Dehydrogenative Coupling Reactions Catalysed by Rose Bengal Using Visible Light Irradiation

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Supporting Information

General procedures and methods

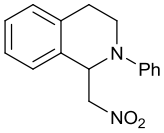
^{1}H and ^{13}C NMR spectra were recorded on a Bruker ACF300 (300MHz), Bruker DPX300 (300MHz) DRX500 (500MHz) or AMX500 (500MHz) spectrometer. Chemical shifts are reported in parts per million (ppm). The residual solvent peak was used as an internal reference. Low resolution mass spectra were obtained on a Finnigan/MAT LCQ spectrometer in ESI mode and a Finnigan/MAT 95XL-T mass spectrometer in FAB mode. All high resolution mass spectra were obtained on a Finnigan/MAT 95XL-T spectrometer. Analytical thin layer chromatography (TLC) was performed with Merck pre-coated TLC plates, silica gel 60F-254, layer thickness 0.25 mm. Flash chromatography separations were performed on Merck 60 (0.040 - 0.063mm) mesh silica gel. Reagents and solvents were commercial grade and were used as supplied without further purification, unless otherwise stated. Irradiation with green light was performed using 0.5-5W LEDs. LEDs were bought from LED POWER SUPPLY, CE-IKEA, TYPE: SLT5-12V. Fluorosence spectra was recorded using SHIMADZU RF-5301.

Representative procedure for oxidative dehydrogenative nitro-Mannich reaction between *N*-aryl-tetrahydroisoquinoline 1a and nitromethane catalyzed by Rose Bengal

1a 2a 3a

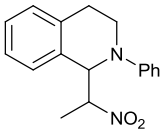
1a (20.9 mg, 0.1 mmol, 1.0 equiv.) was added to a solution of RB (5.0 mg, 0.005 mmol, 5 mol%) in 1.0 ml nitromethane **2a**. The reaction mixture was stirred under green LEDs irradiation at room temperature. After 10 hours, the solvent was removed *in vacuo* and the crude product was directly loaded onto a short silica gel column. Flash chromatography was performed using gradient elution with hexane/EA mixtures (40/1 - 15/1 ratio). After removing solvent, product **3a** (24.7 mg) was obtained as yellow oil in 92% yield.

1-(nitromethyl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3a)[1]



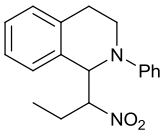
yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.33 – 7.18 (m, 5H), 7.15 (d, *J* = 7.4 Hz, 1H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.86 (t, *J* = 7.2 Hz, 1H), 5.56 (t, *J* = 7.2 Hz, 1H), 4.88 (dd, *J* = 11.8, 7.8 Hz, 1H), 4.57 (dd, *J* = 11.9, 6.7 Hz, 1H), 3.77 – 3.54 (m, 2H), 3.20 – 3.04 (m, 1H), 2.89 – 2.73 (m, 1H). LRMS (ESI) m/z 269.1 ($M + H^+$).

1-(1-nitroethyl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3b)[1]



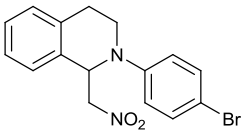
yellow oil, dr = 3:2, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) mixture of the two diastereoisomers: δ 7.31 – 7.08 (m, 6H), 7.03 – 6.96 (m, 2H), 6.85 – 6.79 (m, 1H), 5.31 – 5.18 (m, 1H), 5.08 – 5.02 (m, 0.6H, major isomer), 4.94 – 4.84 (m, 0.4H, minor isomer), 3.89 – 3.77 (m, 0.7H), 3.65 – 3.52 (m, 1.4H), 3.12 – 3.01 (m, 1H), 2.98 – 2.80 (m, 1H), 1.70 (d, *J* = 6.9 Hz, 1.2H, minor isomer), 1.54 (d, *J* = 7.6 Hz, 1.8H, major isomer). LRMS (ESI) m/z 283.2 ($M + H^+$).

1-(1-nitropropyl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3c) [2]



yellow oil, dr = 3:2, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) mixture of the two diastereoisomers: δ 7.54 – 7.10 (m, 6H), 7.07 – 6.90 (m, 2H), 6.88 – 6.68 (m, 1H), 5.25 (d, *J* = 9.2 Hz, 0.3H, minor isomer), 5.14 (d, *J* = 9.5 Hz, 0.5H, major isomer), 4.96 – 4.81 (m, 0.4H, major isomer), 4.77 – 4.62 (m, 0.3H, minor isomer), 4.48 – 4.29 (m, 0.4H), 3.95 – 3.47 (m, 2H), 3.17 – 2.81 (m, 2H), 2.32 – 1.96 (m, 1.5H), 1.94 – 1.75 (m, 0.5H), 1.06 – 0.89 (m, 3H). LRMS (ESI) m/z 297.2 ($M + H^+$).

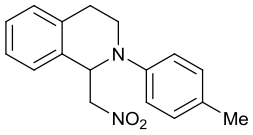
2-(4-bromophenyl)-1-(nitromethyl)-1,2,3,4-tetrahydroisoquinoline (3d) [3]



yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.37 – 7.32 (m, 2H), 7.29 – 7.17 (m, 3H), 7.14 (d, *J* = 7.3 Hz, 1H), 6.85 (d, *J* = 9.1 Hz, 2H),

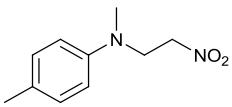
5.49 (t, *J* = 7.2 Hz, 1H), 4.84 (dd, *J* = 12.0, 8.1 Hz, 1H), 4.57 (dd, *J* = 12.0, 6.4 Hz, 1H), 3.72 – 3.54 (m, 2H), 3.12 – 3.03 (m, 1H), 2.79 (dt, *J* = 16.4, 4.8 Hz, 1H). LRMS (ESI) m/z 347.0390, 349.0381 ($M + H^+$).

1-(nitromethyl)-2-(*p*-tolyl)-1,2,3,4-tetrahydroisoquinoline (3e) [3]



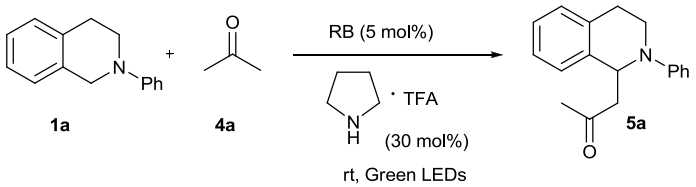
yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.28 – 7.12 (m, 4H), 7.08 (d, *J* = 8.4 Hz, 2H), 6.90 (d, *J* = 8.6 Hz, 2H), 5.50 (t, *J* = 7.2 Hz, 1H), 4.85 (dd, *J* = 11.9, 8.1 Hz, 1H), 4.56 (dd, *J* = 11.9, 6.4 Hz, 1H), 3.72 – 3.52 (m, 2H), 3.16 – 3.00 (m, 1H), 2.76 (dt, *J* = 16.4, 4.5 Hz, 1H), 2.27 (s, 3H). LRMS (ESI) m/z 283.1 ($M + H^+$).

***N*,4-dimethyl-*N*-(2-nitroethyl)aniline (3f)** [1]



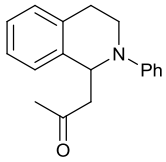
yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.08 (d, *J* = 8.4 Hz, 2H), 6.67 (d, *J* = 8.6 Hz, 2H), 4.56 (t, *J* = 6.4 Hz, 2H), 3.96 (t, *J* = 6.4 Hz, 2H), 2.95 (s, 3H), 2.27 (s, 3H). LRMS (ESI) m/z 195.0 ($M + H^+$).

Representative procedure for dehydrogenative Mannich reaction between *N*-aryl-tetrahydroisoquinoline 1a and acetone catalyzed by Rose Bengal



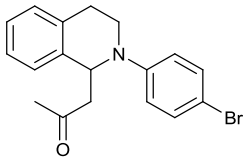
1a (20.9 mg, 0.1 mmol, 1.0 equiv.) was added to a solution of RB (5.0 mg, 0.005 mmol, 5 mol%) in 1.0 ml acetone **4a**, followed by adding pyrrolidine (2.5 ul, 0.03 mmol, 30 mol%) and TFA (2.3 ul, 0.03 mmol, 30 mol%). The reaction mixture was stirred under green LEDs irradiation at room temperature. After 20 hours. the solvent was removed in vacuo and the crude product was directly loaded onto a short silica gel column. Flash chromatography was performed using gradient elution with hexane/EA mixtures (40/1 - 15/1 ratio). After removing solvent, product **5a** (24.1 mg) was obtained as pale yellow solid in 91% yield.

1-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)propan-2-one (5a)[4]



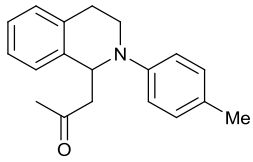
pale yellow solid, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.35 – 7.11 (m, 6H), 6.95 (d, *J* = 8.2 Hz, 2H), 6.79 (t, *J* = 7.3 Hz, 1H), 5.41 (t, *J* = 6.3 Hz, 1H), 3.72 – 3.62 (m, 1H), 3.60 – 3.49 (m, 1H), 3.15 – 3.00 (m, 2H), 2.91 – 2.74 (m, 2H), 2.08 (s, 3H). LRMS (ESI) m/z 266.1 ($M + H^+$).

1-(2-(4-bromophenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)propan-2-one (5b) [5]



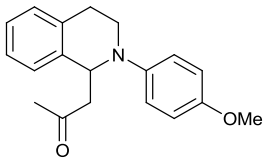
yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.36 – 7.27 (m, 2H), 7.22 – 7.08 (m, 4H), 6.87 – 6.77 (m, 2H), 5.35 (t, *J* = 6.3 Hz, 1H), 3.65 – 3.56 (m, 1H), 3.54 – 3.43 (m, 1H), 3.10 – 2.96 (m, 2H), 2.91 – 2.74 (m, 2H), 2.08 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 206.9, 147.8, 137.9, 134.2, 132.0, 128.6, 127.0, 126.8, 126.4, 116.1, 110.1, 77.2, 77.0, 76.7, 54.6, 50.1, 42.1, 31.1, 27.0. LRMS (ESI) m/z 344.0 ($M + H^+$), HRMS (ESI) m/z 344.0643 calc. for $C_{18}H_{19}{}^{79}BrNO$, 346.0629 calc. for $C_{18}H_{19}{}^{81}BrNO$.

1-(2-*p*-tolyl-1,2,3,4-tetrahydroisoquinolin-1-yl)propan-2-one (5c) [5]



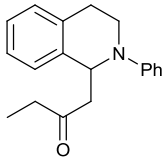
yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.21 – 7.09 (m, 4H), 7.05 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 5.34 (t, *J* = 6.4 Hz, 1H), 3.68 – 3.58 (m, 1H), 3.56 – 3.37 (m, 1H), 3.12 – 2.94 (m, 2H), 2.87 – 2.71 (m, 2H), 2.25 (s, 3H), 2.07 (s, 3H). LRMS (ESI) m/z 280.2 ($M + H^+$).

