

Supporting Information for:

Effect of Heteroatom and Functionality Substitution on the Oxidation Potential of Cyclic Nitroxide Radicals: Role of Electrostatics in Electrochemistry

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Table of Contents

Detailed Experimental Procedures	2
NMR Spectra	15
Theoretical Methodology	18
Supporting computational data.	25

Detailed Experimental Procedures

Materials. The following reagents and solvents were used as received: silica gel 60 (230-400 mesh) ATM (SDS), TLC plates (silica gel 60 F254), sodium chloride (Univar, 99.9%), sodium iodide (Sigma-Aldrich, ACS reagent, $\geq 99.5\%$), lithium chloride (Sigma-Aldrich, BioXtra, $\geq 99.0\%$), methanol (Univar, AR grade), sodium hydrogen carbonate (Merck, AR grade), hydrochloric acid (Vetec, AR, 35-37%), sulfuric acid (Sigma-Aldrich, ACS reagent, 95.0-98.0%), acetic acid glacial (Merck, 100% anhydrous for analysis), sodium azide (Sigma-Aldrich, ReagentPlus®, $\geq 99.5\%$), sodium hydroxide pellets (Thermo Fisher Scientific, CertiFied AR 500g) n-hexane (Scharlau, 96%), acetonitrile (Lab-Scan, HPLC grade), chloroform (CHCl₃, Pronalys, 99%), dichloromethane (DCM, Labscan, AR grade), diethyl ether (Et₂O, Pronalys, AR grade), tetrahydrofuran (THF, HPLC grade, Lichrosolv, 99.8%), ethyl acetate (AR grade), toluene (HPLC, LABSCAN, 99.8%), dimethyl sulfoxide (DMSO, LABSCAN, 99.8%), petroleum spirit (Chem-supply Pty Ltd, 40-60°C AR), triethylamine (TEA, Fluka, purum), magnesium sulfate (Sigma-Aldrich, anhydrous, free-flowing, Redi-Dri™, reagent grade, $\geq 97\%$), potassium hydroxide (Sigma-Aldrich, $\geq 85\%$ KOH basis, pellets, white hydrogen peroxide) 30% w/w (Univar, AR grade), sodium hydride (Aldrich, 60 wt% in mineral oil), N,N'-dicyclohexylcarbodiimide (DCC, Aldrich, 99%), 4-(dimethylamino)pyridine (DMAP, Aldrich, $> 99\%$), N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride (EDC·HCl, Aldrich, 97%), propargyl bromide (Aldrich, 80 wt % in toluene), 2,2,6,6-tetramethyl-4-piperidone (Aldrich, 95%), 4-vinylbenzyl chloride (Aldrich, 90%), p-toluenesulfonyl chloride (Aldrich, $\geq 98\%$), potassium carbonate (Sigma-Aldrich, anhydrous, ACS reagent, $\geq 99\%$), ethylenediaminetetraacetic acid (Sigma-Aldrich, ACS reagent, 99.4-100.6%, powder), sodium borohydride (Aldrich, purum p.a., $\geq 96\%$), sodium tungstate dihydrate (Sigma-Aldrich, ACS reagent, $\geq 99\%$), hydroxylamine hydrochloride (Sigma-Aldrich, ACS reagent, 98.0%), tetrabromomethane (Aldrich, ReagentPlus®, 99%), triphenylphosphine (Sigma-Aldrich, ReagentPlus®, $\geq 98.5\%$), bromine (Sigma-Aldrich, reagent grade), 2-amino-2-methyl-1-propanol (Sigma-Aldrich, BioXtra, $\geq 95\%$), 3-chloroperbenzoic acid (Aldrich, $\leq 77\%$), lithium aluminum hydride (Aldrich, green alternative powder, reagent grade,

95%), *p*-toluenesulfonyl chloride (Sigma-Aldrich, reagent grade, $\geq 98\%$), 2,2,6,6-tetramethylpiperidiyl-1-oxyl (TEMPO) and 4-carboxyl-2,2,6,6-tetramethylpiperidiyl-1-oxyl (4-carboxyl-TEMPO) (Aldrich) were used as received.

Characterization. *¹H and ¹³C Nuclear Magnetic Resonance (NMR) Spectroscopy.* All NMR spectra were recorded on a Bruker DRX 300 MHz or 400 MHz using an external lock (CDCl₃ or DMSO-d₆) and referenced to the residual nondeuterated solvent (CHCl₃ or DMSO). *Electron Spray Ionization-mass spectra (ESI-MS).* All the ESI-MS spectra were recorded on Waters LC-MS system with the condition setting as follows: the capillary voltage as 3.0 KV, extractor voltage 2.0 V, RF Lens 0.5 V, source temperature 120 °C, desolvation temperature 200 °C, desolvation gas flow 500 L/hr, pump flow 20 μ L/min. Sample concentration was 1-5 mg/mL in MeOH, and the cone voltage was varied from 15 to 80V depending on the samples. *Electron Paramagnetic Resonance (EPR).* EPR spectra were recorded with a Bruker E540 spectrometer operating at X-band (~9.8 GHz) and using a Bruker ER4122SQE-W1 high sensitivity resonator. Samples were measure in a 1.5mm internal diameter capillary with the following instrumental parameters, microwave power = 0.635 mW, modulation amplitude = 1 G. The spectra were processed using Bruker Xepr software. *Cyclic Voltammetry (CV).* The electrochemical measurements were performed using a conventional three-electrode cell under standard ambient conditions. A coiled platinum wire and Ag/AgNO₃ were used as the counter and the reference electrodes, respectively. A potentiostat system (CHI-760D) was used for cyclic voltammetry. The cyclic voltammograms were measured using 5 mM solution in MeCN (0.1M tetrabutylammonium hexafluorophosphate). *Attenuated Total Reflectance Fourier Transform Spectroscopy (ATR-FTIR).* ATR-FTIR spectra were obtained using a diamond/ZnSe crystal ATR accessory on a Perkin-Elmer 400 FT-IR/FT-FIR Spectrometer. Spectra were recorded between 4000 and 500 cm⁻¹ by acquiring 24 scans at 4 cm⁻¹ resolution with an OPD velocity of 0.2 cm s⁻¹. Solids were pressed directly onto the diamond internal reflection element of the ATR without further sample preparation. *Elemental Analysis (EA).* Carbon, nitrogen and oxygen content was measured by

dynamic flash combustion of the sample using a Flash 2000 Thermo Fisher organic elemental analyser.

Synthesis of functional nitroxide radicals (b) (g), (k) and (l) was according to previous procedure.⁵¹,

2

Synthesis of functional nitroxide radicals (a and c)

4-oxo-TEMPO (a). Synthesis of (a) was carried out according the reported procedure with modification. Briefly, 2, 2, 6, 6-tetramethylpiperidone (**1**) 6.0 g (3.87×10^{-2} mol), EDTA 0.13 g (4.45×10^{-4} mol), and sodium tungstate dihydrate 1.8 g (5.46×10^{-3} mol) were added to 200 ml methanol/water (1/1, v/v) with stirring and cooling in an ice-water bath. Then 18 mL H₂O₂ (30 wt %) was added dropwise to the mixture. The mixture was kept stirring at room temperature overnight, after which the colour turned to red. The resulting mixture was then condensed under reduced pressure to remove methanol, and the rest was extracted with diethyl ether (3 x 100 mL). The organic phase was collected, dried over MgSO₄ and filtered. The filtrate was concentrated. The crude product was purified by column chromatography (silica gel) using DCM/MeOH mixture (95/5, v/v) as the eluent. Finally, 5.45 g orange solid nitroxide radical (**a**) was obtained with a yield of 82.2%. $R_f=0.68$ (DCM/MeOH, 95/5, v/v). ESI-MS: Cald. (C₉H₁₆NO₂+H⁺) 171.13; Found 171.18. IR $\nu_{\max}/\text{cm}^{-1}$:1380, 1650, 2970. Elemental Analysis: Cald. C, 63.5; H, 9.47; N, 8.23; O, 18.80; Found: C, 63.16; H, 9.24; N, 8.44; O, 19.16%.

1-hydroxy-2, 2, 6, 6-tetramethylpiperidin-4-one oxime (c) To a 50 mL round bottom flask, nitroxide radical (**a**) 2.0 g (1.18×10^{-2} mol) was dissolved in 10 mL water with a few drops of methanol to increase the solubility. In another flask, NH₂OH·HCl 0.69 g (1.0×10^{-2} mol) was pre-neutralized with NaOH 0.4 g (1.0×10^{-2} mol) in 10 mL water. Then, neutralised NH₂OH solution was dropped to the solution of (**a**) in 10 mins. As the reaction proceeds, some orange solid precipitated out. The reaction was stirred at room temperature for 1 h, and checked by TLC to monitor full

conversion of reactant (**a**). The orange solid product **c** (1.63 g) was filtered out from the resulting mixture, washed with deionized water (3 x 20 mL) and dried under high vacuum overnight. Yield: 74.7% $R_f=0.50$ (DCM/MeOH, 90/10, v/v). ESI-MS: Cald. ($C_9H_{17}N_2O_2+H^+$) 186.14; Found 186.28. IR ν_{max}/cm^{-1} : 1134, 1234, 1658, 2976, 3329. Elemental Analysis: C, 58.35; H, 9.25; N, 15.12; O, 17.27; Found: C, 58.39; H, 9.27; N, 14.74; O, 17.60%.

