.2568571923\C,0.0637638585,1.2385266672,-0.00054
86408\C,0.7594386693,0.1236838638,0.4800886833\C,0.0339985032,-1.05080
00983,0.7085158833\C,-1.332967533,-1.1160250037,0.4546812514\C,-2.0406
57208,-0.0041234408,-0.0501004943\H,-1.7927498154,2.0748563941,-0.6237
23331\H,0.5986363799,2.1693839455,-0.1665542684\H,0.5454037155,-1.9249
395431,1.1015635092\H,-1.8463631784,-2.0486198509,0.6534172268\N,-3.40
62139537,-0.0791822685,-0.3497470625\N,2.1347083865,0.2106921435,0.818
7409472\C,-4.1660047281,-1.2093184302,0.1554398012\H,-3.7801652413,-2.
1512561902,-0.2490077266\H,-5.2029243838,-1.1169919489,-0.1729667932\C
,-4.1352409055,1.1563049757,-0.5773281222\H,-5.1764323993,0.9191613985
,-0.8037374125\H,-4.1174773596,1.8404068312,0.2873729187\C,3.078429218
8,-0.7541697777,0.2669443337\H,3.83056364,-1.1302104744,0.956398403\H,
2.6977811581,-1.4861803727,-0.4446756315\C,3.0969682598,0.6721420019,-
0.1748236234\H,3.8628549493,1.3540509481,0.1869456888\H,2.7285622119,0
.8826497853,-1.1783671743\H,-4.1580759094,-1.2851734513,1.2555308098\H
,-3.7301030967,1.6953255145,-1.4404709733\\Version=EM64L-G09RevB.01\St
ate=1-A\HF=-498.9588874\RMSD=3.350e-09\RMSF=6.370e-07\Dipole=-0.429120
3,-0.1273249,-0.429106\Quadrupole=6.3063764,0.1741484,-6.4805248,-0.54
85312,-1.5426308,-2.2552625\PG=C01 [X(C10H14N2)]\\@

DMeDEtPD

1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C12H20N2\CECILIE\28-Dec-2013\
0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\DMeDEtPD\\0,1\C,0.70273
83615,-1.1995879791,-0.1045335062\C,-0.6879928115,-1.1963339829,-0.044
4670513\C,-1.4336641544,0.0001519898,-0.05101962\C,-0.6839355566,1.192
4139527,-0.1113037518\C,0.7073303425,1.1876444367,-0.1624394735\C,1.44
92985647,-0.0084402528,-0.1763115955\H,1.2027986276,-2.1603994979,-0.0
85014805\H,-1.1890307165,-2.1542048119,0.0291114544\H,-1.1831802685,2.
1539361285,-0.1265674105\H,1.2105929529,2.146226583,-0.2021195049\N,2.
8532049973,-0.0137720748,-0.2796899481\N,-2.8298988478,0.0036305283,0.
0075844794\C,3.5568897451,1.2252328325,0.0021862744\H,3.2647805249,2.0
073547676,-0.7060752953\H,4.6295239181,1.0621974656,-0.1222332285\C,3.
5532616073,-1.2374132376,0.0701246205\H,4.6259864919,-1.0858660422,-0.
0673875708\H,3.3804653628,-1.5621702291,1.110783425\C,-3.581395135,1.2
403781374,0.1617170386\H,-4.5138570149,1.0026667301,0.6874474449\H,-3.
0331889816,1.9179737887,0.8260008163\C,-3.5979495793,-1.2283443239,-0.
0950014762\H,-4.5641679734,-0.9847497458,-0.5528745636\H,-3.1019747144
,-1.907861935,-0.7972043145\C,-3.8376946635,-1.9366551932,1.2464656818
\H,-4.3853699859,-1.2874147122,1.9375295849\H,-2.8921879833,-2.2082998
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7967\H,-4.4818159573,2.865998914,-0.977026585\H,-4.4259260219,-2.85006
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28,0.1688624\Quadrupole=6.7604015,0.2526759,-7.0130774,0.0199859,0.764
7992,0.1447009\PG=C01 [X(C12H20N2)]\\@

DMeDiPrPD

1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C14H24N2\HAMMERICH\25-Mar-201
9\0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\DMeDiPrPD_syn_anti_02
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1777737071,-0.1988653658\C,-1.4541272152,0.0419162884,-0.170229319\H,-
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,-2.1186967663,-0.1826099791\N,2.8288622819,-0.1141125986,-0.285527520
2\N,-2.8648955334,0.1101755114,-0.0761520616\C,-3.5696554028,1.0108070
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566033,1.6482394307,-0.3661735601\H,-4.5387895305,2.1192803447,0.58419
34833\H,-5.2266235691,2.4116414193,-1.0280799959\H,-5.5958295957,0.915
6762149,-0.1744631751\C,-3.9115627161,0.3343577835,-2.3561753452\H,-3.
0170919603,-0.1085969217,-2.8054490742\H,-4.6596405694,-0.4556812219,-
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,-0.3187301752,-2.6377940464\H,2.7811343265,0.1277117355,-3.0167049069
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7,-3.3775060911\C,4.7417621969,-1.6490590498,-0.7295781073\H,4.5459645
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41\H,5.5450574008,-0.9178876072,-0.5900734812\H,-2.8689251479,1.819785
9064,-1.2339575018\H,2.7477043754,-1.8138992077,-1.4549014456\C,-3.558
3862032,-1.1244269817,0.2517209311\H,-3.5328781328,-1.8890680464,-0.54
32393904\H,-3.1187987092,-1.5623531485,1.1524462765\H,-4.6067294569,-0
.9077095352,0.4690922573\C,3.5448492185,1.1178952619,0.0011656\H,3.461
5242695,1.8892056295,-0.7833253327\H,3.1724265598,1.5480736221,0.93528
05137\H,4.6062123851,0.8996764214,0.1394736916\\Version=EM64L-G09RevB.
01\State=1-A\HF=-657.4679984\RMSD=7.137e-09\RMSF=1.100e-07\Dipole=-0.0
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0.6529409,-0.3776138,0.0021245\PG=C01 [X(C14H24N2)]\\@

DMeMePiprzA

1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C13H21N3\HAMMERICH\23-Mar-201
9\0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\DMeMePiprzPD Meout sy
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39675561,-0.1858332066\C,-0.0290911752,-0.070617886,-0.0000780898\C,-0
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0070472435\C,-2.8876485937,-0.1297482137,-0.1675543573\N,-4.3022731963
,-0.1290341924,-0.2046134712\N,1.3851409118,-0.0791666926,0.1225922571
\C,2.114250729,-0.9330494245,-0.8229210981\C,2.0537906596,1.206218741,
0.289092182\C,3.5551452776,-1.1307533268,-0.3601483649\C,3.4978464567,
0.9934835899,0.7430631183\H,-2.6990327157,2.0154420018,-0.3564047239\H
,-0.2797036291,2.0623702487,-0.277619722\H,-0.2120880381,-2.1998081796
,0.2818226138\H,-2.6297147249,-2.2678839931,0.0781614228\H,1.620297371
6,-1.9041540673,-0.8918667431\H,2.1187988277,-0.4867036826,-1.83356413

68\H,2.0579493918,1.7968645602,-0.6456507588\H,1.5234068798,1.78470434
75,1.0512983831\H,4.0963255854,-1.7230242462,-1.1073688741\H,3.5545781
055,-1.7049369096,0.5878332696\H,3.9989380585,1.9661416651,0.811812679
7\H,3.4925773087,0.547107011,1.7572545478\C,-4.9427900646,0.6464718822
,-1.2621220236\H,-6.0019443864,0.780023514,-1.0203468803\H,-4.49662055
29,1.6372782345,-1.346206145\H,-4.8748806264,0.1583302072,-2.250349866
2\C,-4.9772768731,-1.3894529465,0.0471089369\H,-6.0492743418,-1.199451
1811,0.1534583712\H,-4.8461609543,-2.1348091054,-0.7585432931\H,-4.620
4818644,-1.8294303194,0.9820751292\C,5.6241232812,0.0091621906,0.15271
199\H,6.1427211142,-0.5805051317,-0.6103556817\H,6.100968021,0.9936210
302,0.2017217917\H,5.773599109,-0.4906609059,1.1294809673\N,4.22405723
35,0.1590159445,-0.2102663762\\Version=EM64L-G09RevB.01\State=1-A\HF=-
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-0.1773755\Quadrupole=5.8488165,0.6835957,-6.5324122,0.5054786,3.09989
65,0.4267585\PG=C01 [X(C13H21N3)]\\@