1-(2-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinolin-1-yl)propan-2-one (5d)[4]



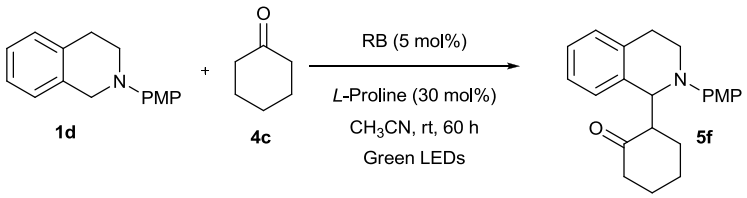
yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.23 – 7.07 (m, 4H), 7.03 – 6.89 (m, 2H), 6.86 – 6.64 (m, 2H), 5.25 (t, *J* = 6.4 Hz, 1H), 3.75 (s, 3H), 3.63 – 3.53 (m, 1H), 3.50 – 3.38 (m, 1H), 3.08 – 2.91 (m, 2H), 2.86 – 2.63 (m, 2H), 2.06 (s, 3H). LRMS (ESI) m/z 296.2 ($M + H^+$).

1-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)butan-2-one (5e) [4]

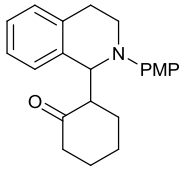


yellow oil, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.36 – 7.21 (m, 2H), 7.21 – 7.06 (m, 4H), 6.95 (d, *J* = 8.2 Hz, 2H), 6.77 (t, *J* = 7.2 Hz, 1H), 5.42 (t, *J* = 6.4 Hz, 1H), 3.72 – 3.60 (m, 1H), 3.59 – 3.48 (m, 1H), 3.15 – 2.97 (m, 2H), 2.92 – 2.68 (m, 2H), 2.46 – 2.17 (m, 2H), 0.99 (t, *J* = 7.3 Hz, 3H). LRMS (ESI) m/z 280.2 ($M + H^+$).

Procedure for *L*-Proline and Rose Bengal co-catalyzed oxidative Mannich reaction between *N*-aryl-tetrahydroisoquinoline 1d and cyclohexanone 4c



1d (23.9 mg, 0.1 mmol, 1.0 equiv.) was added to a solution of RB (5.0 mg, 0.005 mmol, 5 mol%) in 1.0 ml CH_3CN, followed by adding cyclohexanone **4c** (103.5 ul, 1.0 mmol, 10.0 equiv.) and *L*-Proline (3.5 mg, 0.03 mmol, 30 mol%). The reaction mixture was stirred under green LEDs irradiation at room temperature. After 60 hours. the solvent was removed in vacuo and the crude product was directly loaded onto a short silica gel column. Flash chromatography was performed using gradient elution with hexane/EA mixtures (40/1 - 15/1 ratio). After removing solvent, product **5f** (22.1 mg) was obtained as yellow solid in 66% yield with 9:1 dr.



yellow solid, ^{1}H NMR (500 MHz, $CDCl_3$, ppm) major isomer (*syn*): δ 7.21 – 7.05 (m, 4H), 6.88 (d, *J* = 9.0 Hz, 2H), 6.79 (d, *J* = 9.1 Hz, 2H), 5.36 (d, *J* = 5.5 Hz, 1H), 3.74 (s, 3H), 3.70 – 3.58 (m, 1H), 3.52 – 3.40 (m, 1H), 2.97 – 2.72 (m, 3H), 2.51 – 2.41 (m, 1H), 2.32 – 2.21 (m, 1H), 1.91 – 1.60 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm) major isomer (*syn*): δ 212.3, 153.3, 144.2, 136.4, 135.3, 129.1, 128.0, 126.8, 125.8, 118.5, 114.8, 77.6, 77.2, 76.8, 56.6, 56.1, 55.8, 44.1, 41.3, 30.5, 27.7, 26.8, 23.6. LRMS (ESI) m/z 336.2 ($M + H^+$), HRMS (ESI) m/z 336.1975 calc. for $C_{22}H_{26}NO_2$ 336.1958.

Fluorescence quenching study of RB by tertiary amine

Black curve shows the fluorescence spectra of RB (1.6 uM in CH_3CN). Excited at 510nm, PL: 589 nm. Pink curve shows the spectra of amine **1a** (1.0 mM in CH_3CN). Red curve shows the spectra after adding 20 ul of amine **1a** solution to RB (3 ml). The spectra reveals that the fluorescence of RB is quenched with the addition of tertiary amine.

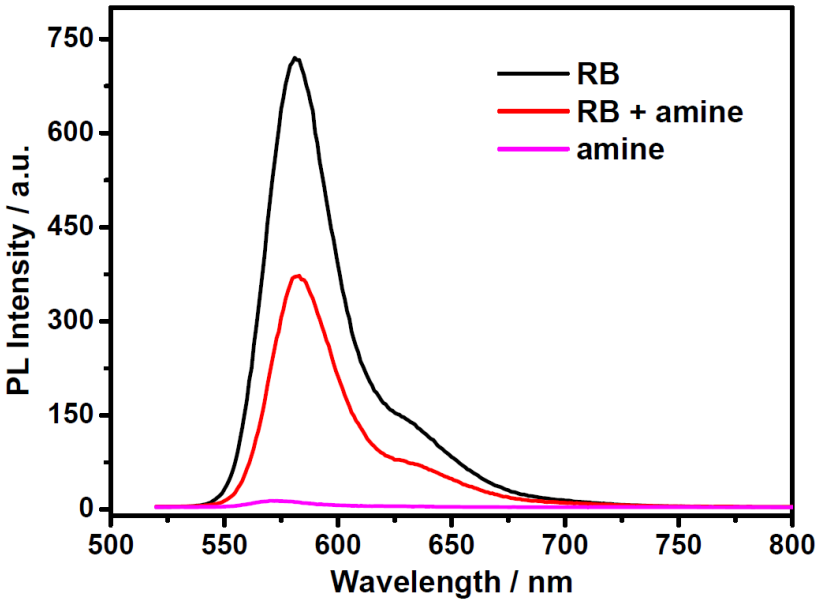
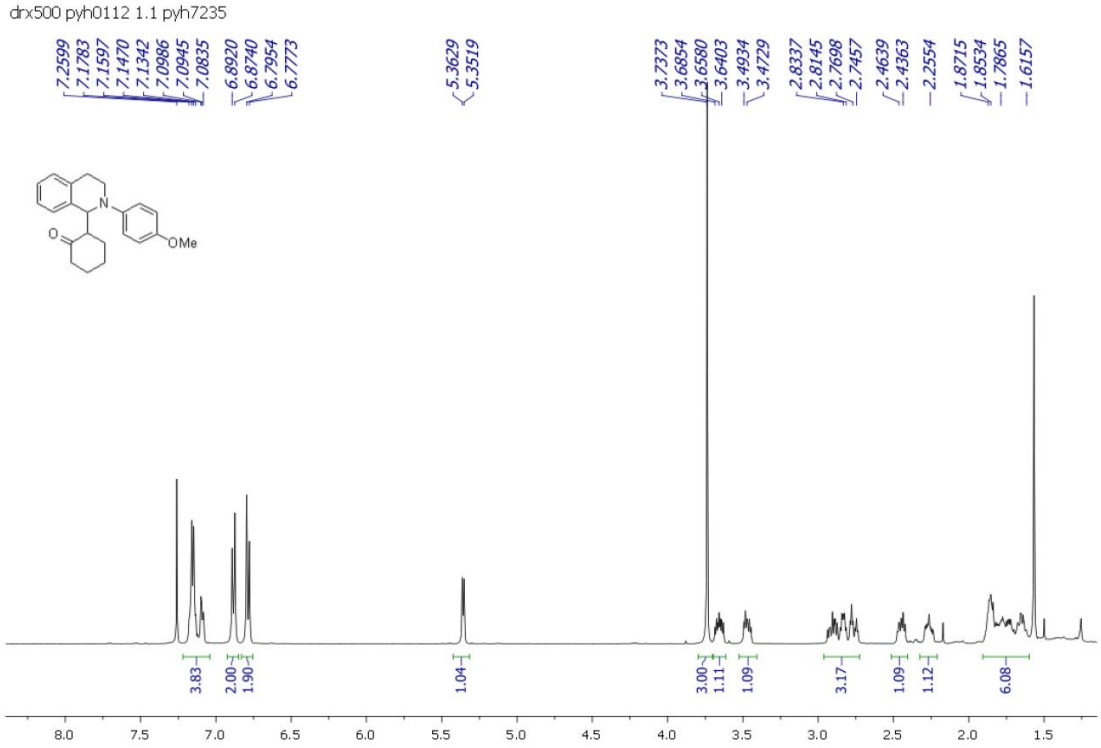
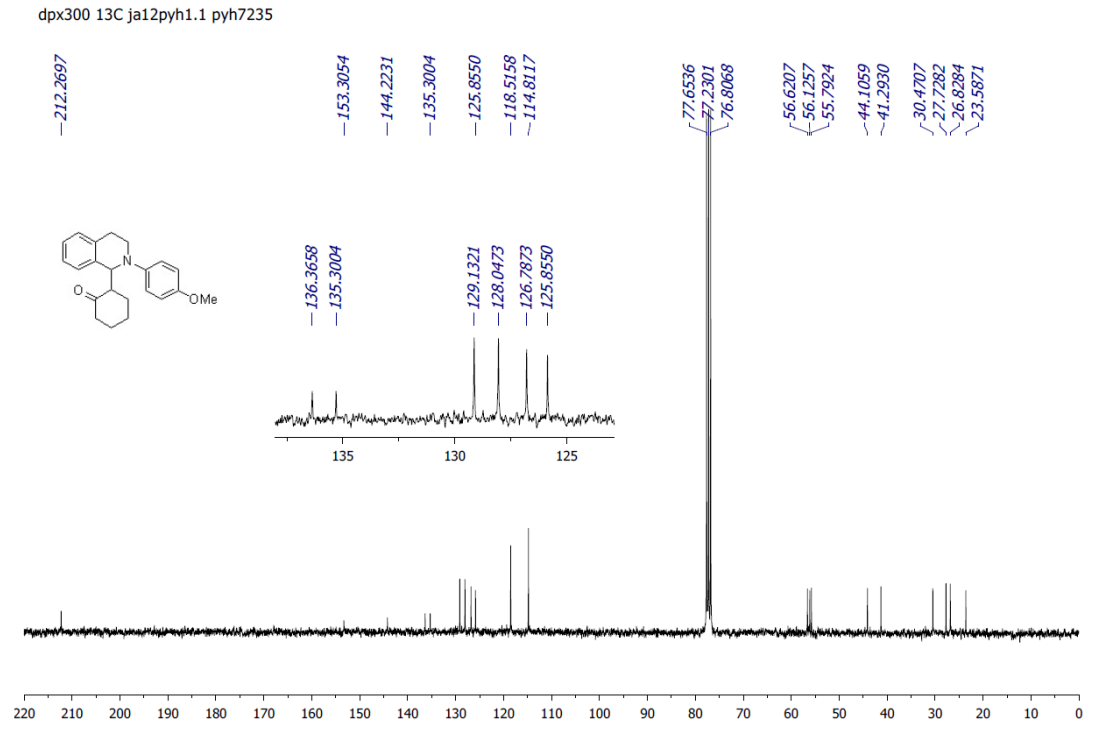


Figure S1 Fluorescence quenching spectra

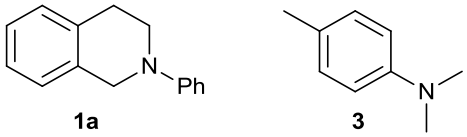
NMR Spectra of New Compounds





Computational Details

All DFT calculations were performed using Gaussian 09 program (Revision A.02).[1] Geometries were optimized at UM06-2X[2]/6-31+G(d,p). The optimized structures were confirmed to be true minima using vibrational frequency analysis: no imaginary frequency. Conformational sampling was performed with MacroModel. Single point calculations were perfomed on the UM06-2X/6-31+G(d,p) geometries at UM06-2X/6-311++G(2df,2p) both in the gas phase and in nitromethane *via* the IEFPCM continuum model with radii and non-electrostatic terms from Truhlar and coworkers' SMD solvation model.[3] Zero point correction and thermal correction to energy, enthalpy and Gibbs free energy are obtained at 298.15 K, 1 atmosphere, and the most abundant isotopes.