Synthesis of functional nitroxide radicals (d-f)

4-oxiranyl-TEMPO (d) To a two neck 100 mL round bottom flask equipped with a magnetic stirrer and Ar flow, sodium hydride (60 % dispersion in mineral oil) 0.8 g (2×10^{-2} mol) was added, followed by 5 mL petroleum ether (40-60 °C) under argon protection. After stirring for a few minutes, the petroleum ether was removed by syringe. Subsequently, dry DMSO 10 mL was added to the flask via syringe and stirred for 30 min. Then 1.42 g (6.45×10^{-3} mol) trimethylsulfoxonium iodide was added proportionally via spatula with positive argon flowing. The mixture was stirred at room temperature for another 30 mins until no bubble produced. Finally, nitroxide radical (**a**) 1.0 g, (5.88×10^{-3} mol) was dissolved in 2 mL dry THF and added to the mixture via syringe during 20 mins. Reaction was left at room temperature for 4 h. The resulting mixture was diluted with Milli-Q water 100 mL and extracted with diethyl ether (3 x 50 mL). The extract was dried with $MgSO_4$ and distilled under reduce pressure. Crude product was purified by column chromatography (silica gel) using EtOAc/Petroleum ether 40-60 °C (1/2, v/v) as the eluent. 0.6 g red solid radical (**d**) was obtained with a yield of 55.5%. $R_f=0.72$ (EtOAc/Petroleum ether 40-60 °C, 1/2, v/v). ESI-MS: Cald. ($C_{10}H_{18}NO_2+Na^+$) 207.12; found 207.18. IR ν_{max}/cm^{-1} : 1160, 1232, 1367, 1463, 2941, 3410. Elemental Analysis: C, 65.19; H, 9.85; N, 7.60; O, 17.37; Found: C, 65.37; H, 9.95; N, 7.56; O, 17.12%.

4-(hydroxymethyl)-2, 2, 6, 6-tetramethylpiperidin-4-ol-1-oxyl (e) 4-spiroepoxy-TEMPO (**d**) 2.55 g (1.38×10^{-2} mol) was dissolved in 20 mL DMSO in a round bottom flask equipped with magnetic stirrer. Then 15% NaOH solution 8 mL was charged to the mixture in one portion. The hydrolysis was carried out at 60 °C over 16 h. The resulting mixture was diluted with 100 mL Milli-Q water and

extracted with EtOAc (5 x 100 mL). The combined organic phase was dried over MgSO₄, filtered and was concentrated under reduced pressure. The crude product was purified by column chromatography (silica gel) using EtOAc/Petroleum ether 40-60 °C (4/1, v/v) as the eluent. Finally, 1.23 g red solid (**e**) was obtained with a yield of 44.9%. R_f=0.43 (EtOAc/Petroleum ether 40-60 °C, 4/1, v/v). ESI-MS: Cald. (C₁₀H₂₀NO₃+Na⁺) 225.13; found 225.27. IR ν_{max}/cm⁻¹: 1043, 1091, 1172, 1242, 1313, 1348, 2920, 3377, 3487. Elemental Analysis: C, 59.38; H, 9.97; N, 6.92; O, 23.73; Found: C, 60.56; H, 10.13; N, 6.65; O, 22.66%.

7, 7, 9, 9-tetramethyl-1, 3-dioxa-8-azaspiro [4.5] decan-2-one-8-oxyl (f). Nitroxide radical (**e**) 0.95 g (4.7 x 10⁻³ mol) was dissolved in 1.5 mL MDF in a 20 mL vial with magnetic stirrer. Then dimethyl carbonate 0.6 mL (7.12 x 10⁻³ mol) was added to the mixture followed with K₂CO₃ 16 mg (1.16 x 10⁻⁴ mol). The reaction was left at 80 °C overnight. After cooling down to room temperature, resulting mixture was diluted with 20 mL Milli-Q water and extracted with diethyl ether (3 x 30 mL). The organic phase was collected and dried with MgSO₄. The crude product obtained after rotavapor was purified by column chromatography (silica gel) using EtOAc/petroleum ether 40-60 °C (3/1, v/v) as the eluent. Finally, 0.55 g pure red colour product was obtained with a yield of 51.4%. R_f=0.77 (EtOAc/Petroleum ether 40-60 °C, 3/1, v/v). ESI-MS: Cald. (C₁₁H₁₈NO₄+Na⁺) 251.11; found 251.18. IR ν_{max}/cm⁻¹: 1060, 1097, 1164, 1240, 1778, 2972. Elemental Analysis: C, 57.88; H, 7.95; N, 6.14; O, 28.04; Found: C, 58.31; H, 8.01; N, 6.16; O, 27.52%.

Synthesis of functional nitroxide radicals (h-j)

4-azido-2, 2, 6, 6-tetramethylpiperidin-1-oxyl (h). Nitroxide radical (**g**) 2.3 g (7.05 x 10⁻³ mol) was dissolved in 12 mL DMSO, 4.6 g (7.07 x 10⁻² mol) sodium azide was added. The mixture was heated to 50 °C for 72h. The solvent was removed by air flow and the residual was dissolved in water and extracted by diethyl ether. The ether phase was dried and concentrated. The crude product was purified by column chromatography (silica gel) using EtOAc/Petroleum ether 40-60 °C (1/8, v/v) as the eluent, R_f=0.24. Finally, 0.83 g pure red colour product was obtained with a yield of 60%. ESI-

MS: Cald. ($C_9H_{17}N_4O+Na^+$) 220.13, Found 220.24. Elemental Analysis: C, 54.80; H, 8.69; N, 28.40; O, 8.11%; Found: C, 54.23; H, 8.76; N, 28.31; O, 8.7 %.

4-bromo-2, 2, 6, 6-tetramethylpiperidin-1-oxyl (i). 4-hydroxyl-TEMPO (**c**) 1.72 g (1.00×10^{-2} mol) and CBR_4 3.97 g (1.20×10^{-2} mol) was dissolved in 30 mL DCM in a 100 mL round bottom flask equipped with magnetic stirrer. Triphenylphosphine 3.67 g (1.40×10^{-2} mol) was added to the mixture proportionally via spatula during 30 mins. Reaction was left at room temperature for overnight. The resulting mixture was then concentrated and purified by column chromatography (silica gel) using EtOAc/Petroleum ether 40-60 °C (1/3, v/v) as the eluent. Finally, 0.23 g pure red colour product was obtained with a yield of 9.8%. $R_f=0.88$ (EtOAc/Petroleum ether 40-60 °C, 1/1, v/v). ESI-MS: Cald. ($C_9H_{17}BrNO+Na^+$) 257.04, 259.04; Found 257.16, 259.17. IR ν_{max}/cm^{-1} : 638, 735, 1173, 1228, 1338, 1466, 2925. Elemental Analysis: C, 45.97; H, 7.29; N, 5.96; Found: C, 46.66; H, 7.59; N, 5.99%.

4-iodo-2,2,6,6-tetramethylpiperidin-1-oxyl (j) 4-tosylate-TEMPO (**g**) 1.9 g (5.82×10^{-3} mol) and NaI 8.8 g (5.87×10^{-2} mol) was dissolved together in 70 mL acetone with magnetic stirring. The mixture was refluxed at 70 °C overnight. Resulting mixture was concentrated by reduce pressure distillation, which was then diluted with 30 mL water. Diluted solution was then extracted with EtOAc (3 x 50 mL). The extract was dried with $MgSO_4$ and distilled to remove the solvent. The crude product was purified by column chromatography (silica gel) using EtOAc/Petroleum ether 40-60 °C (1/3, v/v) as the eluent. Finally, 0.5 g pure red colour product was provided with a yield 30.5%. $R_f=0.76$ (EtOAc/Petroleum ether 40-60 °C, 1/3, v/v). ESI-MS: Cald. ($C_9H_{17}INO+H^+$) 283.04; found 283.16. IR ν_{max}/cm^{-1} : 717, 1169, 1204, 1464, 1718, 2938, 2974, 2992. Elemental Analysis: C, 38.31; H, 6.07; I, 44.98; N, 4.96; Found: C, 40.00; H, 6.28; N, 5.14 %.

Synthesis of functional nitroxide radicals (n-o)

2, 2, 5, 5-tetramethyl-2,5-dihydro-1H-pyrrole-3-carboxamide-1-oxyl (n) With water cooling and vigorous stirring, triacetoneamine (**1**) 17.6 g (1.14×10^{-1} mol) was dissolved in 70 mL glacial acetic

acid. A solution of bromine 36.0 g (2.25×10^{-1} mol) in 50 mL glacial acetic acid was dropped to the mixture during 30 mins. Then the mixture was left at room temperature stirring for overnight, during which, the colour of the mixture gradually fades and some white precipitate formed (a mixture of 3,3-dibromo-2,2,6,6-tetramethylpiperidin-4-one and 3,5-dibromo-2,2,6,6-tetramethylpiperidin-4-one). Subsequently, the precipitate was filtered; washed with acetic acid, water, and diethyl ether sequentially and successively. After drying under high vacuum, a white powder (**3**) 35.0 g was obtained with a yield of 98.8%. The second step was carried out with dissolving (**3**) 16.0 g (5.15×10^{-2} mol) in 200 mL 28% aqueous ammonia under vigorous stirring. When the solution turns to transparent, potassium hydroxide pellet was added proportionally to saturate the solution and get some white precipitate of the amide. The white precipitate was pressed out on a Buchner funnel and dried under high vacuum. Finally, 2, 2, 5, 5-tetramethyl-2, 5-dihydro-1H-pyrrole-3-carboxamide (**4**) (6.5 g) was obtained with a yield of 75.06 %. $R_f=0.2$ (DCM/MeOH, 9/1, v/v). ESI-MS: Cald. ($C_9H_{16}N_2O+Na^+$) 191.12; found 191.10. 1H NMR (300 MHz, DMSO- d_6) δ : 1.16 (6H, s), 1.27 (6H, s), 1.79 (1H, s), 6.32 (1H, s), 6.80 (1H, s), 7.33 (1H, s); ^{13}C NMR (300 MHz, DMSO- d_6) δ : 30.83, 30.88, 63.14, 66.40, 142.04, 142.06 and 166.63.