DMeMorphA

1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C12H18N2O1\CECILIE\28-Dec-201
3\0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\DMeMorphPD\\0,1\C,0.1
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917664951\C,0.0250498029,1.4286501166,0.1142901318\C,0.0502437157,0.67
2630759,1.3079051954\C,0.1016534377,-0.7145297153,1.2846540542\C,0.117
6160612,-1.4366334208,0.0799374064\N,0.1926862412,-2.8573375575,0.1132
2463\N,-0.0570123831,2.8257176365,0.1334172184\C,0.2141012733,3.520062
9466,1.3804943328\C,0.2157435992,3.5508402999,-1.0951863794\C,0.513977
8242,-3.5394306609,-1.1364425705\C,-0.9031666327,-3.5419479814,0.81252
97744\C,0.8412199882,-5.0040684562,-0.8482987547\C,-0.5352338991,-5.00
50980678,1.0405577108\H,0.1160371596,-1.1903962568,-2.0681282897\H,0.0
794492404,1.2216193257,-2.0430854338\H,0.0495131441,1.1676185411,2.271
211722\H,0.1576657247,-1.2507009967,2.2274272848\H,-0.5000600511,3.222
9819915,2.1557070043\H,1.230217047,3.3408830871,1.7695429062\H,1.23210
09341,3.3788901696,-1.4870658313\H,-0.4977371135,3.2732229638,-1.87829
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81060879,-1.5942168477\H,-1.0847422031,-3.0576299544,1.7750855769\H,-1
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,-5.547668805,1.4840724136\H,0.3262078001,-5.0631481006,1.7259144991\O
,-0.2313120087,-5.6590908103,-0.1847347883\H,0.0927883805,4.5935562067
,1.2239647059\H,0.0958466587,4.6203085106,-0.912407609\\Version=EM64L-
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le=0.1695301,0.9309156,0.0730317\Quadrupole=-4.0874984,0.9309919,3.156
5065,-0.21056,-1.9920305,-0.8080653\PG=C01 [X(C12H18N2O1)]\\@

DMePiprzA

1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C12H19N3\HAMMERICH\28-Mar-201
9\0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\DMePiprzA syn NHup\\0
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4212,-0.1977265016\C,-0.3889554155,0.0735779968,0.0262685231\C,0.33070
01806,1.2710263376,0.156486395\C,1.7173600452,1.3084098033,0.044235384
8\C,2.4674867225,0.136208822,-0.1689737057\N,3.8811059438,0.1368884299

,-0.2193135037\N,-1.8032068515,0.0811461648,0.1613092255\C,-2.53667146
34,0.9480257108,-0.7712046787\C,-2.4676689721,-1.2066661099,0.33572551
22\C,-3.9793372135,1.1471474817,-0.2918493434\C,-3.9141667571,-0.99327
92948,0.8065512452\H,2.2752444051,-2.003495832,-0.4127211654\H,-0.1430
967562,-2.051626755,-0.3076004303\H,-0.203092382,2.1939929421,0.362270
4097\H,2.2131518119,2.2673150243,0.1361242533\H,-2.029680914,1.9130815
578,-0.8443454897\H,-2.546061964,0.5080610091,-1.7886010879\H,-2.47647
09553,-1.7984385046,-0.602530546\H,-1.9194117113,-1.7884257364,1.08381
65898\H,-4.535430835,1.7449984442,-1.0224287462\H,-3.964785345,1.70632
43984,0.6523280871\H,-4.4245832053,-1.9597589596,0.8821891446\H,-3.894
3371996,-0.5501050016,1.8100015782\C,4.5138552591,-0.6197673971,-1.294
8492291\H,5.5752654225,-0.7548442265,-1.0643603174\H,4.0694784808,-1.6
102493716,-1.3912677218\H,4.4364163894,-0.115701271,-2.2742858561\C,4.
5591846188,1.391410346,0.0531681241\H,5.6320765314,1.1988539925,0.1441
134403\H,4.4198054768,2.1543579473,-0.734310735\H,4.2125432186,1.81059
24972,1.0013979704\N,-4.6974811487,-0.1082186395,-0.0584585228\H,-4.84
9481316,-0.5718458783,-0.9536951549\\Version=EM64L-G09RevB.01\State=1-
A\HF=-632.9706593\RMSD=7.383e-09\RMSF=3.225e-06\Dipole=0.4780402,-0.06
70748,-0.5734837\Quadrupole=-0.322314,3.246554,-2.92424,2.3446273,1.27
57468,0.695253\PG=C01 [X(C12H19N3)]\\@

TEtPD

1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C14H24N2\HAMMERICH\23-Mar-201
9\0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\TEtPD conf 02\\0,1\C,
0.6877633448,-1.1694278623,-0.1431640855\C,-0.7045061243,-1.1538827236
,-0.1330068193\C,-1.4390061793,0.040121414,0.010859608\C,-0.6760110288
,1.2174046638,0.1438012007\C,0.7162598683,1.2018598557,0.1336441179\C,
1.4507597113,0.0078562939,-0.0102222731\H,1.1767150795,-2.1265454864,-
0.2819013509\H,-1.2166768181,-2.0998226603,-0.2644400745\H,-1.16496174
82,2.1745227867,0.2825391605\H,1.2284292175,2.1478005739,0.2650774544\
N,2.8497318405,-0.0077649275,-0.0204288969\N,-2.8379775786,0.055740403
9,0.0210649397\C,3.6234689895,1.2234759897,-0.0604039459\H,3.097845341
4,1.9626092556,-0.6753808662\H,4.5620256458,1.0143208535,-0.5880531331
\C,3.5962875605,-1.2559800787,0.0084530378\H,4.5468735529,-1.067921634
2,0.5223292934\H,3.0633154956,-1.9832975912,0.6311443623\C,-3.58453444
08,1.3039550358,-0.0078171513\H,-3.0515658077,2.0312714453,-0.63051277
3\H,-4.5351222409,1.1158939516,-0.5216889099\C,-3.6117148152,-1.175499
5618,0.0610511064\H,-3.0860869787,-1.9146318941,0.6760253287\H,-4.5502
667251,-0.9663429002,0.5887082602\C,3.8802863693,-1.8545085628,-1.3774
468507\H,2.9510159718,-2.0748550617,-1.9103034234\H,4.458207631,-1.156
0121134,-1.9915203403\C,3.9409405501,1.8152966551,1.3211064302\H,3.024
6921947,2.0562514641,1.8674228592\H,4.5120177296,1.1039744677,1.926802
8925\C,-3.9291961546,-1.7673256343,-1.3204549343\H,-3.0129502243,-2.00
82834345,-1.8667741143\H,-4.5002757904,-1.0560060696,-1.9261520194\C,-
3.8685281336,1.9024873989,1.3780821242\H,-2.9392558576,2.1228356079,1.
9109346203\H,-4.4464471322,1.2039928944,1.9921599718\H,4.4555641716,-2
.7831768022,-1.2891920801\H,4.5354602193,2.730903435,1.2243144496\H,-4
.4438063553,2.8311552772,1.2898267966\H,-4.5237159312,-2.6829315749,-1
.2236557224\\Version=EM64L-G09RevB.01\State=1-A\HF=-657.4713613\RMSD=6
.665e-09\RMSF=1.972e-06\Dipole=-0.0000005,-0.0000009,0.0000038\Quadrup
ole=6.8068844,0.0449863,-6.8518708,-0.0752034,-0.0991908,0.0445186\PG=
C01 [X(C14H24N2)]\\@