1a **3**

Table 1: UM06-2X/6-31+G(d,p)[a] and single point calculation at UM06-2X/6-311++G(2df,2p)//UM06-2X/6-31+G(d,p)[b] result for neutral species

Compound	**1a**-Conformation 1	**1a**-Conformation 2	**1a**-Conformation 3	**3**-Conformation 1
UM06-2X/6-31+G(d,p)[a]	-635.13745	-635.138668	-635.138786	-405.362897
UM06-2X /6-311++G(2df,2p)[b]	-635.3070798	-635.3078459	-635.3076762	-405.4737776
Zero Point Correction[a]	0.265052	0.264996	0.265379	0.202196
Thermal correction to Enthalpy[a]	0.278519	0.278187	0.278355	0.21353
Thermal correction to Gibbs Free Energy[a]	0.225034	0.22594	0.226459	0.166131

Table 2: UM06-2X/6-31+G(d,p)[a] and single point calculation at UM06-2X/6-311++G(2df,2p)//UM06-2X/6-31+G(d,p)[b] result for cationic species

Compound	**1a**$^+$-Conformation 1	**1a**$^+$-Conformation 2	**1a**$^+$-Conformation 3	**3**$^+$-Conformation 1
UM06-2X/6-31+G(d,p)[a]	-634.877976	-634.876591	-634.876591	-405.106697
UM06-2X /6-311++G(2df,2p)[b]	-635.0460302	-635.0446981	-635.0446981	-405.2162101
Zero Point Correction[a]	0.265393	0.265657	0.265657	0.202666
Thermal correction to Enthalpy[a]	0.27866	0.278948	0.278948	0.214133
Thermal correction to Gibbs Free Energy[a]	0.225673	0.225361	0.225361	0.16584

Table 3: SMD/UM06-2X/6-31+G(d,p)[a] and single point calculation at SMD/UM06-2X/6-311++G(2df,2p)// UM06-2X/6-31+G(d,p)[b] result for neutral species

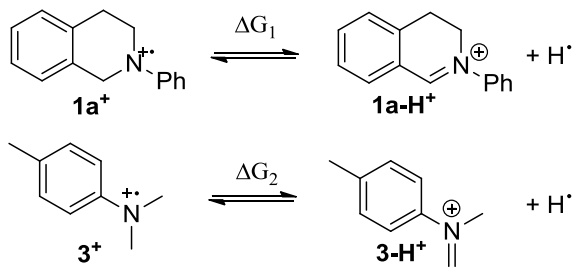
Compound	**1a**-Conformation 1	**1a**-Conformation 2	**1a**-Conformation 3	**3**-Conformation 1
UM06-2X/6-31+G(d,p)[a]	-635.157916	-635.159481	-635.159032	-405.375551
UM06-2X /6-311++G(2df,2p)[b]	-635.32682	-635.3278001	-635.3272353	-405.4858566
Zero Point Correction[a]	0.264543	0.264782	0.265207	0.201894
Thermal correction to Enthalpy[a]	0.278037	0.277938	0.27818	0.213202
Thermal correction to Gibbs Free Energy[a]	0.224514	0.225871	0.226208	0.16583

Table 4: SMD/UM06-2X/6-31+G(d,p) and single point calculation at SMD/UM06-2X/6-311++G(2df,2p)// UM06-2X/6-31+G(d,p) result for cationic species

Compound	**1a**$^+$-Conformation 1	**1a**$^+$-Conformation 2	**1a**$^+$-Conformation 3	**3**$^+$-Conformation 1
UM06-2X/6-31+G(d,p)[a]	-634.96874	-634.96808	-634.96808	-405.192735
UM06-2X /6-311++G(2df,2p)[b]	-635.1358661	-635.1352199	-635.1352198	-405.301676
Zero Point Correction[a]	0.265159	0.265491	0.265492	0.20252
Thermal correction to Enthalpy[a]	0.278373	0.278768	0.278768	0.213819
Thermal correction to Gibbs Free Energy[a]	0.225744	0.225084	0.225088	0.166294

Table 5: SMD/UM06-2X/6-31+G(d,p) and single point calculation at SMD/UM06-2X/6-311++G(2df,2p)// UM06-2X/6-31+G(d,p) result for Iminium

Compound	**1a-H**$^+$-Conformation 1	**1a-H**$^+$-Conformation 2	**3-H**$^+$-Conformation 1
UM06-2X/6-31+G(d,p)[a]	-404.605	-634.403962	-634.403962
UM06-2X /6-311++G(2df,2p)[b]	-404.715	-634.5711347	-634.5706556
Thermal correction to Gibbs Free Energy[a]	0.216064	0.216104	0.157968



The relative stability between the iminium of **1a** and **3** is obtained by ΔG_1-ΔG_2, as the Gibbs free energy of hydrogen radical, ΔG_1-ΔG_2 = ($G_{1a\text{-}H+}$ - G_{1a+}) – ($G_{3\text{-}H+}$ - G_{3+}).

Table 6: Ionization Potential, $\Delta G°_S(X^{+\cdot})$ and $\Delta G°_S(X)$

Compound	Ionization Potential (eV)	$\Delta G°_{ox,gas}$	$\Delta G°_{ox,solv}$
1a	7.14	7.13	5.24
3	7.02	7.00	5.02

Definition for Table 6

For **1a** in which the relative Gibbs free energies for different conformers were sufficiently close, the quantities in Table 6 are calculated as weighted averages over the conformers using the Boltzmann distribution.

Ionization Potential = ($E_{radical\ cation,gas}$ + ZPE) – ($E_{neutral,gas}$ + ZPE), where E refers to the electronic energy from UM06-2X/6-311++G(2df,2p)//UM06-2X/6-31+G(d,p) and ZPE refers to the zero point energy at UM06-2X/6-31+G(d,p)

$\Delta G°_{ox,gas}$ = $G_{radical\ cation,gas}$ – $G_{neutral,gas}$, where G refers to sum the electronic energy from UM06-2X/6-311++G(2df,2p)//UM06-2X/6-31+G(d,p) and thermal correction to Gibbs free energy at UM06-2X/6-31+G(d,p)

$\Delta G°_{ox,solv}$ = $G_{radical\ cation,solv}$ – $G_{neutralsolv}$, where G refers to sum the electronic energy from SMD-UM06-2X/6-311++G(2df,2p)//UM06-2X/6-31+G(d,p) and thermal correction to Gibbs free energy at SMD-UM06-2X/6-31+G(d,p). Solvent being modeled is nitromethane.

Standard Redox Potential Calculation

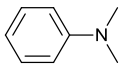
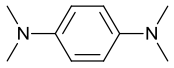
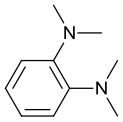
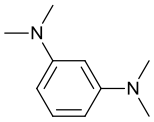
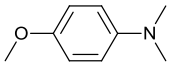
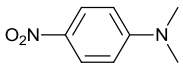
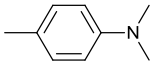
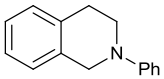
Calculations were performed using a slightly modified methodology from reference Guo and co-workers[9]: Closed-shell restricted wavefunction was used for *N*,*N*-dimethylaniline and its derivatives, Unrestricted open-shell wavefunctions were used for all cationic radical of *N*,*N*-dimethylaniline and its derivatives. The B3LYP functional was used for all calculations. Geometry optimizations were performed at B3LYP/6-31+G(d). Additional single point calculations were performed at B3LYP/6-311++G(2df,2p). Solvation free energies were obtained B3LYP/6-31+G(d,p) using the IEFPCM solvation model from B3LYP/6-31+G(d) optimized structures. Alpha=1.20 was specified in

SCRF calculation. (Guo and coworkers used D-PCM which is not implemented in Gaussian 09). -4.44eV was used for the free energy associated with the NHE half cell.[10]

It was found that experimental E^0 are systematically underestimated by calculations described above (Table 7. Uncorrected). Guo and co-workers added 0.28eV to the calculated adiabiatic ionization potential, which contributes to an improvement in their calculated E^0 when compared with the experimental E^0.

Optimization of the solvation model used to calculate the solvent free energies is important, in this study we used an unoptimized IEFPCM model as implemented in Gaussian 09 with alpha=1.20 (Table 7, Ref 9*). The results for most compound is similar to those reported by Guo and coworkers (Table 7, Ref 9). By applying a simple linear regression model, the corrected E^0 can be obtained which is in excellent agreement with the experimental E^0 (table 7, Corrected). Since this is a preliminary study, a small dataset of 6 compounds (Table 7, entries 1-6) was used to train the linear regression model and no validation of the model was performed. As the compounds which we are interested to predict the E^0 are structurally similar to the compounds in the dataset, it is expected that the predicted E^0 should be fairly accurate, however, further studies would be required to affirm this.

Table 7: Experimental and Calculated E^0 values in MeCN (References for experimental can be found in the supporting information of reference 9)

	Compound	E^0 vs NHE /eV (Experimental)	E^0 vs NHE /eV (Uncorrected)	E^0 vs NHE /eV (Ref 9)	E^0 vs NHE /eV (Ref 9*)	E^0 vs NHE /eV (Corrected)
1		1.10	0.79	1.13	1.07	1.10
2		0.41	-0.08	0.14	0.20	0.47
3		0.79	0.29	0.61	0.57	0.73
4		0.83	0.43	0.67	0.71	0.84
5		0.84	0.40	0.58	0.68	0.82
6		1.52	1.39	1.53	1.67	1.54
7		N/A	0.68	N/A	0.96	1.02
8		N/A	0.84	N/A	1.12	1.14

Cartesian Coordinates

1a-conformation 1 gas phase

C	-0.32874900	-0.85043100	0.48729200
C	-1.77374500	-0.58959700	0.13478000
C	-2.29864800	0.69796500	0.27641600
C	-1.34619800	1.77690900	0.70932800
C	-0.00825700	1.60726200	-0.00650700
H	-2.18617400	-2.62889600	-0.41019000
H	0.02477300	-1.70318300	-0.10573300
C	-2.60004500	-1.63054400	-0.29000000
C	-3.64349600	0.93104300	-0.01213000
H	-1.75598800	2.76792200	0.49182200
H	0.69713700	2.35390100	0.37190300
C	-4.46914900	-0.11209800	-0.42542900
C	-3.94560100	-1.39692900	-0.56415900
H	-4.04381600	1.93696000	0.08750900
H	-5.51458300	0.07835200	-0.64717100
H	-4.58058000	-2.21265200	-0.89508500
H	-0.27246800	-1.15698700	1.54570200
H	-1.17647100	1.72054500	1.79293200
H	-0.14564400	1.79163100	-1.08512800
N	0.54898100	0.28962300	0.24601800
C	1.90340200	0.06234800	0.06694300
C	2.73514600	1.02077700	-0.54842800
C	2.50013500	-1.14040400	0.50015100
C	4.09588800	0.78199900	-0.71051700
H	2.31742300	1.94601600	-0.92705000
C	3.86167200	-1.36304900	0.32539300
H	1.90614900	-1.89647100	1.00005100
C	4.67690100	-0.40826500	-0.27872600
H	4.70556300	1.53965300	-1.19450000
H	4.28817000	-2.29782300	0.67792300
H	5.73810400	-0.58823900	-0.41154700