Oxidation of **4** to give nitrxide radical **n** was carried out in similar procedure as synthesis of **a**. Briefly, 2,2,5,5-tetramethyl-2,5-dihydro-1H-pyrrole-3-carboxamide (**4**) 5 g (2.97×10^{-2} mol) was dissolved in 100 mL water, together with sodium tungstate dihydrate 0.1 g (3.03×10^{-4} mol) and EDTA 0.1 g (3.42×10^{-4} mol). With ice-water cooling, H_2O_2 (30%) 5 ml was dropped to the mixture during five mins. The reaction was left at dark for overnight at room temperature. The yellow solid was filtered and washed with 30 mL Milli-Q water. The rest filtrate was extracted with EtOAc (3 x 100 mL). The organic phase was collected and dried with $MgSO_4$. After evaporation and drying under high vac, total 2.3 g yellow product was obtained with yield 42.3%. $R_f=0.45$ (DCM/MeOH, 9/1, v/v). ESI-MS: Cald. ($C_9H_{15}N_2O_2+Na^+$) 206.10; found 206.18. IR ν_{max}/cm^{-1} : 1363, 1417, 1614, 1643, 1683, 2976,

3172, 3371. Elemental Analysis: C, 59.00; H, 8.25; N, 15.29; O, 17.46; Found: C, 58.50; H, 8.21; N, 14.69; O, 18.60%.

2, 2, 5, 5-tetramethyl-2, 5-dihydro-1H-pyrrole-3-carboxylic-1-oxyl (o) 2, 2, 5, 5-tetramethyl-2, 5-dihydro-1H-pyrrole-3-carboxamide-1-oxyl (**n**) 2 g (1.09×10^{-2} mol) was charged to a 100 mL round bottom flask with 15% (w/w) aqueous NaOH solution 50 mL. The mixture was heated to 95 °C for overnight to get a transparent yellow liquid. Then with ice cooling, resulting mixture was acidified with HCl (36% aqueous solution) until pH=4 and extracted with EtOAc (4 x 100 mL). The organic phase was collected and dried with MgSO₄. After evaporation and drying under high vac, total 1.9 g yellow product was obtained with yield 94.5%. $R_f=0.37$ (DCM/MeOH, 9/1, v/v). ESI-MS: Cald. (C₉H₁₄NO₃+Na⁺) 207.09; found 207.25. IR $\nu_{\max}/\text{cm}^{-1}$: 1630, 1709, 2983, 3093, 3203. Elemental Analysis: C, 58.68; H, 7.66; N, 7.60; O, 26.05; Found: C, 58.36; H, 8.16; N, 7.56; O, 25.91%.

Synthesis of hetero-atom nitroxide radicals (p-r)

4-oxyl-3, 3, 5, 5-tetramethylmorpholin-2-one (p) With magnetic stirring, 2-amino-2-methyl-1-propanol 8.92 g (1.0×10^{-1} mol), CHCl₃ 12.50 mL (1.50×10^{-1} mol) and acetone 75 mL (1.02 mol) were added to a 500 mL three-necked round bottom flask. Under the Ar atmosphere, sodium hydroxide powder 20 g (5.00×10^{-1} mol) was added to the mixture proportionally with the temperature controlled below 5 °C. Resulting mixture was left at room temperature for overnight. The obtained slurry was then filtered on a frit and washed with acetone 100 mL and methanol 200 mL respectively. The filtrates were combined and concentrated under reduce pressure distillation. After further dried under high vacuum an amorphous white crude solid was obtained, to which a concentrated solution of hydrogen chloric acid 120 mL was added. The solution was refluxed at 105 °C for 6h, resulting dark yellow solution was cooled in ice-water bath and neutralised with sodium bicarbonate. The aqueous solution was subsequently extracted by DCM (3 x 200 mL). The DCM phase was collected and dried over MgSO₄ and filtered. Filtrate was concentrated to give a yellow oil crude product, which was purified by distillation under high vacuum. The purified product 3, 3, 5, 5-

tetramethylmorpholin-2-one (**8**) was a colourless transparent liquid (11.31 g, yield: 71.9%). $R_f=0.62$ (DCM/MeOH, 9/1, v/v). ESI-MS: Cald. ($C_8H_{15}NO_2+H^+$) 158.12; found 157.99. 1H NMR (400 MHz, DMSO- d_6) δ : 1.07 (6H, s) , 1.29 (6H, s), 4.15 (2H, s); ^{13}C NMR (100 MHz,) δ : 26.0, 30.7, 48.8, 54.4, 78.0, and 175.3.

To a 250 mL round bottom flask equipped with a magnetic stirrer, 3, 3, 5, 5-tetramethylmorpholin-2-one (**8**) 6.00 g (3.82×10^{-2} mol) was dissolved in 60 mL DCM. Simultaneously, mCPBA 13.12 g (7.60×10^{-2} mol) was dissolved in another vial with 60 mL DCM. With the temperature controlled under 0 °C in an ice-salt bath, mCPBA solution was added to the reactant via a pressure equalising dropping funnel during 1 h. Reaction was kept at 0 °C for 5h and subsequently at room temperature overnight. Resulting mixture was then cooled down again in ice-salt bath, the precipitated salt was filtered out and filtrate was washed with K_2CO_3/Na_2SO_3 solution 100 mL. After drying with $MgSO_4$, DCM was removed to give a yellow liquid, which was further purified by column chromatography (silica gel) using DCM/MeOH mixture (DCM/MeOH, 95/5, v/v) as the eluent. The orange colour product fraction was collected, concentrated and dried under high vacuum to give a bright orange solid (**p**) 5.50 g with yield of 83.7%. $R_f=0.68$ (EtOAc/Petroleum ether 40-60 °C, 1/1, v/v). ESI-MS: Cald. ($C_8H_{14}NO_3+Na^+$) 195.09; found 195.08. IR ν_{max}/cm^{-1} : 1363, 1419, 1643, 1685, 2977, 3172, 3367. Elemental Analysis: C, 55.80; H, 8.19; N, 8.13; O, 27.87; Found: C, 55.96; H, 8.22; N, 8.07; O, 27.75%.

3, 3, 5, 5-tetramethylmorpholine-2-ol-4-oxyl (q) 2, 2, 4, 4-tetramethyl-1, 3-oxazinan-6-one-3-oxyl (**p**) 0.10 g (5.81×10^{-4} mol) and LiCl 0.01 g (2.36×10^{-4} mol) dissolved in $H_2O/MeOH$ (5/1, v/v) mixture 6 mL under magnetic stirring. Then $NaBH_4$ 0.07 g (1.85×10^{-3} mol) was added to the mixture proportionally. Bubbles formed and the colour of the mixture changed to dark red immediately with addition of $NaBH_4$. Reaction was left at room temperature for 30 mins. Resulting solution was diluted with 20 mL Milli-Q water and extracted with EtOAc (3 x 20 mL). The organic phase was collected and dried over $MgSO_4$, filtered. The filtrate was concentrated and dried under high vacuum, a pure

orange colour solid (**q**) 0.07 g was obtained with a yield of 69.3%. $R_f=0.5$ (EtOAc/Petroleum ether 40-60 °C, 3/1, v/v). ESI-MS: Cald. ($C_8H_{16}NO_3+Na^+$) 197.10; found 197.13. IR ν_{max}/cm^{-1} : 678, 1041, 1627, 1708, 2983, 3095. Elemental Analysis: C, 55.15; H, 9.26; N, 8.04; O, 27.55; Found: C, 53.85; H, 9.21; N, 7.80; O, 29.14 %.

3, 3, 5, 5-tetramethylmorpholine-4-oxyl (r) With ice-water cooling, lithium aluminium hydride 0.97g (2.56×10^{-2} mol) was suspended in dry diethyl ether 60 mL in a round bottom flask equipped with magnetic stirrer within argon atmosphere. Then 3, 3, 5, 5-tetramethylmorpholin-2-one (**8**) 2.0 g (1.27×10^{-2} mol) was slowly added to the suspension via syringe. After ten minutes, the ice-water bath was removed and the reaction was left at room temperature for another 20 mins. Subsequently, refluxed at 60 °C for 3h. After cooling down to room temperature, 1 mL H_2O , 1 mL 15% NaOH solution and 3 mL H_2O was added sequentially to quench the reaction. The white salt formed was filtered to provide transparent filtrate, which was concentrated to afford a white solid product (**9**) 1.35 g with yield of 66.0%. The product was used for next step without further purification. ESI-MS: Cald. ($C_8H_{19}NO_2+H^+$) 162.15; Found 162.18. 1H NMR (400 MHz, $CDCl_3$) δ : 1.15 (12H, s), 3.27 (4H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 27.0, 54.8, and 71.2.