TiPrPD


```
1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C18H32N2\HAMMERICH\01-Apr-201
 9\0\\# opt=tight freq=noraman b3lyp/6-31g(d,p)\\TiPrPD conf09\\0,1\C,-
 0.771641144,-0.7254669572,-0.5333338509\C,0.6145745895,-0.8595472101,-
 0.5592445716\C,1.4521431001,-0.079604452,0.2672144012\C,0.8013873777,0
 .843373512,1.113067518\C,-0.5847526569,0.965205166,1.1388366658\C,-1.4
 168397541,0.1815345145,0.3212762162\H,-1.3668478646,-1.3080665924,-1.2
 27709417\H,1.041894012,-1.5547178935,-1.272164832\H,1.3815221604,1.450
 3039068,1.7957760855\H,-1.0255759639,1.6762077173,1.8302713639\N,-2.83
 60873646,0.304840205,0.3104890459\N,2.8508265822,-0.2223587681,0.27056
 14257\C,-3.6506706986,-0.7710235305,0.9149855764\H,-4.6594151742,-0.35
 35345693,1.0036107301\C,-3.4062291285,1.6647983088,0.2951705469\H,-2.5
 879437618,2.31098392,-0.0397383964\C,3.4428197669,-1.4614729919,-0.263
 0509847\H,2.6567028997,-2.217417759,-0.1875970944\C,3.756132875,0.9413
 587762,0.4004334917\H,4.696137972,0.6125931808,-0.0536506348\C,-3.8938
 402462,2.2061609079,1.6552897331\H,-4.226531845,3.24471001,1.550301576
 9\H,-4.7433168984,1.631463709,2.0398405155\H,-3.1040839081,2.181515812
 1,2.4112395175\C,-4.5239277385,1.7707129619,-0.7573510112\H,-4.8816872
 939,2.8030889289,-0.8414567914\H,-4.1574220516,1.4469349812,-1.7350593
 274\H,-5.3857221213,1.1470422303,-0.4944128186\C,-3.7744443366,-2.0107
 966243,0.0131490028\H,-2.8274446204,-2.5545405929,-0.053095897\H,-4.52
 26423587,-2.7014638396,0.418694098\H,-4.0791779623,-1.7248692278,-0.99
 77218261\C,-3.1893357131,-1.1731878997,2.3273651131\H,-2.1799537372,-1
 .5954355964,2.300919759\H,-3.1761351933,-0.3141075866,3.0040068955\H,-
 3.8600184429,-1.9292354899,2.7503933474\C,4.1036599896,1.3080289063,1.
 856874505\H,4.9399538526,2.0163368159,1.873998232\H,3.2683859005,1.777
 9283905,2.3827258476\H,4.3971485148,0.4191002294,2.4209551564\C,3.3085
 868176,2.1675168572,-0.4120355514\H,4.0831139387,2.9404486188,-0.36939
 51264\H,3.1494220166,1.8992649643,-1.4604990555\H,2.3805463056,2.60164
 24628,-0.0334056815\C,4.6014603878,-1.9699139097,0.6114100134\H,4.9371
 589246,-2.9474101303,0.2494036937\H,5.4684971883,-1.3015749495,0.58823
 37162\H,4.2812030381,-2.0805605004,1.651092266\C,3.8642441534,-1.36117
 49653,-1.7420597817\H,4.2088746851,-2.3332648523,-2.1115206231\H,3.031
 8557161,-1.0322161954,-2.3704192471\H,4.6874649536,-0.65085213,-1.8772
 95396\\Version=EM64L-G09RevB.01\State=1-A\HF=-814.7247805\RMSD=1.817e-
 09\RMSF=1.390e-06\Dipole=0.455467,0.0373835,0.0061512\Quadrupole=4.542
 0067,-0.7455611,-3.7964456,-0.9984367,-1.9065881,2.093062\PG=C01 [X(C1
 8H32N2)]\\@
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TMePD