1a-conformation 2 gas phase

C	-0.32818500	-0.90840400	0.19309900
C	-1.79554800	-0.57156100	0.02586000
C	-2.24835400	0.75132900	0.00782400
C	-1.26417100	1.88938800	0.13871000
C	0.04626500	1.40534400	0.74095800

H	-2.35927500	-2.64392200	-0.07482700
H	-0.05452800	-1.67648500	-0.53811600
C	-2.71738300	-1.61662400	-0.09037800
C	-3.61764000	1.00152800	-0.13166500
H	-1.06338200	2.31762000	-0.85113300
H	-0.10427900	1.12948700	1.80079200
C	-4.52998500	-0.04014200	-0.25182000
C	-4.07629100	-1.35982600	-0.22946100
H	-3.96611100	2.03183700	-0.14209700
H	-5.58902200	0.17273900	-0.35912400
H	-4.77874700	-2.18210800	-0.32223400
H	-0.17939700	-1.34717500	1.19965900
H	-1.69287000	2.68332800	0.76052900
H	0.79614300	2.19545000	0.71450700
N	0.52679000	0.24585200	-0.00955700
C	1.91596500	0.01845900	-0.03432200
C	2.78128300	1.06847800	-0.39338000
C	2.48079400	-1.23560700	0.24096400
C	4.15383400	0.87436900	-0.45068100
H	2.36600500	2.03513700	-0.66041200
C	3.86198200	-1.42373600	0.16755200
H	1.85434700	-2.07314900	0.52361900
C	4.70988100	-0.37551700	-0.16907700
H	4.79443800	1.70371100	-0.73540000
H	4.27166300	-2.40547900	0.38666100
H	5.78280800	-0.52681800	-0.22063400

1a-conformation 3 gas phase

C	0.48541200	0.43061700	1.65521500
C	1.58444400	0.00749000	0.69578200
C	1.66076900	0.57740800	-0.58195900
C	0.61886400	1.57538300	-1.04394800
C	-0.17898900	2.14442600	0.13164200
H	2.47193700	-1.36681300	2.08913500
H	0.89811900	1.15193800	2.37328000
C	2.54226300	-0.92765900	1.09571700
C	2.70172600	0.19147200	-1.43304000
H	1.09822500	2.38382800	-1.60757900
H	-1.02634200	2.73377600	-0.22456000
C	3.65246600	-0.74093500	-1.03153800
C	3.57295800	-1.30584900	0.24178000
H	2.76244500	0.63296700	-2.42542400
H	4.45244100	-1.02686900	-1.70739600

H	4.30742000	-2.03734400	0.56434800
H	0.13332000	-0.42360900	2.24103400
H	-0.07670600	1.07413100	-1.73115800
H	0.44927800	2.80713000	0.73817700
N	-0.65133500	1.06887800	1.01054800
C	-1.63193500	0.22116800	0.43824000
C	-2.84995200	0.78895400	0.02871000
C	-1.45606900	-1.16022200	0.28095100
C	-3.85293300	0.00251600	-0.52248800
H	-3.01399100	1.85203200	0.17686600
C	-2.47565900	-1.94582800	-0.25858200
H	-0.51767300	-1.62981100	0.55642900
C	-3.67559600	-1.37483900	-0.66829700
H	-4.78779600	0.46579500	-0.82401400
H	-2.31524100	-3.01413500	-0.37018800
H	-4.46271000	-1.98977200	-1.09190100

1a-conformation 1 scrf=(smd,solvent=nitromethane)

C	-0.34081400	-0.83375400	0.57870700
C	-1.77602800	-0.59704600	0.17751700
C	-2.29709100	0.69750800	0.28739800
C	-1.34448900	1.76163700	0.75328900
C	-0.00611700	1.61777000	0.03131300
H	-2.17885400	-2.64215400	-0.35771800
H	0.00791700	-1.74988500	0.09262600
C	-2.59086900	-1.63996500	-0.26540400
C	-3.62815500	0.93939400	-0.05541600
H	-1.74995800	2.76048200	0.57100600
H	0.70475300	2.33634800	0.45206800
C	-4.44440300	-0.10619700	-0.48954500
C	-3.92561300	-1.39770700	-0.59302300
H	-4.02473900	1.94915600	0.01985100
H	-5.48026700	0.08824100	-0.75214300
H	-4.55532000	-2.21290400	-0.93704900
H	-0.28923200	-1.00779300	1.66691400
H	-1.17544000	1.66348300	1.83418300
H	-0.13663400	1.86466200	-1.03327300
N	0.53561100	0.27075800	0.19186500
C	1.88693300	0.04903300	0.03959100
C	2.72047500	1.01973800	-0.56498800
C	2.49459500	-1.15146600	0.47690400
C	4.08444200	0.79088300	-0.72119900
H	2.29864500	1.94710000	-0.93534700

C	3.86034500	-1.36181900	0.30673500
H	1.90718300	-1.91661400	0.97115500
C	4.67385500	-0.39918100	-0.29187800
H	4.69103500	1.55743200	-1.19650500
H	4.29149600	-2.29470100	0.66058200
H	5.73774300	-0.57112700	-0.41941600

1a-conformation 2 scrf=(smd,solvent=nitromethane)

C	-0.32731500	-0.90344900	0.22181300
C	-1.79379400	-0.57109200	0.04019100
C	-2.25048000	0.75228800	0.01130400
C	-1.27163400	1.89513800	0.14120700
C	0.04911400	1.42174200	0.72640900
H	-2.35007900	-2.64711100	-0.05693200
H	-0.05676200	-1.69849100	-0.47972500
C	-2.71221700	-1.62129200	-0.08019100
C	-3.62091700	0.99847900	-0.14251900
H	-1.08855500	2.33717600	-0.84635200
H	-0.08201400	1.14975600	1.78847500
C	-4.52988200	-0.04796900	-0.26471100
C	-4.07209000	-1.36797100	-0.23180200
H	-3.97147900	2.02816300	-0.16132400
H	-5.58915800	0.16149500	-0.38215000
H	-4.77214200	-2.19286600	-0.32647600
H	-0.17514800	-1.30389500	1.24152500
H	-1.69835800	2.68097000	0.77361300
H	0.78926900	2.21924900	0.67814500
N	0.52576300	0.25082400	-0.01922500
C	1.91430700	0.02143100	-0.03690600
C	2.78659600	1.07358100	-0.38261600
C	2.47452100	-1.23958100	0.22835400
C	4.15971700	0.87207200	-0.44218100
H	2.38089400	2.04985700	-0.63037600
C	3.85641900	-1.43288100	0.15386000
H	1.84509100	-2.07861300	0.50091200
C	4.71090700	-0.38462300	-0.17356100
H	4.80403300	1.70306400	-0.71544400
H	4.26077500	-2.41924500	0.36455800
H	5.78378900	-0.54050400	-0.22578200

1a-conformation 3 scrf=(smd,solvent=nitromethane)

C	0.50927200	0.36241700	1.70629500

C	1.56985200	-0.03515800	0.69464700
C	1.64344600	0.63030100	-0.53869000
C	0.64263900	1.71100800	-0.89964200
C	-0.15888300	2.17881900	0.31648200
H	2.41598200	-1.55782700	1.95353300
H	0.94368500	1.06987400	2.42299200
C	2.48928700	-1.04477500	0.99642800
C	2.64447100	0.26240100	-1.44625800
H	1.15893200	2.55997600	-1.36054200
H	-0.99463200	2.80951300	0.01192400
C	3.55906900	-0.74282200	-1.14174400
C	3.48209000	-1.40174300	0.08762900
H	2.70337700	0.77670300	-2.40343100
H	4.32863400	-1.01261200	-1.85935000
H	4.18664100	-2.19160900	0.33162100
H	0.18150000	-0.50370000	2.28607600
H	-0.04970400	1.31570400	-1.65546300
H	0.47170800	2.77484300	0.98420500
N	-0.63587900	1.02581800	1.09545800
C	-1.60118100	0.21318300	0.46399400
C	-2.72652000	0.81596400	-0.13350600
C	-1.51433300	-1.18965700	0.43311800
C	-3.71886000	0.04594600	-0.72886400
H	-2.83491900	1.89551900	-0.11455000
C	-2.52277200	-1.95346100	-0.15834300
H	-0.65799100	-1.70059700	0.85832000
C	-3.62993700	-1.34857100	-0.74665700
H	-4.57508800	0.54248900	-1.17704800
H	-2.42506000	-3.03558900	-0.16476000
H	-4.40774500	-1.94652800	-1.21106200

3-conformation 1 gas phase

C	-0.06984600	1.20208400	-0.06522700
C	0.66259600	0.00028200	-0.10368000
C	-0.07110300	-1.20176000	-0.06715900
C	-1.46093600	-1.18897200	-0.02160100
C	-2.19053800	0.00114900	0.00300400
C	-1.46050300	1.19003700	-0.01972400
H	0.43973600	2.15769200	-0.07699300
H	0.43817800	-2.15753600	-0.08067700
H	-1.99042000	-2.13917200	-0.00083700
H	-1.98918900	2.14051300	0.00259500
N	2.05328300	-0.00057900	-0.19298800

C	2.75177200	-1.23495600	0.10569100
H	3.82524300	-1.06510400	0.01346400
H	2.53997600	-1.60880200	1.12039100
H	2.48150800	-2.01520300	-0.61187900
C	2.75248400	1.23411700	0.10235800
H	3.82579600	1.06398200	0.00884400
H	2.48104400	2.01295300	-0.61631800
H	2.54216000	1.61002300	1.11663400
C	-3.69608500	-0.00062700	0.08887900
H	-4.03507800	-0.09287700	1.12681600
H	-4.11481900	0.92561200	-0.31395600
H	-4.12416300	-0.83615400	-0.47239700

3-conformation 1 scrf=(smd,solvent=nitromethane)

C	0.07284500	-1.20339600	-0.07617500
C	-0.66451000	0.00004700	-0.11457000
C	0.06829300	1.20350600	-0.05274200
C	1.46073200	1.19233000	0.00992600
C	2.19365600	0.00294200	0.02401400
C	1.46345900	-1.18958800	-0.01389000
H	-0.43572500	-2.16011400	-0.09490300
H	-0.44207500	2.15929700	-0.04830700
H	1.98717400	2.14354000	0.05874400
H	1.99317700	-2.14000000	0.01285800
N	-2.05302900	-0.00431000	-0.22301100
C	-2.75911900	1.22915600	0.08370000
H	-3.82767000	1.06486100	-0.06045100
H	-2.59079600	1.56603400	1.11906000
H	-2.45472100	2.03049300	-0.59434700
C	-2.75256800	-1.23087200	0.12734100
H	-3.82502000	-1.06439500	0.01987400
H	-2.47579200	-2.04602000	-0.54626200
H	-2.54809100	-1.54896000	1.16180900
C	3.70066100	0.00051400	0.06503600
H	4.08497600	0.94680800	0.45610200
H	4.07900600	-0.80920500	0.69644900
H	4.12606900	-0.14000000	-0.93537700