Product (**9**) 0.2 g (1.24×10^{-3} mol) was added to a 50 mL round bottom flask fitted with a reflux condenser. Then H_2SO_4 (98 %) 3 mL was added. The reaction mixture was heated to 140 °C for overnight to provide a black liquid. The resulting mixture was then poured to 20 mL ice in a 250 mL beaker and basified with 50% aqueous KOH. Subsequently, the mixture was extracted with diethyl ether (4 x 50 mL). The organic phase was collected, dried with $MgSO_4$, and concentrated to give a pale yellow liquid 3,3,5,5-tetramethylmorpholine (**10**) 0.12 with a yield of 67.8%. $R_f=0.65$ (DCM/MeOH, 9/1, v/v). ESI-MS: Cald. ($C_8H_{17}NO+H^+$) 144.14; found 144.02. 1H NMR (400 MHz, $CDCl_3$) δ : 1.13 (12H, s), 3.31 (4H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 28.2, 48.7, and 77.6.

To a 20 mL vial equipped with a magnetic stirrer, 3,3,5,5-tetramethylmorpholine (**10**) 0.12 g (8.39×10^{-4} mol), sodium tungstate dihydrate 0.028 g (8.49×10^{-5} mol) and EDTA 0.002 g (6.84×10^{-6} mol)

were dissolved in water/methanol mixture (1/2, v/v) 3 mL. Then hydrogen peroxide (30% wt %) 150 μ L was dropped to the mixture via a pipette. Reaction was left at room temperature for overnight. Resulting mixture was then diluted with 3 mL H₂O and extracted with diethyl ether (3 x 10 mL), organic phase was collected and dried over MgSO₄, the solvent of which was subsequently removed under reduce pressure distillation. The crude product obtained was then purified by column chromatography (silica gel) using DCM/MeOH mixture (9/1, v/v) as the eluent. The yellow product fraction with R_f=0.71 was collected, concentrated. A red liquid product (**r**) 84 mg was obtained with a yield of 63.6%. ESI-MS: Cald. (C₈H₁₆NO₂+Na⁺) 181.11; Found 180.99.

Synthesis of hetero-atom nitroxide radicals (**s-t**)

2, 2, 7, 7-tetramethyl-1, 4-diazepan-5-one (5) First, triacetoneamine (**1**) 3.1 g (2.0 x 10⁻² mol) was dissolved in 50 mL hydrochloride acid (36 %) with magnetic stirrer. Sodium azide 1.64 g (2.52 x 10⁻² mol) was added in small proportions during 20 mins, while keeping temperature below 35 °C. The mixture was left stirring at the room temperature overnight. The resulting solution was concentrated under airflow, and neutralised with saturated sodium carbonate solution in an ice-water bath, which was then further saturated with sodium hydroxide. The resulting basified solution was then extracted by EtOAc (3 x 100 mL). The organic phase was collected and dried over MgSO₄, filtered. Filtrate was concentrated to give 1.8 g of pale yellow solid crude product with yield 52.9%. R_f=0.35 (DCM/MeOH, 9/1, v/v). ESI-MS: Cald. (C₉H₁₈N₂O+H⁺) 171.15; found 171.31. ¹H NMR (300 MHz, DMSO-*d*₆) δ : 1.02 (6H, s) , 1.09 (6H, s), 1.62 (1H, s), 2.39 (2H, s), 2.96 (2H, d, *J*=6 Hz), 7.52 (1H, s); ¹³C NMR (75 MHz, DMSO-*d*₆) δ : 29.0, 31.8, 50.3, 50.5, 52.7, 52.8, and 174.6.

2, 2, 7, 7-tetramethyl-5-homopiperazinone-1-oxyl (s) To a 250 mL round bottom flask equipped with a magnetic stir bar, 2,2,7,7-tetramethyl-1,4-diazepan-5-one (**5**) 2.5 g (1.47 x 10⁻² mol), Sodium tungstate 0.66 g (2.0 x 10⁻³ mol) and EDTA 0.04 g (1.37 x 10⁻⁴ mol) were dissolved in 20 mL water. Then hydrogen peroxide (30% wt %) 8 mL (5.40 x 10⁻² mol) was added dropwise to the mixture via a pressure equalising dropping funnel. The resulting mixture turns to red gradually. After overnight

reaction, the mixture was extracted with EtOAc (3 x 50 mL). Organic phase was collected, dried over MgSO₄ and filtered. Filtrate was concentrated and the crude product obtained was purified by column chromatography (silica gel) using DCM/MeOH mixture (9/1, v/v) as the eluent. The red product fraction at an R_f=0.55 was collected, concentrated and dried under vacuum. A red solid 1.65 g was obtained with a yield of 60.7%. ESI-MS: Cald. (C₉H₁₇N₂O₂+Na⁺) 208.12; found 208.19. IR ν_{max}/cm⁻¹: 1180, 1220, 1290, 1690, 2970, 3320. Elementary Analysis: C, 58.35; H, 9.25; N, 15.12; O, 17.27; Found: C, 58.17; H, 9.23; N, 14.98; O, 17.62 %.

3, 3, 5, 5-tetramethyl-1-tosyl-1,4-diazepane (7) With magnetic stirring, LiAlH₄ 0.50 g (1.32 x 10⁻² mol) was dispersed in 25 mL dry diethyl ether in a 50 mL round bottom flask in an ice-water bath. Then 2, 2, 7, 7-tetramethyl-1, 4-diazepan-5-one (**5**) 1.00 g (5.88 x 10⁻³ mol) was added to the mixture proportionally. Then the reaction was stirred for 10 mins at 0 °C, followed by refluxing at 60 °C for 3 h. The mixture was cooled down and then sequentially quenched by 0.5 mL water, 0.5 mL 15% aqueous NaOH and 1.5 mL water. The white precipitate was filtered and filtrate was dried over MgSO₄. The filtrate was concentrated to give a yellow oil (**6**). The intermediate (**6**) was dissolved in 30 mL DCM in a round bottom flask with magnetic stirring in an ice-water bath. Triethylamine 1 mL (7.17 x 10⁻³ mol) was added to the solution via syringe. After that, *para*-toluenesulfonyl chloride 1.12 g (5.87 x 10⁻³ mol) was added to mixture proportionally. The reaction was left to gradually warm to room temperature and stirring overnight to give a turbidity mixture before being quenched with 20 mL saturate K₂CO₃ solution. The DCM phase was collected, dried over MgSO₄, and filtered. The filtrate was concentrated and dried under high vacuum to give a yellow oil. Crude product was purified via column chromatography (silica gel) using DCM/MeOH mixture (9/1, v/v) as the eluent. The product fraction with an R_f of 0.56 was collected, concentrated and dried under vacuum to give compound (**7**) as a pale yellow solid 0.62g with a total yield of 34.0%. ESI-MS: Cald. (C₁₆H₂₆N₂O₂S+H⁺) 311.18; found 311.20. ¹H NMR (400 MHz, CDCl₃) δ: 1.15 (6H, s), 1.21 (6H, s), 1.80 (2H, t, J=5.88 Hz), 2.41 (3H, s), 3.11 (2H, s), 3.19 (2H, t, J=5.86 Hz), 7.29 (2H, d, J=8.28

Hz), 7.64 (2H, d, $J=8.46$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ :21.5, 29.4, 31.4, 41.7, 45.6, 53.6, 55.1, 59.2, 127.2, 129.7, 135.5, 143.2.

2, 2, 7, 7-tetramethyl-4-tosyl-1,4-diazepan-1-oxyl (t) To a 50 mL round bottom flask equipped with a magnetic stirrer, 3,3,5,5-tetramethyl-1,4-diazepan-1-yl 4-methylbenzenesulfonate (**7**) 0.20 g (6.43×10^{-4} mol), sodium tungstate 0.02 g (6.06×10^{-5} mol) were dissolved in water/methanol mixture (1/1, v/v) 10 mL. Then hydrogen peroxide (30% wt %) 0.50 mL (3.37×10^{-3} mol) was added dropwise to the mixture. The reaction mixture turned to yellow gradually overnight. The mixture was then diluted with 20 mL water and extracted with EtOAc (3 x 20 mL), organic phase was collected and dried over MgSO_4 . After filtration, the filtrate was concentrated to give crude product, which was then purified by column chromatography (silica gel) using EtOAc/ Petroleum ether 40-60 °C mixture (1/1, v/v) as the eluent. The red product fraction at an $R_f=0.74$ was collected, concentrated and dried under vacuum. A red solid (0.14 g) was obtained with a yield of 67.0%. ESI-MS: Cald. ($\text{C}_{16}\text{H}_{25}\text{N}_2\text{O}_3\text{S}+\text{Na}^+$) 348.15; Found 348.11. IR $\nu_{\text{max}}/\text{cm}^{-1}$: 579, 660, 746, 815, 860, 1157, 1334, 2977. Elemental Analysis: C, 59.05; H, 7.74; N, 8.61; Found: C, 59.44; H, 7.82; N, 8.45.