```
1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C10H16N2\CECILIE\23-Dec-2013\
 0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\TMePD pyram\\0,1\C,0.69
 4872,1.195366,-0.039273\C,-0.694873,1.195366,0.039273\C,-1.437192,-0.0
 00002,0.091525\C,-0.694872,-1.195369,0.039276\C,0.694872,-1.195369,-0.
 039271\C,1.437192,0.0000000828,-0.091524\H,1.197127,2.154744,-0.066648
 \H,-1.197128,2.154744,0.066646\H,-1.197128,-2.154747,0.066654\H,1.1971
 27,-2.154747,-0.066646\N,-2.836722,-0.000003,0.218047\C,-3.547339,1.23
 3944,-0.068594\C,-3.54734,-1.23394,-0.068643\N,2.836721,-0.000003,-0.2
 18046\C,3.54734,1.233944,0.068594\C,3.547341,-1.233939,0.068638\H,3.24
```

3573,2.027416,-0.622137\H,4.617123,1.071258,-0.077812\H,3.391223,1.602
707,1.096789\H,3.391209,-1.602674,1.09684\H,4.617125,-1.071253,-0.0777
55\H,3.24359,-2.027433,-0.622075\H,-4.617123,1.071258,0.077805\H,-3.24
3577,2.027415,0.62214\H,-3.391217,1.602709,-1.096787\H,-4.617126,-1.07
1252,0.077736\H,-3.391194,-1.602677,-1.096842\H,-3.243599,-2.027432,0.
622077\\Version=EM64L-G09RevB.01\State=1-A\HF=-500.2005164\RMSD=6.195e
-09\RMSF=4.655e-07\Dipole=0.0000042,0.0000014,-0.0000035\Quadrupole=7.
1209858,0.2343721,-7.3553579,0.0000015,1.2845224,0.0000005\PG=C01 [X(C
10H16N2)]\\@

TrMeEtPD

1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C11H18N2\HAMMERICH\27-Mar-201
9\0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\TrMeEtPD syn 01\\0,1\
C,1.1842097012,1.2368559076,-0.1261180778\C,-0.2008301804,1.3833342049
,-0.0765434802\C,-1.0634098553,0.2727208285,-0.0556057313\C,-0.4506586
637,-0.9950080234,-0.0930565561\C,0.9304935687,-1.1419821561,-0.157152
8667\C,1.79673828,-0.0296141416,-0.1606274585\H,1.7850831821,2.1379493
796,-0.1488318882\H,-0.6039418297,2.3894035435,-0.0741217912\H,-1.0579
607433,-1.8933400285,-0.055400092\H,1.3298379782,-2.1484237792,-0.1892
855609\N,3.1944565904,-0.1799449154,-0.171151522\N,-2.4569485939,0.409
6427898,0.0256169788\C,3.7385378832,-1.469826824,-0.5589954017\H,3.421
0576273,-2.2523654055,0.1379249052\H,4.8286771935,-1.4237315586,-0.516
4142424\C,4.0012353587,0.9819465259,-0.5000365127\H,5.0572534468,0.708
6693642,-0.4495897142\H,3.7973784024,1.3899980726,-1.5049803095\C,-3.3
343128899,-0.5906597799,-0.5813823485\H,-4.0582496768,-0.0787410529,-1
.2314403057\H,-2.742180123,-1.2316339878,-1.2415378956\C,-3.0282042877
,1.7304490639,0.1919199886\H,-4.0900783554,1.6328880989,0.4324700434\H
,-2.550757992,2.2553785913,1.02515691\C,-4.0859899206,-1.444603951,0.4
454187511\H,-4.696421749,-0.818464298,1.1044483939\H,-3.3871511278,-2.
0041903271,1.0742724324\H,-4.7509799306,-2.1582606433,-0.0542369152\H,
3.4450943395,-1.7829785545,-1.5755856013\H,3.8396046145,1.7846263757,0
.2268915504\H,-2.9414972874,2.3667671601,-0.7067691221\\Version=EM64L-
G09RevB.01\State=1-A\HF=-539.5179502\RMSD=2.741e-09\RMSF=7.513e-07\Dip
ole=-0.007105,0.0241616,-0.28435\Quadrupole=6.3937752,0.2638612,-6.657
6364,-0.9688639,-0.8915795,0.7057826\PG=C01 [X(C11H18N2)]\\@

TrMeiPrPD

1\1\GINC-SLEJPNER\FOpt\RB3LYP\6-31G(d,p)\C12H20N2\HAMMERICH\27-Mar-201
9\0\\# opt=tight freq=noraman rb3lyp/6-31g(d,p)\\TrMeiPrPD anti 02\\0,
1\C,0.066486,1.297571,-0.065699\C,1.448916,1.197454,0.096557\C,2.10870
5,-0.044494,0.058545\C,1.30478,-1.176454,-0.201621\C,-0.066973,-1.0661
64,-0.384485\C,-0.734026,0.170584,-0.304943\H,-0.381305,2.283063,-0.00
437\H,2.006357,2.11061,0.2651\H,1.752154,-2.159268,-0.285932\H,-0.6306
68,-1.962369,-0.625579\N,-2.133948,0.244001,-0.52667\N,3.489041,-0.158
416,0.27827\C,4.152765,-1.386892,-0.123612\H,5.212248,-1.318612,0.1312
09\H,3.744743,-2.246042,0.418719\H,4.070212,-1.597624,-1.203145\C,-2.6
75519,1.565366,-0.798777\H,-2.662298,2.255111,0.062569\H,-2.106106,2.0
30665,-1.608407\H,-3.711639,1.474728,-1.133505\C,-2.986993,-0.637039,0
.304166\H,-2.392119,-1.535355,0.486677\C,-4.245866,-1.077929,-0.453554
\H,-4.784362,-1.838675,0.121164\H,-4.941215,-0.248206,-0.619323\H,-3.9

80485,-1.49991,-1.42693\C,-3.328019,-0.031553,1.677924\H,-2.41776,0.27
8367,2.200752\H,-3.983719,0.840598,1.584009\H,-3.845918,-0.766356,2.30
3436\C,4.291405,1.051793,0.247549\H,4.253931,1.578616,-0.72101\H,3.966
61,1.752721,1.023558\H,5.331726,0.795378,0.457509\\Version=EM64L-G09Re
vB.01\State=1-A\HF=-578.8345344\RMSD=5.009e-09\RMSF=3.210e-06\Dipole=0
.2686206,0.0184572,0.0770764\Quadrupole=6.434453,0.300452,-6.734905,-0
.5554895,-0.6942577,-0.0170351\PG=C01 [X(C12H20N2)]\\@

b) Radical cations in the gas phase – lowest free energy conformers
UB3LYP/6-31G(d,p)

BMorphB$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C14H20N2O2(1+,2)\HAMMERICH\28
-Mar-2019\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\BMorphB_RC sy
n anti\\1,2\C,-0.7032322169,1.2012997132,0.0344068514\C,0.6524574664,1
.2058767736,0.2380991806\C,1.4312175442,0.0076222796,0.1951063835\C,0.
7117177583,-1.1932365506,-0.0935822088\C,-0.6456721012,-1.199443545,-0
.2855739641\C,-1.4274427456,-0.0040761738,-0.2218565922\H,-1.214939235
7,2.1524272753,0.0836249568\H,1.1253797028,2.1629018762,0.4101725806\H
,1.2259189081,-2.1419720845,-0.159974607\H,-1.1102298306,-2.1484465732
,-0.5152289259\N,-2.777140493,-0.0149022378,-0.4050193898\N,2.77688264
43,0.0145816298,0.4060248657\C,3.66476753,-1.1374119394,0.170178625\H,
3.0980878927,-2.0231353607,-0.1044583763\H,4.3226416984,-0.8813625925,
-0.6695946333\C,3.5371256425,1.1942492819,0.8534722931\H,4.1774191352,
1.5303110916,0.0289919212\H,2.8689081185,2.005765344,1.1307411706\C,-3
.5855970507,-1.2408062709,-0.5205686873\H,-3.9565356351,-1.3187217909,
-1.5496534722\H,-2.990362838,-2.1222751561,-0.295488734\C,-3.607939543
5,1.1918125088,-0.5620743156\H,-3.0220127735,2.0959902206,-0.419912680
7\H,-3.9945932531,1.1957332423,-1.5887501213\C,-4.7737804998,-1.174423
5881,0.453219371\H,-5.4233073729,-2.0376005027,0.2901400853\H,-4.40106
74879,-1.2032402293,1.4890532916\C,-4.7893547836,1.1576857685,0.416955
7662\H,-5.4497236289,2.0059026526,0.2224805375\H,-4.4195695271,1.22682
24913,1.4519251861\C,4.5234500635,-1.412635855,1.4120827333\H,5.244328
6516,-2.2028527134,1.190112758\H,3.8822826982,-1.7418888895,2.24465668
68\C,4.4076725758,0.8234112041,2.065527819\H,5.042814712,1.6727861862,
2.3276561564\H,3.7596436768,0.58834908,2.9243071758\O,-5.5544276303,-0
.0173618146,0.2319791177\O,5.2634321581,-0.2616531218,1.769793135\\Ver
sion=EM64L-G09RevB.01\State=2-A\HF=-805.2504157\S2=0.759945\S2-1=0.\S2
A=0.750031\RMSD=6.539e-09\RMSF=8.827e-07\Dipole=0.0530216,0.0507995,-0
.3646839\Quadrupole=14.5682717,0.1129913,-14.681263,-0.5205572,4.31078
46,2.1133314\PG=C01 [X(C14H20N2O2)]\\@

BPipB$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C16H24N2(1+,2)\HAMMERICH\28-M
ar-2019\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\BPipB RC anti a
nti\\1,2\C,-0.6201416994,-1.210511645,0.2665527089\C,0.7246346121,-1.1
80930656,0.0039380604\C,1.4169077007,0.0374114113,-0.2829565662\C,0.61

83297017,1.2240720042,-0.2703460952\C,-0.7239547419,1.1962212548,0.006
8794858\C,-1.4174658274,-0.023168219,0.2864866881\H,-1.063227112,-2.17
29243876,0.4817489331\H,1.2509847964,-2.1252900024,0.0003427625\H,1.06
66747671,2.1892909589,-0.4614228798\H,-1.2555565434,2.1375771446,-0.01
36178401\N,-2.7491703671,-0.0502521365,0.5636730805\N,2.7485847265,0.0
651052548,-0.5602142748\C,3.6698315702,-1.0621816221,-0.3231248457\H,3
.1205156965,-1.9497163829,-0.0214857128\H,4.1684119742,-1.2879495066,-
1.2739849507\C,3.4709653797,1.2665400197,-1.0173495096\H,3.9932000684,
0.9841153908,-1.9407563245\H,2.7703858632,2.0543644523,-1.2818371773\C
,-3.5766564324,1.1553190082,0.7537191147\H,-4.0814308423,1.0379000241,
1.721494309\H,-2.9490756789,2.0392516909,0.8327034337\C,-3.5676176508,
-1.2771360353,0.5878070738\H,-2.9410596296,-2.1584851118,0.4824440182\
H,-4.0539673634,-1.331447221,1.5697454008\C,-4.6221359331,1.287987265,
-0.3638323376\H,-5.2336868555,2.1745967131,-0.1672321928\H,-4.10762399
04,1.4545757728,-1.3181569219\C,-4.6244283278,-1.234268309,-0.53047015
84\H,-5.2382728691,-2.1379911351,-0.4571263129\H,-4.1115461751,-1.2710
628795,-1.4992601149\C,-5.4935337524,0.0267604815,-0.4376246582\H,-6.1
242906993,-0.0301653412,0.4592597685\H,-6.1715424446,0.0819940839,-1.2
945575528\C,4.708291216,-0.6848217659,0.7485236033\H,5.3983472111,-1.5
263950271,0.8688419619\H,4.1912489269,-0.5527645103,1.7067427816\C,4.4
904115179,1.730049492,0.0340490229\H,5.0251970963,2.601438934,-0.35762
33486\H,3.9543702812,2.0564828996,0.9336658811\C,5.4664301396,0.595369
6947,0.3736990168\H,6.1289443805,0.8949456662,1.1912622697\H,6.1082881
297,0.3981035971,-0.4949786601\\Version=EM64L-G09RevB.01\State=2-A\HF=
-733.4885756\S2=0.760436\S2-1=0.\S2A=0.750033\RMSD=2.880e-09\RMSF=8.20
7e-07\Dipole=0.0029838,-0.0682571,0.0075731\Quadrupole=31.9893617,-10.
6099021,-21.3794596,1.4241599,-3.8935453,-1.3751207\PG=C01 [X(C16H24N2
)]\\@

BPyrB$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C14H20N2(1+,2)\CECILIE\17-Dec
-2013\0\\# freq=noraman opt=tight ub3lyp/6-31g(d,p)\\BPyrB_RC (unrestr
icted open shell)\\1,2\C,0.6851678289,-1.2220462395,0.0004700644\C,-0.
6851693998,-1.2220452573,-0.0004696708\C,-1.4278425972,0.0000020308,-0
.0000002935\C,-0.6851676612,1.2220479238,0.0004694977\C,0.685169862,1.
2220469851,-0.0004692202\C,1.4278429687,-0.0000001377,0.0000010647\H,1
.2074674222,-2.1704272047,-0.0062325911\H,-1.2074705673,-2.1704253627,
0.0062314854\H,-1.2074662235,2.1704294236,-0.0062336763\H,1.2074702252
,2.1704275087,0.0062317976\N,2.777980733,-0.0000010661,-0.0000006271\N
,-2.777980503,0.0000017836,-0.0000016077\C,-3.6110809145,-1.2200376524
,-0.0733316505\H,-3.2466545718,-1.8825882169,-0.8629523981\H,-3.554681
2357,-1.7574273188,0.8820889182\C,-3.6110845846,1.2200390743,0.0733256
185\H,-3.2466527084,1.8825993225,0.8629351786\H,-3.5546984898,1.757418
516,-0.8821016778\C,3.6110831629,1.2200376587,-0.0733248977\H,3.246655
027,1.8825949813,-0.862938886\H,3.5546884025,1.757419734,0.8821003502\
C,3.6110829122,-1.2200394701,0.0733289153\H,3.2466530885,-1.8825949543
,0.8629437242\H,3.5546904778,-1.7574243758,-0.8820948486\C,5.023286318
9,0.6869007703,-0.3437436116\H,5.1813982078,0.5767022792,-1.4213605611
\H,5.7920166456,1.359827451,0.0407140187\C,5.0232859071,-0.6869024353,
0.3437494896\H,5.7920166376,-1.3598288183,-0.0407079257\H,5.1813968587
,-0.5767043423,1.4213665699\C,-5.0232869473,-0.686902191,-0.3437411511

\H,-5.792013812,-1.3598309287,0.0407198148\H,-5.1814053458,-0.57670214
12,-1.4213569559\C,-5.0232850239,0.6868996318,0.3437543489\H,-5.181387
751,0.5766991294,1.4213724633\H,-5.7920193498,1.3598259213,-0.04069606
91\\Version=EM64L-G09RevB.01\State=2-A\HF=-654.8601016\S2=0.759819\S2-
1=0.\S2A=0.75003\RMSD=8.357e-09\RMSF=1.705e-07\Dipole=0.0000054,0.0000
019,-0.0000034\Quadrupole=32.4080217,-10.5835299,-21.8244918,-0.000004
4,0.0000121,0.0000037\PG=C01 [X(C14H20N2)]\\@

DHDiPrPD$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C12H20N2(1+,2)\HAMMERICH\26-M
ar-2019\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\DHDiPrPD_RC_ant
i_syn_02_B3LYP_6-31G_dp\\1,2\C,-0.6660059406,1.144127187,-0.1533602572
\C,0.6620565548,1.1443032295,0.164823848\C,1.3807358652,-0.0824225706,