$1a^{+}$-conformation 1 gas phase

C	-0.35775000	-0.78083500	0.76361500
C	-1.75706700	-0.58744900	0.23710900
C	-2.30160100	0.69685000	0.29114200

C	-1.37939800	1.77562600	0.78563100
C	-0.02197300	1.63841800	0.09815400
H	-2.07528800	-2.65357500	-0.29643200
H	0.03302300	-1.74085700	0.43053900
C	-2.50536200	-1.65664000	-0.24897300
C	-3.60598500	0.91169200	-0.14464400
H	-1.77062100	2.77224300	0.56687600
H	0.69007200	2.36543200	0.49393500
C	-4.36402300	-0.15915800	-0.61690900
C	-3.81600600	-1.43982900	-0.67009600
H	-4.03000400	1.91145600	-0.11328600
H	-5.38259800	0.00788100	-0.95113200
H	-4.40630600	-2.26918000	-1.04459900
H	-0.34490900	-0.75811800	1.86376100
H	-1.24643000	1.71320800	1.87372600
H	-0.13739900	1.79934100	-0.98123700
N	0.55436200	0.28975800	0.29593000
C	1.86799200	0.05755800	0.07456700
C	2.66953200	1.03159000	-0.60252300
C	2.48916100	-1.15452600	0.51585100
C	4.00463500	0.78961000	-0.83218200
H	2.22306200	1.94548000	-0.97326600
C	3.82983600	-1.36594600	0.28737100
H	1.92560900	-1.89166600	1.07276300
C	4.59741100	-0.40526900	-0.39106700
H	4.59832500	1.52432500	-1.36465800
H	4.29519400	-2.27863300	0.64282100
H	5.65132600	-0.58579300	-0.57359400

$1a^{+}$-conformation 2 gas phase

C	-0.39301800	-0.97762700	0.75310700
C	-1.76507300	-0.56902500	0.23567300
C	-2.07832200	0.74959400	-0.10139100
C	-1.05313400	1.84516900	0.07054900
C	-0.00066400	1.41071600	1.08721900
H	-2.47372900	-2.60214100	0.35995800
H	-0.02955600	-1.81588400	0.16114100
C	-2.72241400	-1.57738100	0.09400900
C	-3.35714300	1.03988200	-0.58629800
H	-0.56759800	2.08346400	-0.88418600
H	-0.47837000	1.22558800	2.05682600
C	-4.30822500	0.03742900	-0.73098100
C	-3.99089600	-1.27712900	-0.38610500

H	-3.60522800	2.06559300	-0.84595700
H	-5.29718000	0.27907000	-1.10559500
H	-4.72975700	-2.06406600	-0.49194800
H	-0.45494000	-1.29086800	1.80505500
H	-1.52858100	2.76187700	0.43171300
H	0.78749200	2.14366900	1.23714700
N	0.57035000	0.12556800	0.66848000
C	1.84036900	-0.02521200	0.22770500
C	2.62422000	1.11249800	-0.14689700
C	2.43138800	-1.32518600	0.13370600
C	3.91538500	0.94539000	-0.59342200
H	2.19421600	2.10582300	-0.13292800
C	3.73063600	-1.46404800	-0.29883100
H	1.88365000	-2.20187700	0.45435200
C	4.48253500	-0.33709300	-0.66951800
H	4.49280200	1.81169400	-0.89640600
H	4.17727600	-2.45118400	-0.34329700
H	5.50320300	-0.45761100	-1.01639300

$1a^{+}$-conformation 3 gas phase

C	0.39301400	-0.97763400	0.75306600
C	1.76507800	-0.56902600	0.23565900
C	2.07833100	0.74959400	-0.10139500
C	1.05313800	1.84516600	0.07053700
C	0.00066700	1.41070900	1.08720300
H	2.47373600	-2.60214200	0.35995100
H	0.45492200	-1.29090400	1.80500600
C	2.72242300	-1.57738100	0.09400900
C	3.35715900	1.03988600	-0.58628100
H	1.52858000	2.76187600	0.43170200
H	-0.78748700	2.14366200	1.23713600
C	4.30824500	0.03743400	-0.73095100
C	3.99091200	-1.27712500	-0.38608400
H	3.60524600	2.06559800	-0.84593200
H	5.29720600	0.27907900	-1.10554900
H	4.72977700	-2.06406100	-0.49191700
H	0.02955600	-1.81587400	0.16107300
H	0.56760500	2.08345800	-0.88420100
H	0.47837300	1.22557400	2.05680900
N	-0.57035000	0.12556500	0.66845600
C	-1.84037600	-0.02521200	0.22769800
C	-2.62423200	1.11250000	-0.14688700
C	-2.43139500	-1.32518600	0.13369700

C	-3.91540300	0.94539500	-0.59339700
H	-2.19422900	2.10582500	-0.13291700
C	-3.73064900	-1.46404500	-0.29882400
H	-1.88365200	-2.20187800	0.45433100
C	-4.48255200	-0.33708800	-0.66949400
H	-4.49282400	1.81170000	-0.89636800
H	-4.17728800	-2.45118100	-0.34329100
H	-5.50322600	-0.45760500	-1.01635700

$1a^{+}$-conformation 1 scrf=(smd,solvent=nitromethane)

C	-0.35491900	-0.77738400	0.76469300
C	-1.75535000	-0.58425400	0.24248600
C	-2.29773900	0.70272600	0.28129600
C	-1.37558300	1.77994400	0.77409900
C	-0.01283500	1.64047800	0.10356300
H	-2.07471100	-2.65268200	-0.26416000
H	0.02917900	-1.74124000	0.43901900
C	-2.50937100	-1.65695100	-0.23018600
C	-3.60270200	0.91575300	-0.15974600
H	-1.76338000	2.77593500	0.54868300
H	0.69244000	2.36066400	0.52042600
C	-4.36574200	-0.15842700	-0.62048500
C	-3.82089100	-1.44277800	-0.65559400
H	-4.01914900	1.91968800	-0.14172600
H	-5.38386300	0.00842600	-0.95964600
H	-4.41321800	-2.27620800	-1.02076500
H	-0.34336000	-0.74520800	1.86387600
H	-1.25033900	1.70825800	1.86205700
H	-0.10265800	1.81536600	-0.97558800
N	0.55287100	0.28867500	0.29338000
C	1.86638500	0.05264400	0.07174800
C	2.67040700	1.03774100	-0.58371400
C	2.47946200	-1.16957800	0.49158600
C	4.00740700	0.79615600	-0.81017700
H	2.22849600	1.96091500	-0.93678500
C	3.82244800	-1.37765000	0.26518800
H	1.91212500	-1.92239000	1.02340300
C	4.59575400	-0.40651100	-0.38874900
H	4.60474800	1.54160900	-1.32393900
H	4.28250500	-2.29975800	0.60371500
H	5.65070000	-0.58554600	-0.56828100

$1a^{+}$-conformation 2 scrf=(smd,solvent=nitromethane)

C	-0.39793200	-0.94872600	0.83468400
C	-1.75397400	-0.56007200	0.26720800
C	-2.06224200	0.75160300	-0.10762300
C	-1.04183900	1.85064400	0.06268900
C	0.00439200	1.43895400	1.09275200
H	-2.45487600	-2.59015200	0.41332600
H	-0.03837400	-1.83130800	0.31102100
C	-2.70740400	-1.57350600	0.12080300
C	-3.33073100	1.02761300	-0.63147600
H	-0.54665100	2.07167100	-0.89053700
H	-0.47187300	1.27381900	2.06598200
C	-4.27833800	0.01976100	-0.77850800
C	-3.96604800	-1.28766700	-0.39738800
H	-3.57054100	2.04865300	-0.91848300
H	-5.25871900	0.25109900	-1.18422200
H	-4.70015700	-2.08005100	-0.50673300
H	-0.48452500	-1.18446600	1.90355400
H	-1.52564600	2.77005700	0.40434700
H	0.78741300	2.18012200	1.21928300
N	0.56810000	0.14346300	0.69942600
C	1.82751100	-0.02321600	0.23778900
C	2.61944000	1.10785600	-0.13954600
C	2.39956000	-1.33008300	0.12418800
C	3.90299300	0.92699100	-0.60431700
H	2.20658800	2.10749900	-0.10593000
C	3.69119700	-1.47981500	-0.32945300
H	1.84573200	-2.20577900	0.43529900
C	4.45312900	-0.36057300	-0.69945300
H	4.48694200	1.79020900	-0.90454100
H	4.12187900	-2.47328000	-0.39181900
H	5.46781900	-0.49091700	-1.06062200

1a^{+}-conformation 3 scrf=(smd,solvent=nitromethane)

C	0.39788700	-0.94878000	0.83428700
C	1.75402100	-0.56008800	0.26706700
C	2.06236000	0.75159900	-0.10765300
C	1.04194800	1.85063800	0.06259500
C	-0.00436900	1.43891700	1.09254900
H	2.45490000	-2.59017500	0.41323300
H	0.48433300	-1.18476600	1.90311600
C	2.70747400	-1.57352000	0.12078300
C	3.33093700	1.02762700	-0.63128600

H	1.52574000	2.77002200	0.40436000
H	-0.78736800	2.18010400	1.21908100
C	4.27856300	0.01977700	-0.77820500
C	3.96620500	-1.28766500	-0.39718600
H	3.57079600	2.04867900	-0.91820800
H	5.25901400	0.25113000	-1.18374200
H	4.70033100	-2.08004700	-0.50643500
H	0.03836100	-1.83123100	0.31037500
H	0.54686900	2.07174200	-0.89066800
H	0.47182200	1.27372000	2.06580800
N	-0.56810600	0.14346200	0.69914000
C	-1.82759500	-0.02319900	0.23770500
C	-2.61959400	1.10787800	-0.13947100
C	-2.39965400	-1.33006700	0.12413300
C	-3.90320200	0.92701600	-0.60409200
H	-2.20678200	2.10753700	-0.10583200
C	-3.69134800	-1.47979500	-0.32934600
H	-1.84578300	-2.20577400	0.43513600
C	-4.45333500	-0.36054900	-0.69921900
H	-4.48719800	1.79024100	-0.90420500
H	-4.12202800	-2.47326200	-0.39168600
H	-5.46806600	-0.49089300	-1.06027300

$3a^{+}$-conformation 1 gas phase

C	0.08631700	-1.22703000	0.06120400
C	-0.64814200	0.00063600	0.00081800
C	0.08049400	1.22967400	-0.06212900
C	1.45570000	1.21583900	-0.07137300
C	2.17966400	0.00751100	-0.00750800
C	1.45874200	-1.20667800	0.06159300
H	-0.43399800	-2.17386700	0.13792600
H	-0.44359200	2.17457900	-0.13729600
H	1.99732000	2.15459300	-0.13765400
H	2.00626600	-2.14294600	0.12259600
N	-1.99431000	-0.00172800	0.00142100
C	-2.77115000	1.23042300	0.12567100
H	-3.75607000	0.96989800	0.51086300
H	-2.28825900	1.92055700	0.81528200
H	-2.88053000	1.69687400	-0.85936800
C	-2.76688500	-1.23647200	-0.12301800
H	-3.75217900	-0.97945500	-0.50964800
H	-2.28078900	-1.92540700	-0.81155600
H	-2.87597500	-1.70268600	0.86217600

C	3.67354500	-0.00201500	0.00478900
H	4.08120500	0.98297300	-0.22944800
H	4.03543800	-0.30043300	0.99629300
H	4.06162400	-0.73390900	-0.71038700