NMR Spectra

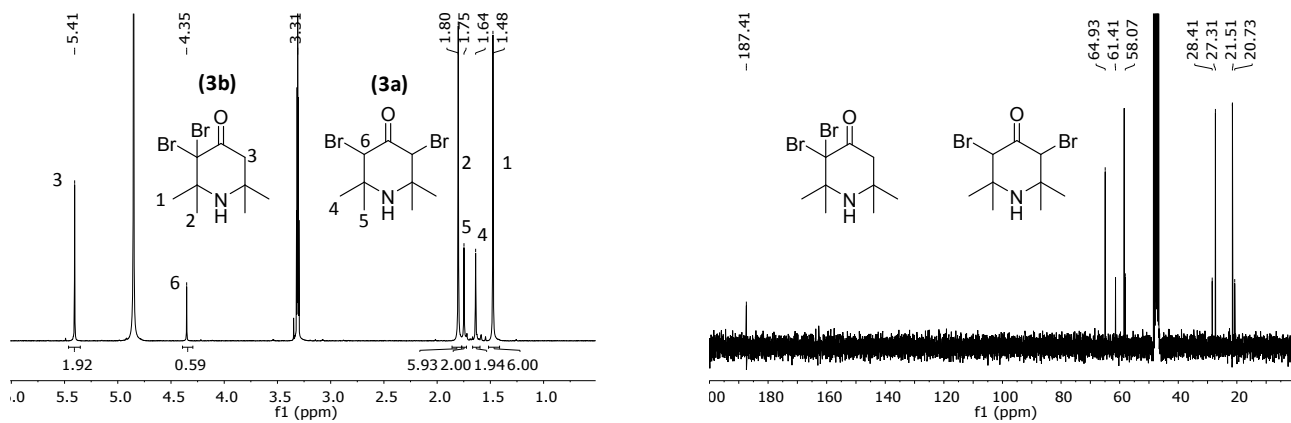


Figure S1. (A) ^1H NMR and (B) ^{13}C NMR of compound **3** in $\text{MeOD-}d_4$.

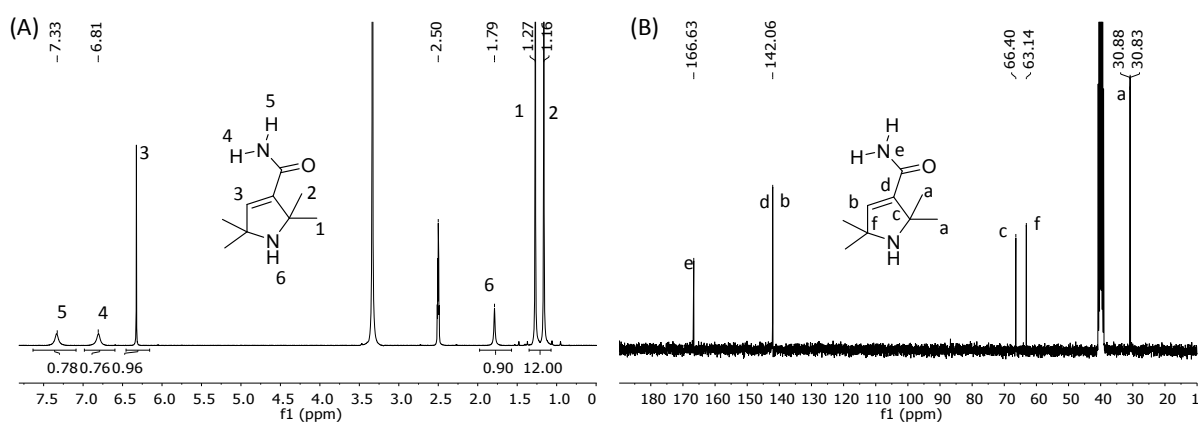


Figure S2. (A) ^1H NMR and (B) ^{13}C NMR of compound **4** in $\text{DMSO-}d_6$.

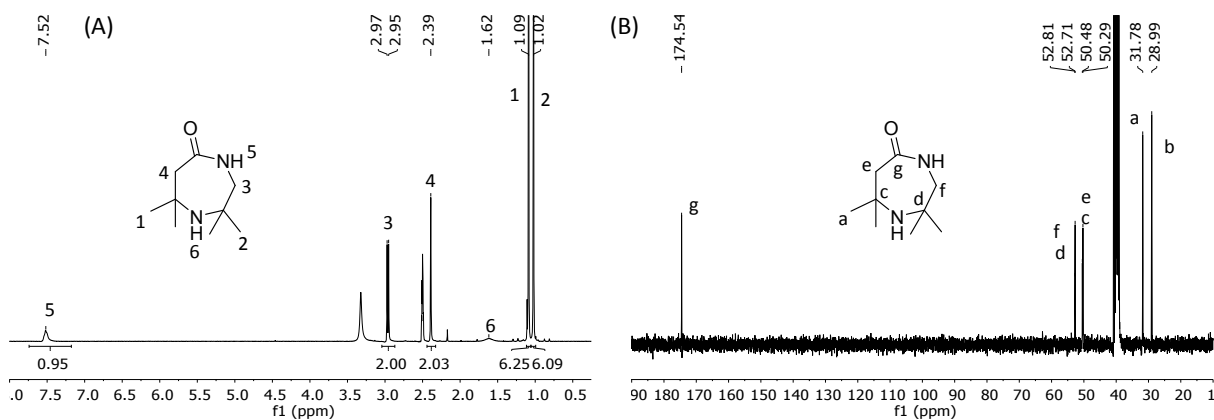


Figure S3. (A) ^1H NMR and (B) ^{13}C NMR of compound **5** in $\text{DMSO-}d_6$.

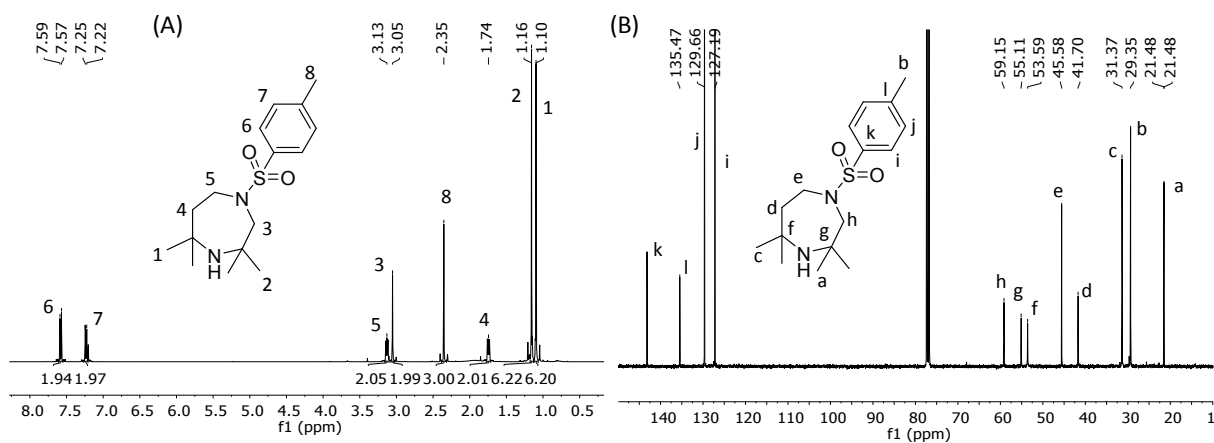


Figure S4. (A) ^1H NMR and (B) ^{13}C NMR of compound **7** in CDCl_3 .

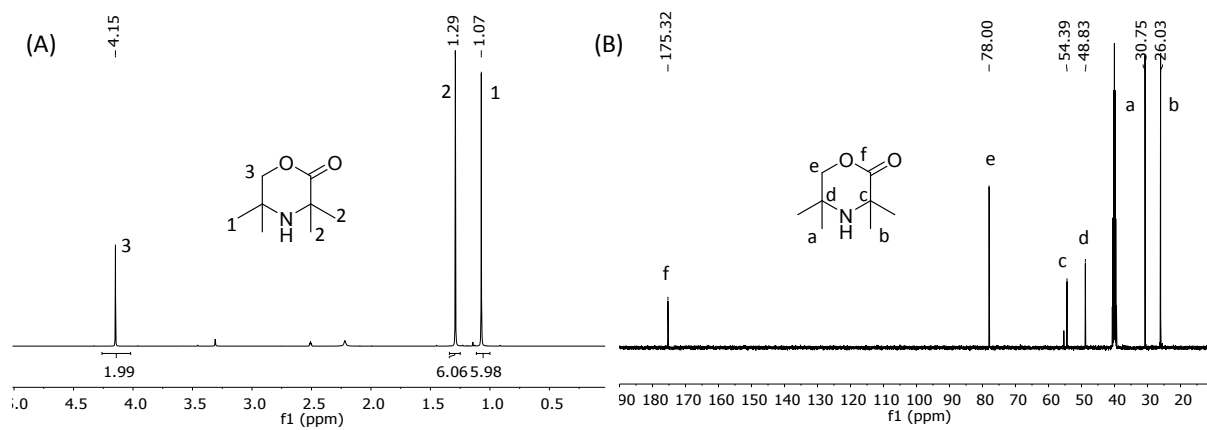


Figure S5. (A) ^1H NMR and (B) ^{13}C NMR of compound **8** in $\text{DMSO-}d_6$.