0.3323884102\C,0.6673106016,-1.3068229656,0.1588801437\C,-0.6671635771
,-1.306996465,-0.1618042143\C,-1.3826337522,-0.0827929497,-0.328129339
3\H,-1.1923335275,2.0863979292,-0.2750457782\H,1.1868096114,2.08672191
71,0.2920413486\H,1.1780985742,-2.2534694415,0.2828233771\H,-1.1763708
598,-2.253750912,-0.2912996811\N,2.6936318812,-0.0391719215,0.63397698
32\N,-2.6955994612,-0.039968293,-0.62947043\H,3.0950510362,0.881781165
5,0.7711421263\H,-3.0985598478,0.8811007969,-0.7612256313\C,-3.6074091
717,-1.1726529758,-0.8847919407\C,-3.5015249033,-1.6382474931,-2.34458
10712\H,-4.1524410596,-2.5020885816,-2.5050088473\H,-3.8153827063,-0.8
44462185,-3.0294444303\H,-2.4787937097,-1.9278809522,-2.6014126808\C,-
5.0279771368,-0.7478753398,-0.5055724667\H,-5.715313335,-1.5832601906,
-0.6571010054\H,-5.0883217872,-0.442000738,0.5422803545\H,-5.373549962
,0.0799570961,-1.1356428668\C,3.6073418815,-1.1718072109,0.8826372043\
C,5.0271855385,-0.7424407346,0.5058799671\H,5.3713944936,0.0822629174,
1.1407816373\H,5.7159222908,-1.5775488693,0.6524959074\H,5.0869839304,
-0.4303313409,-0.5401642858\C,3.5022823611,-1.6461214141,2.3396762067\
H,3.8148353148,-0.8558381626,3.0291712837\H,2.4800443945,-1.9389628622
,2.5948285274\H,4.1546463486,-2.5097982845,2.4950267632\H,-3.298749818
,-1.9842845448,-0.2181819373\H,3.3000169578,-1.9800339196,0.2112907651
\\Version=EM64L-G09RevB.01\State=2-A\HF=-578.6551672\S2=0.758661\S2-1=
0.\S2A=0.750024\RMSD=4.894e-09\RMSF=1.006e-06\Dipole=-0.0004138,0.4940
121,0.0014529\Quadrupole=24.2616452,-7.6767777,-16.5848675,-0.0070447,
11.4950243,0.0357817\PG=C01 [X(C12H20N2)]\\@

DMeAzetA$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C11H16N2(1+,2)\CECILIE\25-Apr
-2014\0\\# freq=noraman opt=tight ub3lyp/6-31g(d,p)\\DMeAzetA_RC (Unre
stricted open shell)\\1,2\C,-1.1011321857,-1.1095010467,-0.2897605688\
C,0.2558622562,-1.2943293102,-0.2472572996\C,1.1138585317,-0.286554598
4,0.2859482767\C,0.5232227519,0.917479394,0.7733158953\C,-0.8340050069
,1.1003774219,0.7299219588\C,-1.7030264057,0.0950804369,0.1968024724\H
,-1.7184207605,-1.8969220679,-0.7014581399\H,0.6836028226,-2.217242250
6,-0.6231405863\H,1.1567044348,1.6966130762,1.1827914036\H,-1.24410401
52,2.0269868631,1.1091129297\N,-3.0472966885,0.2772079137,0.1542529496
\C,-3.9280432768,-0.7600877176,-0.394362234\C,-3.6529244036,1.51588642
14,0.6558163616\H,-3.8408318346,-1.6899014963,0.1765568365\H,-3.690711

7386,-0.9602790773,-1.4439836446\H,-4.9588921841,-0.4178072884,-0.3357
487805\H,-3.4365484814,1.6546299472,1.719789974\H,-4.7319699335,1.4594
501298,0.5304505448\H,-3.2864273084,2.3842214598,0.0992356986\N,2.4414
747647,-0.466418401,0.3279562212\C,3.551378446,0.3761776603,0.81013282
02\H,3.6415503049,1.3186430813,0.2597277283\H,3.4911912182,0.587811646
1,1.8829359773\C,3.3151896851,-1.5777547307,-0.0914509512\H,3.26761681
97,-1.7748180541,-1.1676575615\H,3.1172627794,-2.5056076856,0.45556997
53\C,4.5369739632,-0.7503071831,0.3942463763\H,5.085083316,-1.19866089
88,1.2223397855\H,5.2348195191,-0.4707424044,-0.3944478913\\Version=EM
64L-G09RevB.01\State=2-A\HF=-538.079687\S2=0.759484\S2-1=0.\S2A=0.7500
3\RMSD=7.976e-09\RMSF=2.422e-07\Dipole=-0.2779728,0.0376621,-0.0088009
\Quadrupole=26.5314332,-9.171166,-17.3602672,-5.0695193,1.9734326,4.13
84152\PG=C01 [X(C11H16N2)]\\@

DMeAzirA$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C10H14N2(1+,2)\CECILIE\25-Apr
-2014\0\\# freq=noraman opt=tight ub3lyp/6-31g(d,p)\\DMeAzirA_RC (Unre
stricted open shell)\\1,2\C,-0.8249150392,-1.2302321293,0.0672218592\C
,0.539610689,-1.2328252837,0.1938968603\C,1.2618431179,-0.0105117131,0
.2959646387\C,0.5391999322,1.2157466192,0.2831122665\C,-0.8253264393,1
.2219218163,0.1565676835\C,-1.5628139646,-0.0017859702,0.0434748584\H,
-1.3420560079,-2.1770836346,-0.0132558571\H,1.0828819473,-2.1713540152
,0.2192235963\H,1.0821569435,2.1501255619,0.3766801454\H,-1.3427855294
,2.1719460879,0.1452047198\N,2.6005035725,-0.01739181,0.4909721767\C,3
.6876394805,-0.7508559741,-0.1146393682\C,3.6873854744,0.758563808,-0.
0596473766\N,-2.912880946,0.0024434345,-0.078833089\C,-3.663604545,-1.
2557158675,-0.1826414494\C,-3.6640285196,1.264568954,-0.0908179982\H,-
3.5251763608,-1.8667164297,0.7146290432\H,-3.3454912965,-1.8268701939,
-1.0599383526\H,-4.7223817489,-1.0294503664,-0.2854998123\H,-3.5258024
857,1.8086964756,0.8485420898\H,-4.7227298943,1.0460331531,-0.20989173
84\H,-3.346111081,1.8981614286,-0.9242158592\H,4.3298808628,-1.2997605
701,0.568771873\H,3.4899867184,-1.2331400701,-1.069577902\H,3.48955764
17,1.3089896872,-0.9769629847\H,4.3294524879,1.2565000016,0.6618999568
\\Version=EM64L-G09RevB.01\State=2-A\HF=-498.737988\S2=0.759602\S2-1=0
.\S2A=0.750031\RMSD=6.981e-09\RMSF=3.664e-07\Dipole=-0.3204351,0.01318
87,-0.363466\Quadrupole=24.4312984,-6.3798855,-18.0514129,-0.0062194,0
.3125756,0.4258699\PG=C01 [X(C10H14N2)]\\@

DMeDEtPD$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C12H20N2(1+,2)\HAMMERICH\27-M
ar-2019\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\DMeDEtPD RC con
f01\\1,2\C,-1.2879144906,1.1831890129,-0.2730738825\C,0.0826396459,1.1
840555886,-0.2834131055\C,0.837726929,0.0086500856,0.0286163691\C,0.08
89542043,-1.168295639,0.3499201483\C,-1.2816220294,-1.1702359286,0.356
4867046\C,-2.0321734279,0.0057114249,0.0463166269\H,-1.8030759261,2.10
58157144,-0.5058084462\H,0.5894591023,2.110980239,-0.5152879028\H,0.60
04925672,-2.0941772764,0.5755141809\H,-1.7919835312,-2.0939127604,0.59
55455262\N,-3.388899918,0.0043221058,0.0546871598\N,2.194893018,0.0100
403584,0.0202502604\C,-4.134691483,-1.2103906298,0.4015182935\H,-3.932

0367899,-2.0128564235,-0.3151840916\H,-5.2000458246,-0.9915694012,0.37
9436635\C,-4.1414025064,1.2175012644,-0.2828917144\H,-5.2059522412,0.9
964926579,-0.2476859109\H,-3.9315770489,2.0203809269,0.4312794446\C,2.
9885510866,-1.1616752205,0.4395413321\H,3.9247887795,-0.7724476363,0.8
478581253\H,2.4786649444,-1.6609448347,1.2657442116\C,2.9809217026,1.1
833721757,-0.4087765348\H,3.9128422344,0.7960566526,-0.8286254517\H,2.
4598611983,1.6815982535,-1.2286126854\C,3.280986972,2.1558760789,0.736
2851819\H,3.8326457741,1.6633628206,1.5419588212\H,2.3642842148,2.5756
262451,1.1592493625\C,3.2764529584,-2.1335883995,-0.7091388712\H,3.817
1232792,-1.6399648588,-1.5215539641\H,2.3554633345,-2.5552209642,-1.12
07657075\H,3.8970781457,-2.9561169603,-0.3431777651\H,3.8953676571,2.9
796700776,0.3627130932\H,-3.874968781,-1.5544936199,1.4073113578\H,-3.
89480575,1.5621378703,-1.291800801\\Version=EM64L-G09RevB.01\State=2-A
\HF=-578.6327789\S2=0.759961\S2-1=0.\S2A=0.750032\RMSD=6.464e-09\RMSF=
2.908e-06\Dipole=-0.7458388,-0.0007618,0.0046037\Quadrupole=25.8638164
,-6.7743763,-19.08944,0.0168145,-0.2745094,-2.6912364\PG=C01 [X(C12H20
N2)]\\@

DMeDiPrPD$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C14H24N2(1+,2)\HAMMERICH\26-M
ar-2019\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\DMeDiPrPD_RC_an
ti_anti_03_B3LYP_6-31G_dp\\1,2\C,-0.7615736202,1.1609392673,0.12516036
3\C,0.6058348398,1.2548723772,0.1038571\C,1.4363645778,0.0966045069,-0
.0201970944\C,0.7608189639,-1.1603392648,-0.1256022082\C,-0.6065891925
,-1.2542726341,-0.1042976335\C,-1.4371197774,-0.0960041094,0.019751551
9\H,-1.3328310071,2.0782275362,0.1787411082\H,1.0434766849,2.243581800
8,0.1353127416\H,1.3320771046,-2.0776273585,-0.1791794508\H,-1.0442297
16,-2.2429827465,-0.135750008\N,2.7936667866,0.1646807466,-0.047099490
5\N,-2.7944225794,-0.1640778035,0.0466488334\C,-3.5489672185,-1.403194
115,-0.2936871979\C,-4.0670205635,-2.0958222849,0.9737354948\H,-4.5684
993868,-3.0287529203,0.7020550457\H,-3.2498386959,-2.3324809892,1.6607
471176\H,-4.7932147495,-1.4742735653,1.5063304023\C,-4.660898597,-1.11
39844936,-1.3124738039\H,-4.2716680661,-0.5888978943,-2.1890281085\H,-
5.0808147581,-2.065759973,-1.6487370536\H,-5.4814681666,-0.5299586854,
-0.8881048339\C,3.5482035128,1.4038022169,0.2932358205\C,4.0661683356,
2.0964833929,-0.9741944771\H,3.2489409368,2.3331601063,-1.6611459232\H
,4.5676574953,3.0294082156,-0.7025133325\H,4.7923319956,1.4749574969,-
1.5068578445\C,4.6602034348,1.1145858948,1.3119454376\H,5.4807703584,0
.530610935,0.8875019552\H,5.0801031717,2.0663619886,1.6482272469\H,4.2
710438065,0.5894457898,2.1884991057\H,-2.8388247711,-2.0627043959,-0.7
916639456\H,2.8380734463,2.0632770293,0.7912786106\C,-3.5815506789,1.0
138363471,0.4262829724\H,-3.6617457002,1.7284760912,-0.4003870985\H,-4
.5854065303,0.6989783822,0.7037343947\H,-3.1340781046,1.5094363175,1.2
895540954\C,3.5807966415,-1.0132232016,-0.4267605675\H,4.5846361904,-0
.698351141,-0.7042557938\H,3.6610375244,-1.7278581689,0.3999092478\H,3
.1332960221,-1.5088335938,-1.2900106592\\Version=EM64L-G09RevB.01\Stat
e=2-A\HF=-657.266264\S2=0.760422\S2-1=0.\S2A=0.750033\RMSD=9.906e-09\R
MSF=4.113e-06\Dipole=-0.0000022,-0.0000049,-0.0000014\Quadrupole=27.80
86203,-7.7213173,-20.087303,5.7512743,0.0347956,1.9648901\PG=C01 [X(C1
4H24N2)]\\@

DMeMePiprzA$^{\bullet+}$

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1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C13H21N3(1+,2)\CECILIE\05-Mar
 -2014\0\\# freq=noraman opt=tight ub3lyp/6-31g(d,p)\\DMeMePiprzPD conf
 2\\1,2\C,2.189310199,-1.2188096453,-0.1404315606\C,0.8187285432,-1.232
 5954667,-0.1699722765\C,0.0499811141,-0.0265409399,-0.1207330225\C,0.7
 901367653,1.1953835923,-0.0362893189\C,2.160189299,1.2100143254,0.0021
 701944\C,2.923046302,0.0034049239,-0.0510910398\N,4.279177587,0.018376
 2854,-0.0218386799\N,-1.3100923286,-0.0427086301,-0.1603955112\C,-2.14
 51614953,1.1393397432,-0.4337168635\C,-2.1242133639,-1.2579420744,0.01
 13263238\C,-3.2108246265,1.3225667751,0.6509345224\C,-3.1972914553,-1.
 0272763282,1.0861457778\H,2.7124458936,-2.163554986,-0.2092069708\H,0.
 3273843644,-2.1896825451,-0.2798201171\H,0.2755127859,2.1435424419,0.0
 389459581\H,2.6593636749,2.1660040494,0.0900996871\H,-1.5318065408,2.0
 306460979,-0.5316876788\H,-2.6431511195,0.9648072983,-1.3953308742\H,-
 2.6059308901,-1.4928135872,-0.9449961094\H,-1.4977200243,-2.0953905933
 ,0.3079887236\H,-3.8477961,2.1663508292,0.3671310058\H,-2.7181661226,1
 .5836365097,1.6081226363\H,-3.825223191,-1.9227001597,1.1329297041\H,-
 2.7000723491,-0.9183741106,2.0699415363\C,5.0128392151,1.2875774177,0.
 0255375119\H,6.0804674836,1.0823647013,-0.0139091681\H,4.7527702143,1.
 9209471244,-0.827983469\H,4.7994191021,1.8303616544,0.9523381204\C,5.0
 428531235,-1.2335925668,-0.0486075105\H,6.1025053553,-1.0054430883,0.0
 446387516\H,4.7567979145,-1.8829536231,0.7841642795\H,4.8860935899,-1.
 7694090767,-0.9907887686\C,-5.1640719038,0.2780994503,1.645888337\H,-5
 .7834791408,1.1119616246,1.3048225168\H,-5.7750127105,-0.6282626317,1.
 6224693547\H,-4.8686183329,0.4704373089,2.6921005453\N,-4.0234324015,0
 .1197449598,0.7465294325\\Version=EM64L-G09RevB.01\State=2-A\HF=-672.0
 763983\S2=0.760018\S2-1=0.\S2A=0.750032\RMSD=2.612e-09\RMSF=2.270e-06\
 Dipole=1.926489,-0.0183356,-0.1387791\Quadrupole=31.7411684,-9.3805547
 ,-22.3606137,-0.6781327,-4.8032084,-0.1084575\PG=C01 [X(C13H21N3)]\\@
```