3a^{+}-conformation 1 scrf=(smd,solvent=nitromethane)

C	0.08631700	-1.22703000	0.06120400
C	-0.64814200	0.00063600	0.00081800
C	0.08049400	1.22967400	-0.06212900
C	1.45570000	1.21583900	-0.07137300
C	2.17966400	0.00751100	-0.00750800
C	1.45874200	-1.20667800	0.06159300
H	-0.43399800	-2.17386700	0.13792600
H	-0.44359200	2.17457900	-0.13729600
H	1.99732000	2.15459300	-0.13765400
H	2.00626600	-2.14294600	0.12259600
N	-1.99431000	-0.00172800	0.00142100
C	-2.77115000	1.23042300	0.12567100
H	-3.75607000	0.96989800	0.51086300
H	-2.28825900	1.92055700	0.81528200
H	-2.88053000	1.69687400	-0.85936800
C	-2.76688500	-1.23647200	-0.12301800
H	-3.75217900	-0.97945500	-0.50964800
H	-2.28078900	-1.92540700	-0.81155600
H	-2.87597500	-1.70268600	0.86217600
C	3.67354500	-0.00201500	0.00478900
H	4.08120500	0.98297300	-0.22944800
H	4.03543800	-0.30043300	0.99629300
H	4.06162400	-0.73390900	-0.71038700

1a-H^{+}-conformation 1 scrf=(smd,solvent=nitromethane)

C	-0.33099300	-0.74057000	-0.10010600
C	-1.75973600	-0.54248200	-0.10201300
C	-2.27795000	0.71348100	0.26515200
C	-1.29798000	1.77139100	0.69519200
C	0.00933900	1.64816900	-0.06773300
H	-2.17411300	-2.57108600	-0.70943600
C	-2.60431600	-1.61036000	-0.43972100
C	-3.65693400	0.88644000	0.28001900
H	-1.70543300	2.77100600	0.52738900
H	0.78078900	2.27993300	0.36954300
C	-4.49918700	-0.17049600	-0.07527500

C	-3.97965200	-1.41733100	-0.43447900
H	-4.07535200	1.84656900	0.56842800
H	-5.57448900	-0.01901300	-0.06812100
H	-4.64564500	-2.23017700	-0.70349300
H	0.07565100	-1.74642800	-0.17845000
H	-1.10937900	1.66689700	1.77132400
H	-0.11644300	1.90782300	-1.12454900
N	0.50908000	0.24608300	-0.02870000
C	1.92925200	0.01694400	-0.01180300
C	2.75573200	0.83816400	-0.77840000
C	2.44895200	-1.01613300	0.76635500
C	4.12782700	0.60077200	-0.77658300
H	2.33481300	1.63721900	-1.38043700
C	3.82336200	-1.24271800	0.75541500
H	1.79463600	-1.61815200	1.38951000
C	4.66306700	-0.43827000	-0.01444200
H	4.77683900	1.22872400	-1.37831300
H	4.23614800	-2.04144200	1.36333800
H	5.73371700	-0.61646300	-0.01529500

1a-H^+-conformation 2 scrf=(smd,solvent=nitromethane)

C	-0.32803200	-0.68932700	-0.29340900
C	-1.75759700	-0.52294200	-0.18071500
C	-2.28040000	0.76430900	0.04619400
C	-1.30927800	1.91323700	0.09581600
C	0.01100100	1.48125500	0.70723700
H	-2.16182200	-2.61485500	-0.51756900
C	-2.59648500	-1.63658800	-0.33101700
C	-3.65939800	0.91513500	0.13807400
H	-1.14037400	2.28215800	-0.92412100
H	-0.08790600	1.25487500	1.77534200
C	-4.49571900	-0.19694600	0.01231400
C	-3.97114600	-1.47117800	-0.22228500
H	-4.08265700	1.90154500	0.30510900
H	-5.57078300	-0.06601500	0.09328000
H	-4.63398300	-2.32404300	-0.32237600
H	0.08368300	-1.61363900	-0.69368300
H	-1.71432700	2.74040800	0.68339300
H	0.77799900	2.24301800	0.57953500
N	0.50739700	0.23112800	0.07303600
C	1.93030500	0.00896000	0.02436500
C	2.74017400	0.95235300	-0.60593700
C	2.46048300	-1.13921600	0.60831800

C	4.11256000	0.72534000	-0.66272100
H	2.30195400	1.83573000	-1.06091100
C	3.83637600	-1.35194500	0.54471900
H	1.80829900	-1.84435000	1.11565600
C	4.66079200	-0.42341700	-0.08933000
H	4.75309000	1.44639900	-1.16034000
H	4.26118900	-2.24073600	1.00004000
H	5.73204400	-0.59256500	-0.13433600

3-H^+-conformation 1 scrf=(smd,solvent=nitromethane)

C	0.00373900	-1.14770600	-0.32780500
C	-0.65582200	0.04471800	-0.03876800
C	0.04614200	1.20381900	0.27885700
C	1.43739100	1.16705300	0.28933700
C	2.13195000	-0.01101400	-0.00508800
C	1.39461600	-1.16121000	-0.31488300
H	-0.55006200	-2.04499800	-0.58353700
H	-0.48688700	2.11502600	0.53297900
H	1.98994300	2.06826200	0.53981500
H	1.91775000	-2.08319600	-0.55337100
N	-2.10210800	0.08392600	-0.05791100
C	-2.73119900	1.03648800	-0.63411300
H	-3.81518700	1.05974200	-0.58534000
H	-2.17346700	1.80203000	-1.16451000
C	-2.81380700	-1.00025900	0.64403400
H	-3.87751000	-0.77194600	0.65571500
H	-2.63587600	-1.93658900	0.11449800
H	-2.41609600	-1.06438100	1.65720300
C	3.63526700	-0.05308400	0.04220600
H	3.97605000	-0.41018400	1.02040800
H	4.03422800	-0.73410700	-0.71406200
H	4.06220700	0.94003000	-0.11708500

Table 7 Entry 1 RB3LYP/6-31+G(d)

C	-1.94550100	-1.19970400	0.01703100
C	-0.55159200	-1.20879200	-0.03194200
C	0.18362200	0.00000600	-0.07227600
C	-0.55159800	1.20879900	-0.03195500
C	-1.94550800	1.19970200	0.01701500
C	-2.66095000	-0.00000200	0.03906000
H	-2.47456000	-2.14973700	0.04330200
H	-0.03928800	-2.16370200	-0.04088700

H	-0.03930400	2.16371300	-0.04093200
H	-2.47457200	2.14973300	0.04326800
H	-3.74650700	-0.00000500	0.07961800
N	1.57536100	0.00000200	-0.16251300
C	2.29717900	-1.24218500	0.06287300
H	3.36648800	-1.06061700	-0.06602200
H	2.13445700	-1.65533200	1.07314700
H	2.00382400	-2.00375700	-0.66872300
C	2.29719700	1.24217900	0.06290100
H	3.36651800	1.06056100	-0.06581200
H	2.00397500	2.00374900	-0.66875300
H	2.13435000	1.65536100	1.07313700

Table 7 Entry 1 RB3LYP/6-31+G(d) cationic radical

C	-0.56134700	-1.23144200	-0.07346100
C	0.17034000	0.00000000	0.00000000
C	-0.56134800	1.23144300	0.07346100
C	-1.94162400	1.21781000	0.07934000
C	-2.64514200	0.00000000	0.00000000
C	-1.94162300	-1.21781000	-0.07934000
H	-0.03964600	-2.17624900	-0.16234200
H	-0.03964800	2.17625000	0.16234300
H	-2.48604900	2.15401700	0.15295100
H	-2.48604700	-2.15401700	-0.15295100
N	1.53042300	0.00000000	0.00000000
C	2.31635200	1.23451600	-0.14676800
H	3.28864900	0.97465200	-0.56774200
H	1.82035700	1.93364100	-0.81922900
H	2.46981300	1.70203500	0.83389000
C	2.31634800	-1.23451700	0.14676800
H	3.28865500	-0.97465300	0.56771900
H	1.82036300	-1.93363000	0.81924800
H	2.46978700	-1.70205100	-0.83388700
H	-3.73093900	0.00000000	0.00000000

Table 7 Entry 2 RB3LYP/6-31+G(d)

C	0.69716600	1.19588700	-0.10561900
C	1.44311700	0.00000600	-0.12468900
C	0.69720300	-1.19591500	-0.10582400
C	-0.69716200	-1.19594200	-0.10578900
C	-1.44311800	-0.00005000	-0.12460900
C	-0.69721200	1.19586000	-0.10558100

H	1.19722600	2.15655500	-0.08718400
H	1.19730300	-2.15656500	-0.08756400
H	-1.19723200	-2.15661000	-0.08750000
H	-1.19732200	2.15650200	-0.08711100
N	2.84879900	0.00003100	-0.17827700
C	3.54303200	-1.23135600	0.16431100
H	4.61821300	-1.07467600	0.05472700
H	3.34356800	-1.56981200	1.19649700
H	3.26214400	-2.03903000	-0.51859100
C	3.54298400	1.23138700	0.16451600
H	4.61817300	1.07476400	0.05491900
H	3.26207300	2.03916200	-0.51825800
H	3.34349300	1.56967000	1.19675400
N	-2.84879200	-0.00006000	-0.17810800
C	-3.54295600	1.23147400	0.16405100
H	-3.26256200	2.03873900	-0.51955500
H	-4.61818000	1.07460400	0.05526800
H	-3.34287600	1.57062500	1.19588100
C	-3.54305900	-1.23138100	0.16466200
H	-4.61823100	-1.07471700	0.05499900
H	-3.26215900	-2.03918600	-0.51807500
H	-3.34364700	-1.56965100	1.19691100

Table 7 Entry 2 RB3LYP/6-31+G(d) cationic radical

C	-0.68607600	-1.22041600	0.00003000
C	-1.43296700	-0.00001300	0.00003000
C	-0.68605000	1.22037300	0.00008400
C	0.68620200	1.22035800	0.00008400
C	1.43310500	-0.00004600	0.00006500
C	0.68617700	-1.22043400	0.00005500
H	-1.19890100	-2.17338900	0.00000300
H	-1.19885700	2.17335700	0.00013500
H	1.19901300	2.17333300	0.00011900
H	1.19895400	-2.17342600	0.00007900
N	-2.79015900	0.00000500	-0.00001700
C	-3.54200300	1.26150100	0.00001900
H	-4.60686100	1.03900400	-0.00008800
H	-3.31284100	1.85240800	0.89266200
H	-3.31274900	1.85244800	-0.89257000
C	-3.54204800	-1.26146400	-0.00012600
H	-4.60689800	-1.03892800	-0.00015700
H	-3.31279500	-1.85239200	-0.89273100
H	-3.31293000	-1.85240600	0.89250100

N	2.79028000	-0.00000800	-0.00002800
C	3.54196700	-1.26155600	0.00004100
H	3.31279900	-1.85224400	0.89284500
H	3.31239300	-1.85261900	-0.89236700
H	4.60684700	-1.03929700	-0.00023200
C	3.54179500	1.26164200	-0.00014800
H	3.31200900	1.85258800	-0.89263700
H	3.31265900	1.85238900	0.89257400
H	4.60670000	1.03952900	-0.00063400

Table 7 Entry 3 RB3LYP/6-31+G(d)