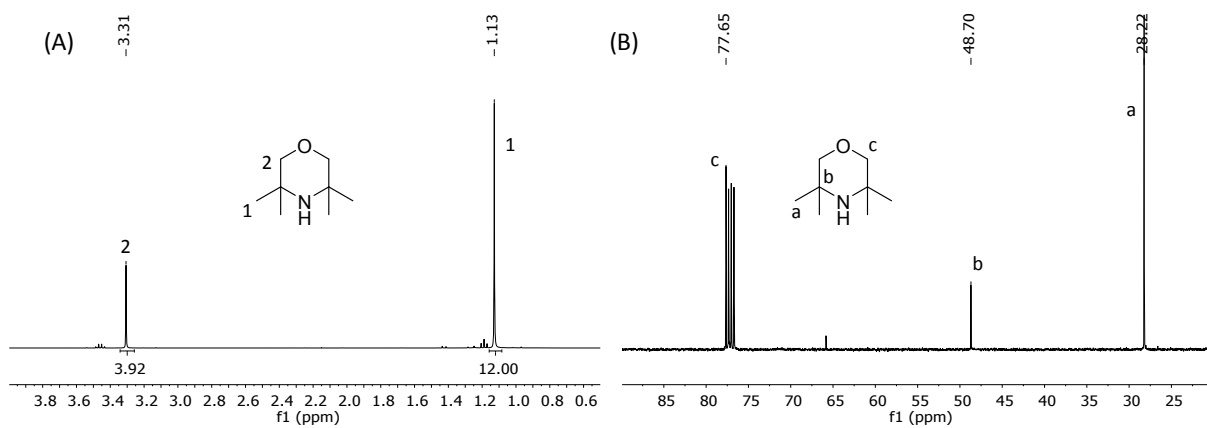


Figure S6. (A) ^1H NMR and (B) ^{13}C NMR of compound **10** in CDCl_3 .

Theoretical Methodology

Standard *ab initio* molecular orbital theory and density functional theory (DFT) calculations were carried out using Gaussian 09³ with the exception of URCCSD(T) calculations, which were performed using Molpro 2015.^{4, 5} Calculations on radicals were performed with an unrestricted wavefunction. Calculations were performed at a high-level of theory, with very similar theory shown to predict accurate values for the oxidation potential of a range of nitroxides.⁶ Geometries of all species were optimised at the M06-2X^{S7} level of theory using the 6-31+G(d,p)⁸⁻¹² basis set and frequencies, entropies and thermal corrections were also calculated at this level of theory. All geometries were verified as local minima (possessing no imaginary frequencies). Improved single-point energies were calculated using the high-level composite *ab initio* G3(MP2,CC)(+) method, a variation of standard G3(MP2,CC)¹³ where calculations with the 6-31G(d) basis set are replaced with 6-31+G(d).

Although the more modern family of G4 methods^{14, 15} include an extra basis set correction at the HF level (and utilise basis sets with additional polarisation functions), we used the older G3 variant because of previously noted concerns^{16, 17} with the (non-cancelling) higher-level correction (HLC) of standard G4 theory. In G3 theory, the HLC term is generally small and only makes a minor contribution to absolute oxidation potentials. Moreover, this contribution is constant for all the oxidation reactions that we considered in this work. Thus, the G3 HLC fully cancels when calculating relative oxidation potentials and so G3(MP2,CC)(+) can be considered fully *ab initio* once applied to these reaction energies. In contrast, the HLC of standard G4 theory does not cancel for any radical reaction and has the potential (due to its mathematical formulation) to grow rapidly with system size.^{16, 17} Some of the more recently developed G4 variants¹⁸ do address this HLC ‘explosion’ problem, albeit through the introduction of several empirically fitted (energy component based) scaling

parameters. However, we should note that the performance of G3(MP2,CC)(+) has already been verified in previous studies of nitroxide oxidation potentials.^{6, 19}

High-level calculations were utilized in conjunction with the ONIOM approximation^{20, 21} for larger systems, with UMP2 used to model remote substituents effects. Solvation corrections were calculated using the polarisable continuum model (PCM)²² (as implemented in Gaussian 09) at UB3LYP/6-31G(p) with $\alpha = 1.45$.³ For consistency with experiment acetonitrile was used as the solvent. For all species in this study full systematic conformational searches (at a resolution of 120°) were performed to ensure global, and not merely local minima were located. In addition, we performed a thorough search of chair (with substituents axial and equatorial) and twist boat conformations. Lowest energy conformations were generally selected on the basis of their G3MP2-CC(+) solution-phase free-energies, although if several conformations were close in energy ($< 5 \text{ kJ mol}^{-1}$, of the global minimum oxoammonium cation or nitroxide radical) then Boltzmann averaging of these conformations (and the respective oxidation potentials and dipole/quadrupole terms) were performed. Relative oxidation potentials were calculated taking TEMPO as a reference. Theory was compared directly with experiment and the mean absolute deviation was 33 mV and maximum deviation 64 mV (Figure S7).

Dipole and quadrupole moments were calculated on the model species (see Figure S11) using M06-2X/6-31+G(d,p), preserving the substituent conformation of the nitroxide/oxoammonium analogue. If several nitroxide/oxoammonium conformations were close in energy (within 5 kJ/mol of the global minimum), the dipole and quadrupole parameters for the corresponding substituent conformations were weighted according to a Boltzmann distribution (using the nitroxide and oxoammonium conformational energies). Natural charges were calculated in Gaussian software via its built-in Natural Bond Orbital population analysis²³ at the M06-2X/6-31+G(d,p) level. If several nitroxide conformations were close in energy

(within 5 kJ/mol of the global minimum), the natural charges were weighted according to a Boltzmann distribution (using the nitroxide conformational energies).

Table S1. Comparison between oxidation potentials measured in this work and those in previous studies.

Nitroxide	E_{ox} (mV vs. Fc/Fc ⁺)		Reference
	This study	Previous work	
TEMPO	234	226, 238, 239	24, 25, 26
Nitroxide a	410	428	25
Nitroxide b	284	296	25
Nitroxide m	315	300	24
Nitroxide p	636	691	26

Table S2. Oxidation potentials for previously studied nitroxides converted to Fc/Fc⁺. Chemical structures of these nitroxides are given in Figure S10.

Nitroxide	E_{ox} (mV vs. Fc/Fc ⁺)	Reference
Nitroxide 1	352	24
Nitroxide 3a	386	24
Nitroxide 3b	472	24
Nitroxide 3c	551	24
Nitroxide 4a	421	24
Nitroxide 4b	471	24
Nitroxide 4c	499	24
Nitroxide 4d	399	24
Nitroxide 4e	406	24
Nitroxide 4f	383	24
Nitroxide 4g	475	24
Nitroxide 4h	506	24
Nitroxide 4j	524	24
Nitroxide 4k	336	24
Nitroxide 7	443	24
Nitroxide 8	340	25
Nitroxide 9	299	25
Nitroxide 10	276	26

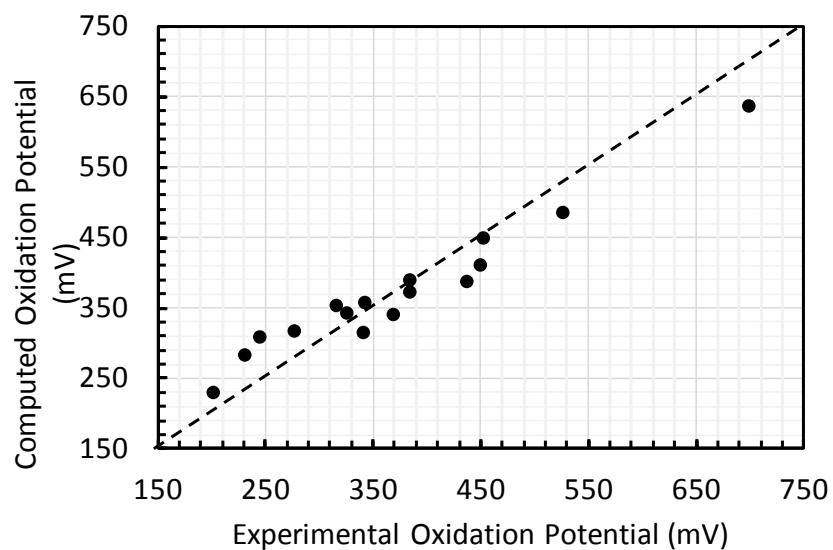


Figure S7. Comparison of computed and experimental oxidation potentials.

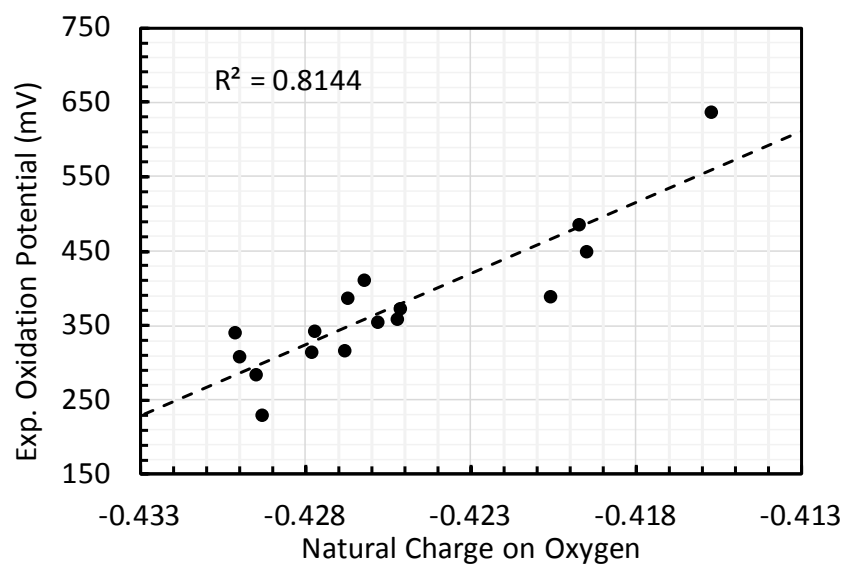


Figure S8. The correlation between the natural charge on oxygen of nitroxide radicals and their experimental oxidation potentials (vs Fc/Fc⁺).