DMeMorphA$^{\bullet+}$

```
1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C12H18N2O1(1+,2)\CECILIE\29-D
 ec-2013\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\DMeMorphPD_RC\\
 1,2\C,-0.7391473448,1.1927270195,0.0295520128\C,0.6161126622,1.2134390
 022,0.2350200329\C,1.4026870963,0.0188405526,0.2050400372\C,0.69752914
 38,-1.200598342,-0.044055268\C,-0.6566038989,-1.2221641649,-0.25655802
 86\C,-1.4373086859,-0.0260918111,-0.2301313991\H,-1.2806553117,2.12755
 75225,0.0909711843\H,1.0744706503,2.1652824352,0.4663373778\H,1.228994
 3444,-2.140562305,-0.1043727583\H,-1.1270618135,-2.1746758552,-0.46188
 56113\N,-2.7775767701,-0.0475686824,-0.4364769273\N,2.748913549,0.0441
 066096,0.4121320014\C,3.5573092854,1.2750265022,0.4331864526\H,2.96236
 10445,2.1346094047,0.1332364249\H,3.9259547521,1.4358077125,1.45324641
 04\C,3.5755711242,-1.1474509271,0.6699514021\H,3.9626419638,-1.0611210
 5,1.6928303456\H,2.9835800114,-2.057089202,0.6121750054\C,-3.482800242
 5,-1.3160704496,-0.6505364859\H,-3.151294228,-1.7986328207,-1.57596672
 55\H,-3.3196355547,-1.999330181,0.1882429111\C,-3.5555881146,1.1962174
 695,-0.4387697202\H,-3.1635494905,1.8993297361,-1.179425439\H,-4.58775
 41412,0.9689332336,-0.6966434136\C,4.7486084697,1.1252253205,-0.529966
 7854\H,5.4006236069,1.9967780759,-0.4361079871\H,4.3774272692,1.071088
```