C	0.71569100	0.25857200	-0.01707000
C	-0.71579800	0.25829700	0.01706600
C	-1.38182900	1.49327600	0.06689700
C	-0.69480000	2.71041700	0.04288000
C	0.69374400	2.71068300	-0.04290000
C	1.38124100	1.49380500	-0.06689800
H	-2.46603800	1.50884500	0.09437500
H	-1.25104900	3.64387300	0.07206200
H	2.46544500	1.50980100	-0.09434900
N	-1.43805400	-0.96611100	0.02502600
C	-2.82131200	-0.92118100	0.47328700
H	-3.50771800	-0.44680200	-0.25341000
H	-3.16783600	-1.94838600	0.63253700
H	-2.89429800	-0.38275900	1.42304000
C	-1.27879900	-1.79999400	-1.17020500
H	-1.83556700	-1.38859500	-2.03166000
H	-0.22202800	-1.87518300	-1.43020700
H	-1.66203600	-2.80576800	-0.96141300
H	1.24963500	3.64435200	-0.07208900
N	1.43841000	-0.96559600	-0.02501700
C	1.27955600	-1.79944100	1.17030000
H	1.66298900	-2.80514600	0.96151300
H	1.83638400	-1.38785200	2.03162900
H	0.22285000	-1.87486300	1.43047900
C	2.82163600	-0.92023200	-0.47337200
H	3.50794400	-0.44572600	0.25332800
H	3.16844400	-1.94733100	-0.63271500
H	2.89440600	-0.38171700	-1.42308600

Table 7 Entry 3 RB3LYP/6-31+G(d) cationic radical

C	0.72833100	0.28068300	-0.04070700

C	-0.72833200	0.28067800	0.04070900
C	-1.38354300	1.52987200	0.23795700
C	-0.69473700	2.71752400	0.13952400
C	0.69471700	2.71752900	-0.13952400
C	1.38353300	1.52988300	-0.23795600
H	-2.45810200	1.55296000	0.36751600
H	-1.22891300	3.65779400	0.23447000
H	2.45809100	1.55297800	-0.36751500
N	-1.47147100	-0.86155400	-0.11077600
C	-2.88207800	-0.89329200	0.29237200
H	-3.52739100	-0.43159000	-0.46691800
H	-3.17814500	-1.93875800	0.40580400
H	-3.01961000	-0.38746000	1.24942700
C	-1.11315500	-1.93457700	-1.04859100
H	-1.88083800	-1.97880400	-1.83060300
H	-0.14880500	-1.74246900	-1.51421500
H	-1.08957800	-2.90226900	-0.53667400
H	1.22888500	3.65780300	-0.23447300
N	1.47147900	-0.86154200	0.11078000
C	1.11316800	-1.93456900	1.04859200
H	1.08958000	-2.90225900	0.53667000
H	1.88085900	-1.97880400	1.83059600
H	0.14882300	-1.74245600	1.51422600
C	2.88208400	-0.89327300	-0.29237600
H	3.52740100	-0.43157300	0.46691200
H	3.17815400	-1.93873800	-0.40581400
H	3.01960800	-0.38743600	-1.24942900

Table 7 Entry 4 RB3LYP/6-31+G(d)

C	0.00000100	0.47554100	0.00000000
C	-1.23301600	-0.20767400	0.06993100
C	-1.21931000	-1.62102200	0.05399900
C	0.00000000	-2.29217600	-0.00000300
C	1.21931100	-1.62102200	-0.05400500
C	1.23301700	-0.20767400	-0.06993500
H	0.00000200	1.55472300	0.00000300
H	-2.13740800	-2.19353000	0.09174200
H	0.00000000	-3.38011500	-0.00000400
N	-2.43431800	0.50018400	0.17247800
C	-3.68548200	-0.21439400	-0.02801200
H	-4.51756600	0.47924100	0.11311300
H	-3.77005700	-0.65950900	-1.03442700
H	-3.79910000	-1.01615600	0.70993300

C	-2.44101100	1.92747400	-0.10404300
H	-3.45601800	2.31019600	0.02483400
H	-1.79739400	2.46730600	0.60022900
H	-2.10668600	2.16745600	-1.12835400
H	2.13740800	-2.19353100	-0.09174900
N	2.43431900	0.50018400	-0.17248200
C	3.68548200	-0.21439200	0.02802700
H	4.51756700	0.47924000	-0.11310100
H	3.77005000	-0.65949400	1.03445000
H	3.79910400	-1.01616400	-0.70990500
C	2.44100800	1.92747400	0.10403900
H	2.10668100	2.16745700	1.12834900
H	3.45601400	2.31019900	-0.02483800
H	1.79739000	2.46730200	-0.60023600

Table 7 Entry 4 RB3LYP/6-31+G(d) cationic radical

C	**0.72833100**	**0.28068300**	**-0.04070700**
C	**-0.72833200**	**0.28067800**	**0.04070900**
C	**-1.38354300**	**1.52987200**	**0.23795700**
C	**-0.69473700**	**2.71752400**	**0.13952400**
C	**0.69471700**	**2.71752900**	**-0.13952400**
C	**1.38353300**	**1.52988300**	**-0.23795600**
H	**-2.45810200**	**1.55296000**	**0.36751600**
H	**-1.22891300**	**3.65779400**	**0.23447000**
H	**2.45809100**	**1.55297800**	**-0.36751500**
N	**-1.47147100**	**-0.86155400**	**-0.11077600**
C	**-2.88207800**	**-0.89329200**	**0.29237200**
H	**-3.52739100**	**-0.43159000**	**-0.46691800**
H	**-3.17814500**	**-1.93875800**	**0.40580400**
H	**-3.01961000**	**-0.38746000**	**1.24942700**
C	**-1.11315500**	**-1.93457700**	**-1.04859100**
H	**-1.88083800**	**-1.97880400**	**-1.83060300**
H	**-0.14880500**	**-1.74246900**	**-1.51421500**
H	**-1.08957800**	**-2.90226900**	**-0.53667400**
H	**1.22888500**	**3.65780300**	**-0.23447300**
N	**1.47147900**	**-0.86154200**	**0.11078000**
C	**1.11316800**	**-1.93456900**	**1.04859200**
H	**1.08958000**	**-2.90225900**	**0.53667000**
H	**1.88085900**	**-1.97880400**	**1.83059600**
H	**0.14882300**	**-1.74245600**	**1.51422600**
C	**2.88208400**	**-0.89327300**	**-0.29237600**
H	**3.52740100**	**-0.43157300**	**0.46691200**
H	**3.17815400**	**-1.93873800**	**-0.40581400**

H	**3.01960800**	**-0.38743600**	**-1.24942900**

Table 7 Entry 5 RB3LYP/6-31+G(d)

C	-0.22661700	-1.10596300	-0.06662900
C	-1.07560800	0.01737400	-0.10312400
C	-0.45168100	1.28775300	-0.06546100
C	0.93193500	1.41639100	-0.02349300
C	1.75997800	0.28768800	-0.00630100
C	1.16712900	-0.97648600	-0.02532500
H	-0.63756200	-2.10862000	-0.07350700
H	-1.04621300	2.19372900	-0.07280400
H	1.38981400	2.40125600	0.00245700
H	1.76839300	-1.87913400	-0.00191100
N	-2.47052800	-0.11181500	-0.19552000
C	-3.29157200	1.04346500	0.13323300
H	-4.34366300	0.77955000	0.00164400
H	-3.14752100	1.39542500	1.17036100
H	-3.07970000	1.87819800	-0.54346900
C	-3.05646100	-1.41338100	0.08201000
H	-4.13974700	-1.35000700	-0.04579900
H	-2.68821400	-2.16424600	-0.62570500
H	-2.84614000	-1.77279800	1.10539600
C	3.98699500	-0.59021100	0.06416700
H	3.87437400	-1.21016900	-0.83624500
H	4.99793000	-0.17891300	0.09553000
H	3.81929100	-1.21105900	0.95537100
O	3.11350800	0.52621500	0.03785500

Table 7 Entry 5 RB3LYP/6-31+G(d) cationic radical

C	-0.44795300	1.31078800	-0.00001000
C	-1.06930800	0.01642600	-0.00000200
C	-0.21594100	-1.13507800	0.00000600
C	1.15524700	-1.00985900	0.00000700
C	1.74886200	0.27838900	0.00000100
C	0.91616300	1.43303600	-0.00000800
H	-1.05188300	2.20932600	-0.00001500
H	-0.64243100	-2.13036500	0.00000900
H	1.76911100	-1.90294200	0.00001300
H	1.39160200	2.40856600	-0.00001200
N	-2.41993100	-0.11325300	-0.00000300
C	-3.05433800	-1.44068100	0.00001800
H	-4.13547300	-1.31688400	0.00004100

H	-2.76802000	-2.00425900	-0.89393800
H	-2.76798200	-2.00424900	0.89396800
C	-3.29146700	1.07226000	-0.00002500
H	-4.33040600	0.74874800	-0.00004600
H	-3.11429500	1.67912500	0.89379100
H	-3.11425800	1.67911800	-0.89383900
O	3.05389900	0.51476600	0.00000200
C	4.00952700	-0.56808000	0.00001200
H	4.98406100	-0.08287900	0.00001200
H	3.89177800	-1.17592800	0.90192000
H	3.89178300	-1.17593800	-0.90189000

Table 7 Entry 6 RB3LYP/6-31+G(d)

C	-0.57855600	-1.21599600	0.00000100
C	-1.31586500	0.00000000	0.00000300
C	-0.57855600	1.21599600	0.00000100
C	0.80718700	1.21340000	-0.00000200
C	1.50246600	0.00000000	-0.00000400
C	0.80718700	-1.21340000	-0.00000200
H	-1.09295400	-2.16908200	0.00000300
H	-1.09295400	2.16908200	0.00000200
H	1.36076800	2.14519200	-0.00000300
H	1.36076800	-2.14519200	-0.00000300
N	-2.68946300	0.00000000	0.00000600
C	-3.42373800	1.25818800	0.00000800
H	-4.49388500	1.04699600	0.00001100
H	-3.19643100	1.85988400	0.89074300
H	-3.19643500	1.85988500	-0.89072700
C	-3.42373800	-1.25818800	0.00000900
H	-4.49388500	-1.04699600	0.00001100
H	-3.19643500	-1.85988600	-0.89072600
H	-3.19643100	-1.85988400	0.89074400
N	2.95464500	0.00000000	-0.00000700
O	3.53770500	-1.09161300	-0.00000800
O	3.53770500	1.09161300	-0.00000900

Table 7 Entry 6 RB3LYP/6-31+G(d) cationic radical

C	-0.56134700	-1.23144200	-0.07346100
C	0.17034000	0.00000000	0.00000000
C	-0.56134800	1.23144300	0.07346100
C	-1.94162400	1.21781000	0.07934000
C	-2.64514200	0.00000000	0.00000000

C	-1.94162300	-1.21781000	-0.07934000
H	-0.03964600	-2.17624900	-0.16234200
H	-0.03964800	2.17625000	0.16234300
H	-2.48604900	2.15401700	0.15295100
H	-2.48604700	-2.15401700	-0.15295100
N	1.53042300	0.00000000	0.00000000
C	2.31635200	1.23451600	-0.14676800
H	3.28864900	0.97465200	-0.56774200
H	1.82035700	1.93364100	-0.81922900
H	2.46981300	1.70203500	0.83389000
C	2.31634800	-1.23451700	0.14676800
H	3.28865500	-0.97465300	0.56771900
H	1.82036300	-1.93363000	0.81924800
H	2.46978700	-1.70205100	-0.83388700
H	-3.73093900	0.00000000	0.00000000