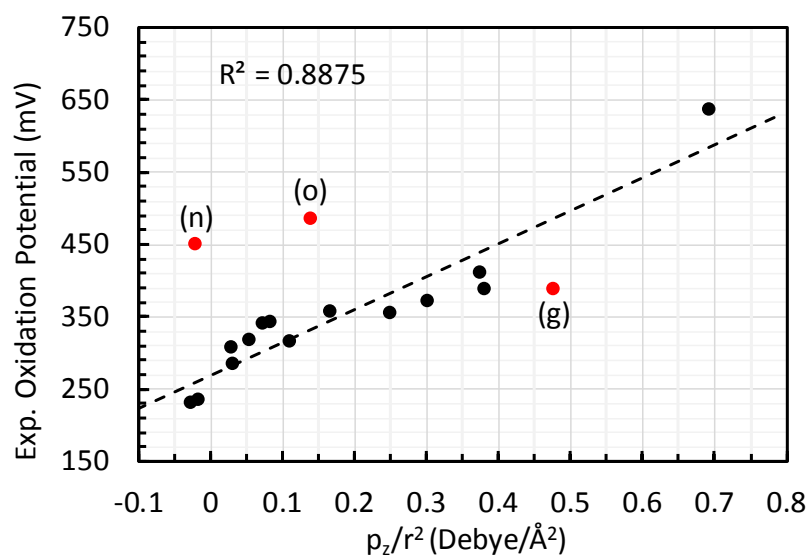


Figure S9. The correlation between the distance-scaled substituent dipole moment of the substituent and the experimentally determined oxidation potential of the nitroxide radicals (vs Fc/Fc⁺).

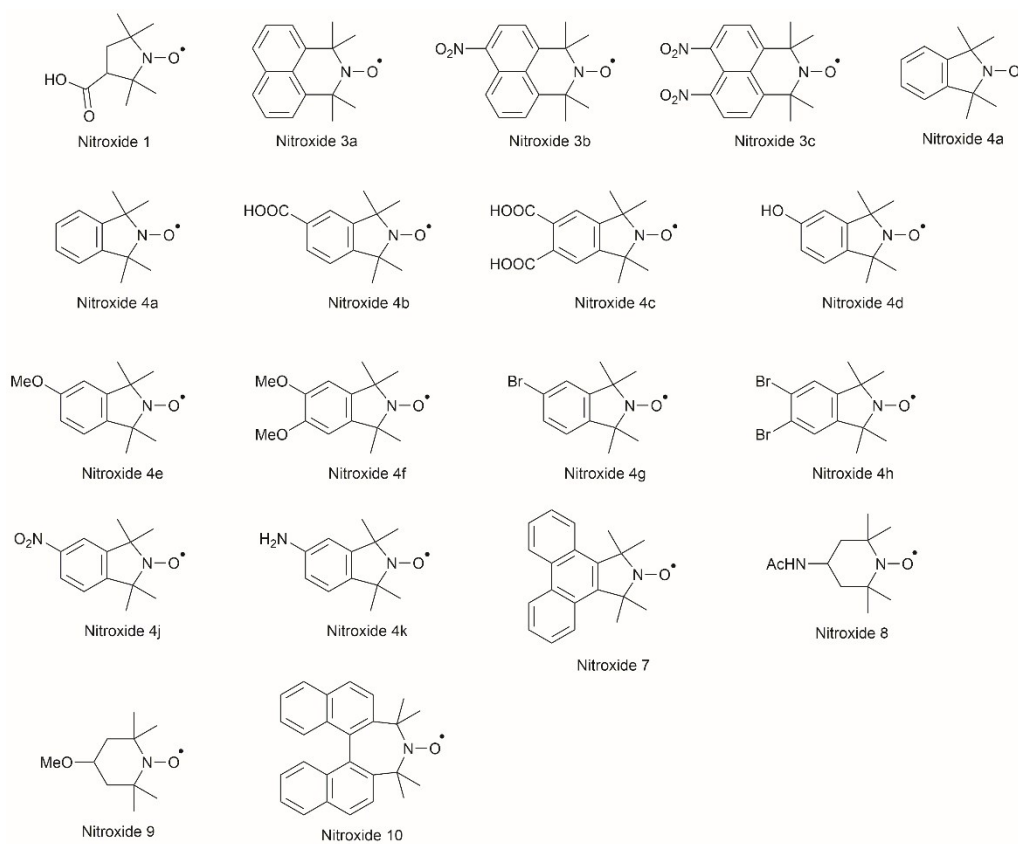


Figure S10. The chemical structures and abbreviations for the additional nitroxides, taken from previous work.

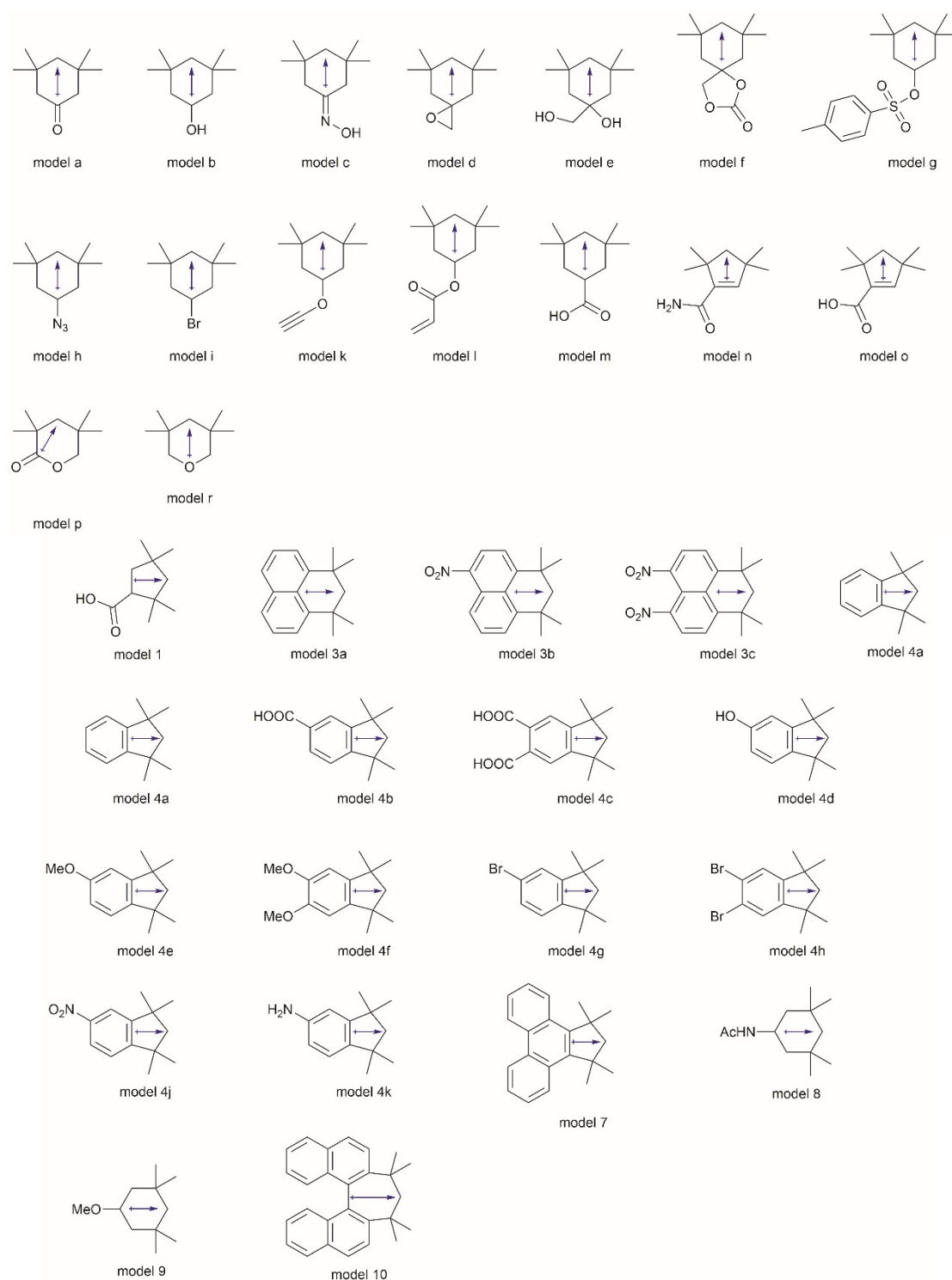


Figure S11. The model species used for the dipole and quadrupole analysis.

Note: The blue arrow depicts the defined z-axis. For all 6-membered species, the origin was defined by the atom in the 3-positions (except for model p, for which a larger dipole interaction with the carbonyl C atom in the 2 position would be anticipated). For 5- and 7-membered species, the origin was defined as the midpoint between the atoms in the 3- and 4- positions and 4- and 5- positions, respectively. The z axis was then defined from this origin to the opposite C atom (flanked by the tetra methyl groups).