0162,-1.5652455307\C,4.7587831079,-1.1979429614,-0.3061429773\H,5.4173
136788,-2.0282782124,-0.0412813367\H,4.3919673392,-1.3500054781,-1.333
1879474\O,5.5245444743,-0.0123092266,-0.2133726347\H,-4.5499781227,-1.
1199974876,-0.7288467885\H,-3.5416181343,1.6701663341,0.5484606859\\Ve
rsion=EM64L-G09RevB.01\State=2-A\HF=-652.6218002\S2=0.75987\S2-1=0.\S2
A=0.750031\RMSD=6.434e-09\RMSF=2.364e-06\Dipole=-1.9542683,-0.0065538,
-0.0389109\Quadrupole=21.9156168,-4.0724976,-17.8431192,0.1906289,4.74
54288,0.7101443\PG=C01 [X(C12H18N2O1)]\\@

DMePiprzA$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C12H19N3(1+,2)\CECILIE\05-Mar
-2014\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\DMeMePiprzPD\\1,2
\C,2.1237545398,-1.2185088434,-0.1361168353\C,0.7571544544,-1.24441082
29,-0.2414092718\C,-0.0247046814,-0.0457129995,-0.2285843648\C,0.69880
41067,1.1822973715,-0.0988357797\C,2.0645686055,1.2090172169,0.0150981
588\C,2.8402505309,0.0096691627,-0.0008318008\N,4.1924576244,0.0363055
891,0.103918938\N,-1.3807235412,-0.0740632829,-0.3432494927\C,-2.21012
6929,1.108270351,-0.643324817\C,-2.1920572002,-1.2976201763,-0.1996557
959\C,-3.3007273548,1.2913060591,0.4187416228\C,-3.2901430365,-1.07453
49412,0.8535105883\H,2.6586521075,-2.158091345,-0.1813559551\H,0.28228
60254,-2.2055637469,-0.3833920334\H,0.172330537,2.1255432278,-0.047235
8331\H,2.5492583299,2.1688783895,0.1357958058\H,-1.592924871,1.9974338
548,-0.7351124822\H,-2.6887422039,0.9255434157,-1.6128503953\H,-2.6527
330161,-1.5248245443,-1.1677438349\H,-1.5669771348,-2.1335649556,0.103
0587128\H,-3.9360861194,2.1310642183,0.1226436883\H,-2.8215320636,1.54
96261015,1.3809735054\H,-3.9191677598,-1.9689578555,0.8851629143\H,-2.
8061820741,-0.9651924998,1.8413952586\C,4.9121367698,1.3114259396,0.18
99646912\H,5.9822577741,1.1154768263,0.1945597737\H,4.6832692375,1.947
4587341,-0.6703373049\H,4.6550936177,1.8471445766,1.1099305911\C,4.967
113246,-1.2090536797,0.1223343814\H,6.0160841404,-0.972409901,0.287565
9688\H,4.6317683452,-1.8647892679,0.9312445376\H,4.8784191129,-1.74153
59432,-0.8306323457\N,-4.0948818401,0.0730351817,0.46667711\H,-4.90310
02492,0.1790923791,1.0713388657\\Version=EM64L-G09RevB.01\State=2-A\HF
=-632.7639054\S2=0.760051\S2-1=0.\S2A=0.750032\RMSD=8.542e-09\RMSF=2.1
31e-06\Dipole=1.2640413,0.0401254,0.2164692\Quadrupole=29.013402,-8.08
42984,-20.9291037,-0.4286088,-2.4408161,-0.0446223\PG=C01 [X(C12H19N3)
]\\@

TEtPD$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C14H24N2(1+,2)\HAMMERICH\17-M
ay-2019\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\TEtPD_RC conf03
in MeCN\\1,2\C,0.6853038475,-1.2160907525,0.0019843057\C,-0.685304254
7,-1.2160905589,-0.0019841018\C,-1.4389900077,0.0000000597,0.000000296
5\C,-0.6853041866,1.216090645,0.0019843844\C,0.6853039114,1.2160907669
,-0.0019845491\C,1.4389898351,-0.0000000133,-0.0000002552\N,2.79657789
56,-0.0000000039,-0.0000005297\N,-2.7965775553,0.0000000549,0.00000054
06\C,3.5857672577,1.2420639462,-0.1075241232\C,3.5857673548,-1.2420639
396,0.1075227571\C,-3.5857668828,1.2420636739,0.1075248843\C,-3.585766
8637,-1.2420635779,-0.10752354\C,3.8798167011,-1.8865275032,-1.2506706

551\C,3.8798171462,1.88652749,1.2506691805\C,-3.8798170888,-1.88652762
52,1.2506694904\C,-3.8798175417,1.8865277438,-1.2506680425\H,1.1928971
064,-2.1712815277,-0.0071498844\H,-1.1928973172,-2.1712812394,0.007150
3172\H,-1.1928971938,2.1712813528,-0.0071498752\H,1.1928972365,2.17128
1511,0.0071494146\H,3.0702895525,1.9359726594,-0.7744193563\H,4.520139
4958,0.9748027772,-0.6080204404\H,4.5201397958,-0.9748027162,0.6080186
663\H,3.0702899805,-1.9359726642,0.7744182305\H,-4.5201388661,0.974802
4661,0.6080213231\H,-3.0702892602,1.9359723072,0.774419981\H,-4.520139
0036,-0.9748024248,-0.6080197145\H,-3.0702893874,-1.9359721988,-0.7744
187652\H,2.9608591154,-2.1854805353,-1.7619707197\H,4.4247603081,-1.20
06209647,-1.9053492507\H,2.9608597616,2.1854804515,1.7619696469\H,4.42
47610779,1.2006209689,1.9053475242\H,-4.4247610031,-1.2006214009,1.905
3479521\H,-2.9608599762,-2.1854808648,1.7619700211\H,-4.424761618,1.20
06215119,-1.9053463609\H,-2.9608605924,2.1854810365,-1.7619688349\H,4.
4980900109,-2.7768826418,-1.1065963337\H,4.4980903385,2.776882671,1.10
65946168\H,-4.4980907908,2.7768827422,-1.1065929302\H,-4.4980903392,-2
.7768826552,1.1065945817\\Version=EM64L-G09RevB.01\State=2-A\HF=-657.2
724732\S2=0.76005\S2-1=0.\S2A=0.750031\RMSD=6.109e-09\RMSF=1.501e-07\D
ipole=-0.0000027,0.,0.\Quadrupole=26.605475,-6.4336196,-20.1718554,-0.
0000015,-0.0000088,0.000002\PG=C01 [X(C14H24N2)]\\@

TiPrPD$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C18H32N2(1+,2)\HAMMERICH\24-A
pr-2019\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\TiPrPD RC conf1
2\\1,2\C,0.6945310825,-1.2927791523,-0.1152028051\C,-0.673922512,-1.30
41588576,-0.0318960792\C,-1.4559416697,-0.1084001622,-0.1318755898\C,-
0.7091017173,1.0977619416,-0.3152579058\C,0.6593522668,1.1091419178,-0
.3985629306\C,1.4413698906,-0.086618124,-0.2985959551\H,1.2115064721,-
2.2298782786,0.0198102676\H,-1.1486454581,-2.25339341,0.1754492164\H,-
1.2260744398,2.0348635243,-0.4502607203\H,1.134076759,2.0583784506,-0.
605896588\N,2.8025719797,-0.075193968,-0.3693743195\N,-2.817143986,-0.
119826874,-0.0611124482\C,3.6239026383,-1.2858435857,-0.691612898\H,4.
6059991201,-0.8688168837,-0.9179410931\C,3.5569108092,1.2103468296,-0.
2625245558\H,2.8612320019,1.9309660338,0.1653913322\C,-3.5714833562,-1
.4053678115,-0.1679567706\H,-2.8757928768,-2.1260024881,-0.5958261481\
C,-3.6384839305,1.0908279553,0.2610850301\H,-4.6205872705,0.6738045352
,0.4873874394\C,4.0026324591,1.7148459093,-1.6423963634\H,4.4780362805
,2.6942963184,-1.538586112\H,4.7327206219,1.0437620577,-2.1048011722\H
,3.1532392558,1.8170684682,-2.3237625645\C,4.7199007537,1.117241398,0.
7368032495\H,5.1403849488,2.1183254278,0.8667874227\H,4.3772879501,0.7
686290332,1.7144129475\H,5.531398326,0.4693701033,0.3959071997\C,3.830
0689431,-2.2350329917,0.5021014938\H,2.9380420303,-2.8091657268,0.7609
46841\H,4.6144831642,-2.9530648999,0.2456899649\H,4.1513283619,-1.6896
771696,1.3919962548\C,3.1665088637,-1.9960450225,-1.9748327649\H,2.219
9778245,-2.5279727997,-1.8655038308\H,3.0662386865,-1.285405884,-2.799
4744762\H,3.9263013207,-2.7313181739,-2.2543314035\C,-3.8446136505,2.0
400013136,-0.9326482863\H,-4.6290321937,2.7580396138,-0.6762679479\H,-
2.9525782658,2.6141265779,-1.1914795425\H,-4.1658517404,1.4946336382,-
1.8225434126\C,-3.1811300172,1.8010430087,1.544311606\H,-3.9409300209,
2.5363204609,1.8237784312\H,-3.0808875041,1.0904122085,2.3689637204\H,
-2.2345944735,2.3329678856,1.4350084963\C,-4.7344335148,-1.3122847362,