Table 7 Entry 7 RB3LYP/6-31+G(d)

C	1.46944900	1.19271900	0.00412600
C	0.07478000	1.20437400	-0.04283200
C	-0.66350800	0.00055800	-0.08639400
C	0.07679100	-1.20373400	-0.04690800
C	1.47003000	-1.19124300	-0.00011100
C	2.20477400	0.00175500	0.02045700
H	1.99465400	2.14595300	0.03599300
H	-0.43215000	2.16232500	-0.04338500
H	-0.42979000	-2.16189900	-0.05111900
H	1.99602100	-2.14435900	0.02822100
N	-2.05846900	-0.00098000	-0.17716000
C	-2.77571500	1.23840300	0.07606400
H	-3.84570400	1.06385300	-0.05867900
H	-2.61259900	1.62969200	1.09553600
H	-2.47854800	2.01389900	-0.63870200
C	-2.77444000	-1.23974100	0.08343800
H	-3.84487700	-1.06602400	-0.04875700
H	-2.47964100	-2.01842600	-0.62881500
H	-2.60818600	-1.62639700	1.10412000
C	3.71659000	-0.00083500	0.04303900
H	4.13661900	-0.17700000	-0.95728000
H	4.11185300	0.95802300	0.39734000
H	4.10912200	-0.78631500	0.70037300

Table 7 Entry 7 RB3LYP/6-31+G(d) cationic radical

C	-0.08851700	1.22737600	0.06198800
C	0.64964700	-0.00028600	-0.00196400
C	-0.08867600	-1.22741700	-0.07309600
C	-1.46554400	-1.21175800	-0.08441800
C	-2.19753200	0.00040300	-0.01240800
C	-1.46530600	1.21253200	0.06125700
H	0.42857900	2.17551300	0.14364200
H	0.42846700	-2.17539200	-0.15645800
H	-2.00423000	-2.15221000	-0.15884400
H	-2.00413700	2.15376700	0.12485700
N	2.00742000	-0.00031800	0.00277600
C	2.78970000	-1.23800700	0.13997200
H	3.76839500	-0.98385600	0.54888600
H	2.29949800	-1.93341200	0.82117400
H	2.92822100	-1.71074600	-0.84027000
C	2.79002300	1.23789700	-0.12858100
H	3.77579100	0.98310100	-0.51951700
H	2.30993100	1.92838000	-0.82204300
H	2.91132100	1.71683800	0.85091400
C	-3.69465400	-0.00022300	0.01464700
H	-4.11007000	-0.86700200	-0.50814800
H	-4.04991700	-0.04897600	1.05544900
H	-4.10863400	0.91312400	-0.42346100

Table 7 Entry 8 RB3LYP/6-31+G(d) Conformation 1

C	-0.32978700	-0.86528000	0.38241600
C	-1.79005100	-0.58411600	0.09474100
C	-2.31038200	0.70694000	0.26120700
C	-1.34645200	1.79682900	0.65221300
C	-0.00243500	1.60663400	-0.05798500
H	-2.23484000	-2.62717900	-0.43461800
H	0.00718400	-1.67762000	-0.27673500
C	-2.64058600	-1.62694300	-0.29408700
C	-3.67301500	0.93747100	0.03556300
H	-1.75096800	2.78401800	0.39898100
H	0.69996400	2.36098800	0.31051600
C	-4.52016900	-0.10697800	-0.33961200
C	-4.00089000	-1.39468400	-0.50551400
H	-4.07009600	1.94391100	0.15348500
H	-5.57637200	0.08391300	-0.51172800
H	-4.64999600	-2.21224500	-0.80841500
H	-0.24402800	-1.25135000	1.41325300
H	-1.17746100	1.78850900	1.73939600

H	-0.13360100	1.77907900	-1.14106700
N	0.55898200	0.28877300	0.21430500
C	1.92376800	0.05987900	0.05907200
C	2.78380100	1.03419300	-0.50231100
C	2.50753000	-1.16462500	0.46532100
C	4.15193400	0.79460900	-0.63127400
H	2.38610000	1.97561300	-0.86358400
C	3.87685800	-1.38891300	0.32522000
H	1.89742600	-1.93872900	0.91685400
C	4.71709600	-0.41523200	-0.22071500
H	4.77893700	1.56659700	-1.07184500
H	4.28857900	-2.33965600	0.65655200
H	5.78299400	-0.59597500	-0.32670300

Table 7 Entry 8 RB3LYP/6-31+G(d) cationic radical Conformation 1

C	-0.36735800	-0.76951300	0.78818300
C	-1.76545900	-0.58447400	0.24519300
C	-2.31524200	0.70376600	0.27549500
C	-1.40125100	1.79656000	0.76478700
C	-0.01728400	1.65434200	0.11952600
H	-2.08095700	-2.66348800	-0.26007200
H	0.02824700	-1.73691600	0.48379400
C	-2.51200500	-1.66532100	-0.23158700
C	-3.62256600	0.90682900	-0.17180700
H	-1.78495200	2.79006600	0.51224400
H	0.68429900	2.37793800	0.54277800
C	-4.37826300	-0.17546000	-0.63218400
C	-3.82494500	-1.45881600	-0.66344300
H	-4.05150400	1.90588500	-0.16019400
H	-5.39674200	-0.01530400	-0.97382700
H	-4.41138400	-2.29695700	-1.02791500
H	-0.36044300	-0.72771300	1.88888900
H	-1.29907900	1.76821300	1.85954200
H	-0.09628000	1.83365300	-0.96047800
N	0.55741700	0.29710500	0.31199200
C	1.87940700	0.05750200	0.07987600
C	2.68527900	1.03270400	-0.59446700
C	2.50131200	-1.16099500	0.50809300
C	4.02368700	0.78787600	-0.83196900
H	2.24448900	1.95356800	-0.95453100
C	3.84516000	-1.37743900	0.27107100
H	1.93928200	-1.90428600	1.05866400
C	4.61750200	-0.41394800	-0.40316500

H	4.61711600	1.52747800	-1.36044100
H	4.30692500	-2.29696000	0.61700700
H	5.67121900	-0.59658800	-0.59101800

Table 7 Entry 8 RB3LYP/6-31+G(d) Conformation 2

C	-0.33259500	-0.90219600	0.22181900
C	-1.80379200	-0.57096900	0.03603200
C	-2.26452000	0.75379800	-0.00302600
C	-1.28021700	1.89785200	0.11457500
C	0.03685400	1.43756600	0.73701400
H	-2.36321400	-2.65138700	-0.04411400
H	-0.04756100	-1.67078400	-0.50500700
C	-2.72343400	-1.62418500	-0.07533900
C	-3.63844300	0.99525400	-0.15480200
H	-1.07587400	2.31630900	-0.88133800
H	-0.11331400	1.20387400	1.80838400
C	-4.54781800	-0.05516800	-0.26875900
C	-4.08649600	-1.37556500	-0.22807300
H	-3.99452300	2.02372400	-0.18102400
H	-5.60853500	0.15226200	-0.38525200
H	-4.78430700	-2.20434100	-0.31629600
H	-0.19359500	-1.34806500	1.22815000
H	-1.71073900	2.70713700	0.71915300
H	0.77837700	2.23472700	0.68586500
N	0.53567200	0.25201900	0.03216200
C	1.92745300	0.02697300	-0.01131300
C	2.80336600	1.07833300	-0.36244200
C	2.49377300	-1.23990200	0.23538000
C	4.17729800	0.87125000	-0.44638800
H	2.40187800	2.05810200	-0.60294500
C	3.87457400	-1.44020900	0.13590100
H	1.86652700	-2.07767800	0.51779000
C	4.72967700	-0.39107600	-0.19839700
H	4.82114200	1.70228500	-0.72495800
H	4.27802000	-2.43058100	0.33413700
H	5.80194000	-0.55025300	-0.27077000

Table 7 Entry 1 RB3LYP/6-31+G(d) cationic radical Conformation 2

C	-0.39196600	-0.95027200	0.73617200
C	-1.77912900	-0.56573700	0.22940200
C	-2.12171000	0.75360400	-0.09507800
C	-1.10520600	1.86387800	0.05533500

C	0.00258000	1.45091300	1.03164100
H	-2.45624800	-2.61517700	0.35087400
H	-0.02482000	-1.80105900	0.16435200
C	-2.72385500	-1.59216600	0.09381100
C	-3.41710900	1.02407900	-0.56054100
H	-0.65993200	2.12724600	-0.91407500
H	-0.42489500	1.29196600	2.03019500
C	-4.35519000	0.00317300	-0.69904400
C	-4.00843600	-1.31081700	-0.36791200
H	-3.68865500	2.04651500	-0.81283500
H	-5.35458000	0.23068100	-1.05803100
H	-4.73498900	-2.11182300	-0.46670100
H	-0.43723900	-1.24691500	1.79550300
H	-1.57737200	2.77357100	0.44368800
H	0.78526100	2.19956000	1.12423300
N	0.57514200	0.15583600	0.62681600
C	1.86431700	-0.01263900	0.21216100
C	2.67098200	1.11227900	-0.15991600
C	2.44841000	-1.31949300	0.14287200
C	3.97342100	0.92780600	-0.58235400
H	2.25745600	2.11260600	-0.16009700
C	3.75833800	-1.47713700	-0.26681300
H	1.88874600	-2.19077600	0.45808900
C	4.53206400	-0.36199100	-0.63724200
H	4.56414400	1.78798000	-0.88161900
H	4.19344600	-2.47137100	-0.29204500
H	5.55860700	-0.49673800	-0.96421100

Table 7 Entry 8 RB3LYP/6-31+G(d) Conformation 3

C	0.47483000	0.12634800	1.62554000
C	1.62687700	-0.14339900	0.66431300
C	1.77761000	0.64441800	-0.49108600
C	0.75495100	1.71442800	-0.83388800
C	-0.13079000	2.07735600	0.36935000
H	2.44935600	-1.74428300	1.84945100
H	0.85244500	0.72353400	2.47005700
C	2.57093400	-1.13823200	0.95251600
C	2.87529800	0.41080500	-1.33264800
H	1.26020500	2.61384200	-1.21144400
H	-0.96364000	2.70978400	0.05478600
C	3.81095600	-0.58247700	-1.04235200
C	3.65800900	-1.36379200	0.10769200
H	2.99448700	1.01920400	-2.22768900

H	4.65458100	-0.74638800	-1.70813600
H	4.37852500	-2.14339600	0.34216200
H	0.09925900	-0.80442000	2.05984300
H	0.11135600	1.35388100	-1.64979900
H	0.44666900	2.64754700	1.10875700
N	-0.63497300	0.87189400	1.04117400
C	-1.68658300	0.16492800	0.40985100
C	-2.87360000	0.85234100	0.07771800
C	-1.62777700	-1.21466600	0.13395900
C	-3.94872800	0.18795900	-0.50751100
H	-2.96303200	1.90936200	0.31144500
C	-2.71900700	-1.87723500	-0.43709300
H	-0.72375500	-1.77743600	0.34022300
C	-3.88473300	-1.18600400	-0.76773100
H	-4.85166900	0.74593200	-0.74460800
H	-2.64174400	-2.94328900	-0.63814000
H	-4.72773000	-1.70380800	-1.21689600

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