-1.1673330647\H,-5.1549216448,-2.313369052,-1.297302121\H,-5.5459393169,-0.6643946791,-0.8264919776\H,-4.391777661,-0.9637064681,-2.1449398269\C,-4.0172561906,-1.9098315568,1.2119112416\H,-4.492655474,-2.8892848086,1.1081068269\H,-3.1678871224,-2.0120380303,1.8933098413\H,-4.7473618334,-1.2387383065,1.6742746409\\Version=EM64L-G09RevB.01\State=2-A\HF=-814.5261055\S2=0.760917\S2-1=0.\S2A=0.750036\RMSD=2.783e-09\RMSF=2.377e-06\Dipole=-0.0000059,-0.0000015,-0.0000022\Quadrupole=28.6476438,-7.8228243,-20.8248195,0.5445857,-3.5386079,0.1892555\PG=C01 [X(C18H32N2)]\\@

TMePD$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C10H16N2(1+,2)\CECILIE\11-Dec-2013\0\\# UB3LYP/6-31G(d,p) Freq=noraman Opt=Tight Guess=save\\TMePD_RC (Unrestricted open shell)\\1,2\C,0.685273,1.22,0.00001\C,-0.685273,1.22,-0.000023\C,-1.43104,-0.0000001037,-0.000034\C,-0.685273,-1.220001,-0.000009\C,0.685273,-1.220001,0.000022\C,1.431041,-0.0000001105,0.000034\H,1.199641,2.1719,0.000022\H,-1.199641,2.1719,-0.00003\H,-1.19964,-2.171902,-0.000024\H,1.199642,-2.171901,0.000034\N,-2.78745,-0.0000000968,-0.000066\C,-3.53791,1.261202,-0.000144\C,-3.537912,-1.261201,-0.000008\N,2.787449,-0.0000001255,0.000065\C,3.537911,1.261201,0.000062\C,3.537911,-1.261201,0.000091\H,3.307995,1.85254,0.89188\H,3.308039,1.85251,-0.891787\H,4.603,1.040488,0.000093\H,3.307985,-1.852526,0.891916\H,4.603001,-1.040487,0.000131\H,3.30805,-1.852524,-0.891752\H,-4.602999,1.04049,-0.000294\H,-3.308134,1.852512,0.891731\H,-3.307896,1.852538,-0.891937\H,-3.308076,-1.852534,-0.891852\H,-3.307961,-1.852516,0.891815\H,-4.603001,-1.040486,0.000061\\Version=EM64L-G09RevB.01\State=2-A\HF=-499.9929221\S2=0.75975\S2-1=0.\S2A=0.75003\RMSD=9.018e-09\RMSF=3.431e-07\Dipole=0.0000041,0.0000002,0.0000011\Quadrupole=24.4849187,-5.7570166,-18.7279021,0.0000013,0.000931,-0.000219\PG=C01 [X(C10H16N2)]\\@

TrMeEtPD$^{\bullet+}$

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C11H18N2(1+,2)\HAMMERICH\27-Mar-2019\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\TrMeEtPD conf02\\1,2\C,-1.130156168,1.2568490683,-0.3033148938\C,0.2198728306,1.4006804534,-0.1142042376\C,1.0705213185,0.2719711866,0.106557883\C,0.4475726302,-1.0162913519,0.1103982814\C,-0.9014325095,-1.1603779125,-0.0826489243\C,-1.751373297,-0.030345597,-0.2942664319\H,-1.7260275676,2.1478398886,-0.451213886\H,0.6338678512,2.4003268948,-0.1149995626\H,1.0421874043,-1.91010525,0.2438703921\H,-1.3156124107,-2.1599459746,-0.0831316277\N,-3.0875674211,-0.1735808969,-0.479544064\N,2.4040019174,0.4279780888,0.3023414437\C,-3.9398828757,0.9947301324,-0.7269006571\H,-3.9289580631,1.6765949486,0.1296400336\H,-4.9627668651,0.6607403911,-0.8864447852\C,-3.7122379003,-1.5005740505,-0.4396500288\H,-4.7887216857,-1.3898133911,-0.5502125906\H,-3.3440844915,-2.1325721035,-1.254561989\C,3.2984136239,-0.6963958892,0.63965657\H,4.0750607962,-0.2920128502,1.2941050447\H,2.7434291085,-1.4217012716,1.236516205\C,3.0380058401,1.7432166954,0.1584548116\H,4.1191554195,1.6130482092,0.1629906635\H,2.7540701005,2.2139029922,-0.7857667476\C,3.9265720725,-1.3526166112,-0.59

33519004\H,4.5096548795,-0.6325428116,-1.1742940462\H,3.1648384913,-1.
7832070406,-1.2491890689\H,4.6003422435,-2.1535279221,-0.2767491683\H,
-3.6115571033,1.5354976685,-1.6197140578\H,-3.5140228681,-1.9957921566
,0.5155166535\H,2.7648137591,2.4043368732,0.9882950756\\Version=EM64L-
G09RevB.01\State=2-A\HF=-539.313031\S2=0.759879\S2-1=0.\S2A=0.750031\R
MSD=5.615e-09\RMSF=1.964e-06\Dipole=-0.4354316,0.1436441,0.0123089\Qua
drupole=24.5462782,-6.0230317,-18.5232465,2.2895079,5.286146,-0.624643
7\PG=C01 [X(C11H18N2)]\\@

TrMeiPrPD•+

1\1\GINC-SLEJPNER\FOpt\UB3LYP\6-31G(d,p)\C12H20N2(1+,2)\HAMMERICH\27-M
ar-2019\0\\# opt=tight freq=noraman ub3lyp/6-31g(d,p)\\TrMeiPrPD RC an
ti 02\\1,2\C,0.1627032811,1.4210334304,-0.0899620084\C,1.5255741327,1.
2808826482,-0.1357005371\C,2.1448961834,-0.0054856175,-0.0828789327\C,
1.2773881662,-1.1371022367,0.0130625839\C,-0.084907752,-0.9961210914,0
.0648812777\C,-0.7098198039,0.2914813835,0.0222064445\H,-0.2469616269,
2.4220182295,-0.1087394277\H,2.1317880524,2.1750877463,-0.1974030947\H
,1.6889747724,-2.1377090245,0.0272304887\H,-0.6826519006,-1.8965870728
,0.1007543247\N,-2.0580868312,0.4568069338,0.0727799994\N,3.4934902099
,-0.1463243348,-0.1247474749\C,4.1123776082,-1.4724781289,-0.023920922
5\H,5.1939241264,-1.3584073369,0.0035179088\H,3.7974993819,-1.98020830
18,0.8924079997\H,3.851888698,-2.0952708136,-0.8863528718\C,-2.6467842
858,1.7725049914,-0.2016384217\H,-2.5151738482,2.4548305242,0.64510702
96\H,-2.1984832694,2.213360157,-1.0940547682\H,-3.7124442703,1.6551769
364,-0.3837273218\C,-3.0028051086,-0.6465865078,0.4070147598\H,-2.3937
243611,-1.4626851201,0.7932848355\C,-3.7423787682,-1.1333035433,-0.846
1825292\H,-4.3793603376,-1.9831230799,-0.5860254327\H,-4.3870813685,-0
.3554666816,-1.2663533322\H,-3.0417447287,-1.4545149609,-1.6218133482\
C,-3.9519914929,-0.2365308817,1.5426771281\H,-3.3981387058,0.133173594
7,2.409917384\H,-4.6745607852,0.5246491639,1.2368166649\H,-4.520814454
8,-1.1161617495,1.855659794\C,4.3650027516,1.0244635298,-0.2724480576\
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