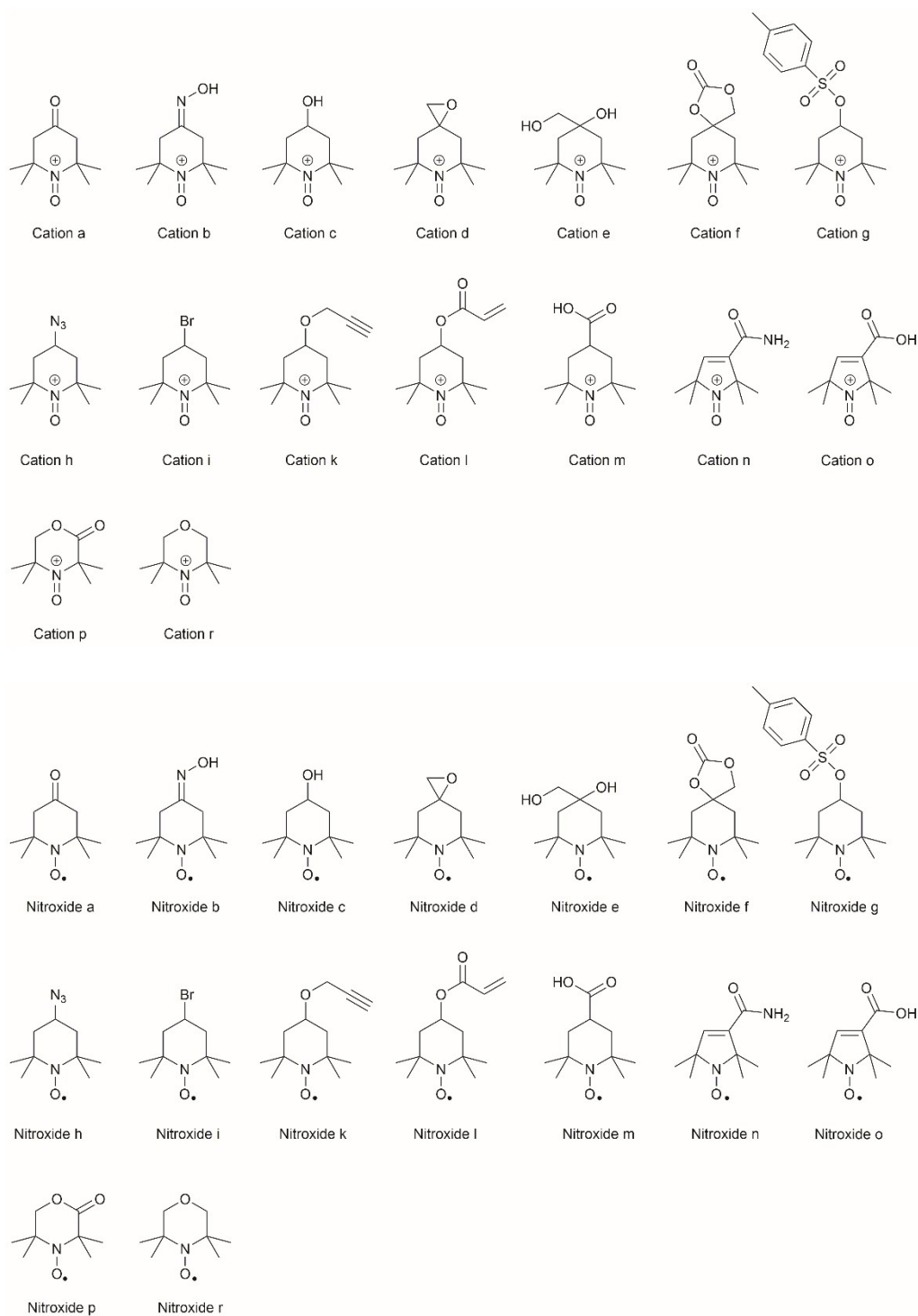


Figure S12. The chemical structures and abbreviations for nitroxides and cations studied in this work.

Supporting computational data

Table S3. Conformational Populations of the Radicals and Cations for Nitroxides a - r

Species	Relative free-energy (kJ mol ⁻¹)	Relative Number of Degenerate Conformations	Relative Mole Fraction	Dipole (D)	Quadrupole (DÅ)	r	Natural Charge on Nitroxide O
Cation TEMPO	-	-	1.000	-0.1401	-0.0100	2.924	-
Radical TEMPO	-	-	1.000	-0.1401	-0.0100	2.924	-0.4331
Cation a.1	7.89	1	0.040	2.9928	-1.5329	2.863	-
Cation a.2	0.0	1	0.960	3.3714	-2.5577	2.993	-
Radical a.1	1.93	1	0.315	2.9928	-1.5329	2.863	-0.4201
Radical a.2	0.0	1	0.685	3.3714	-2.5577	2.993	-0.4290
Cation b.1	6.56	1	0.030	1.7581	-3.0668	2.928	-
Cation b.2	4.78	2	0.123	0.7033	0.6688	2.924	-
Cation b.3	0.00	2	0.847	-0.4893	0.6158	2.949	-
Radical b.1	0.38	1	0.255	1.7581	-3.0668	2.928	-0.4285
Radical b.2	0.00	2	0.594	0.7033	0.6688	2.924	-0.4298
Radical b.3	3.39	2	0.151	-0.4893	0.6158	2.949	-0.4303
Cation c.1	3.19	1	0.216	-0.1073	-0.0997	2.902	-
Cation c.2	0.0	1	0.784	0.9522	3.7357	2.956	-
Radical c.1	1.16	1	0.385	-0.1073	-0.0997	2.902	-0.4255
Radical c.2	0.0	1	0.615	0.9522	3.7357	2.956	-0.4330
Cation d.1	7.99	1	0.038	1.8062	-2.1486	2.883	-
Cation d.2	0.0	1	0.962	0.0869	2.1414	2.884	-
Radical d.1	1.28	1	0.374	1.8062	-2.1486	2.883	-0.4266
Radical d.2	0.0	1	0.626	0.0869	2.1414	2.884	-0.4269
Cation e.1	0.00	1	0.386	-1.6438	5.2222	2.957	-
Cation e.2	0.00	1	0.386	0.4918	-3.4874	2.960	-
Cation e.3	1.31	1	0.228	1.1616	-2.2300	2.961	-
Radical e.1	0.00	1	0.441	-1.6438	5.2222	2.957	-0.4311
Radical e.2	0.51	1	0.359	0.4918	-3.4874	2.960	-0.4289
Radical e.3	1.97	1	0.199	1.1616	-2.2300	2.961	-0.4282
Cation f	-	-	1.000	3.2880	-2.1385	2.943	-

Radical f	-	-	1.000	3.2880	-2.1385	2.943	-0.4206
Cation g.1	0.00	2	0.927	4.1948	-17.4025	2.897	-
Cation g.2	4.60	1	0.073	-0.0932	9.9204	2.899	-
Radical g.1	0.00	2	0.988	4.1948	-17.4025	2.897	-0.4268
Radical g.2	9.17	1	0.012	-0.0932	9.9204	2.899	-0.4261
Cation h.1	0.66	2	0.372	2.5498	-2.2085	2.917	-
Cation h.2	4.68	1	0.037	2.4374	0.2885	2.920	-
Cation h.3	0.00	2	0.485	1.1146	1.4126	2.952	-
Cation h.4	3.76	2	0.106	1.9470	-0.9430	3.023	-
Radical h.1	0.00	2	0.799	2.5498	-2.2085	2.917	-0.4259
Radical h.2	2.14	1	0.168	2.4374	0.2885	2.920	-0.4248
Radical h.3	8.42	2	0.027	1.1146	1.4126	2.952	-0.4266
Radical h.4	12.23	2	0.006	1.9470	-0.9430	3.023	-0.4315
Cation i	-	-	1.000	2.5359	-1.0463	2.901	-
Nitroxide i	-	-	1.000	2.5359	-1.0463	2.901	-0.4251
Cation k.1	0.00	1	0.572	-0.2435	-0.1484	2.948	-
Cation k.2	6.50	1	0.042	0.6030	-0.0648	2.924	-
Cation k.3	4.23	1	0.104	0.5988	-0.5868	2.920	-
Cation k.4	2.77	1	0.187	0.0595	1.5051	3.026	-
Cation k.5	4.42	1	0.096	0.1881	1.5005	3.027	-
Nitroxide k.1	5.32	1	0.087	-0.2435	-0.1484	2.948	-0.4298
Nitroxide k.2	4.27	1	0.133	0.6030	-0.0648	2.924	-0.4297
Nitroxide k.3	0.00	1	0.746	0.5988	-0.5868	2.920	-0.4298
Nitroxide k.4	10.90	1	0.009	0.0595	1.5051	3.026	-0.4354
Nitroxide k.5	8.45	1	0.025	0.1881	1.5005	3.027	-0.4346
Cation l.1	0.36	1	0.268	0.4358	6.5036	2.905	-
Cation l.2	2.37	1	0.119	0.7817	4.2685	2.905	-
Cation l.3	0.00	1	0.309	0.9904	-3.3120	2.944	-
Cation l.4	2.45	1	0.115	1.5286	-4.7545	2.946	-
Cation l.5	3.78	1	0.067	0.8493	1.3671	3.018	-
Cation l.6	2.29	1	0.123	0.7716	1.2295	3.020	-
Nitroxide l.1	0.00	1	0.615	0.4358	6.5036	2.905	-0.4276

Nitroxide l.2	1.85	1	0.292	0.7817	4.2685	2.905	-0.4274
Nitroxide l.3	6.22	1	0.050	0.9904	-3.3120	2.944	-0.4290
Nitroxide l.4	7.83	1	0.026	1.5286	-4.7545	2.946	-0.4287
Nitroxide l.5	10.82	1	0.008	0.8493	1.3671	3.018	-0.4334
Nitroxide l.6	10.50	1	0.009	0.7716	1.2295	3.020	-0.4340
Cation m.1	0.11	1	0.241	1.8599	-2.9961	2.923	-
Cation m.2	0.00	2	0.503	0.7583	4.3022	2.920	-
Cation m.3	2.95	2	0.153	0.2460	3.9157	3.024	-
Cation m.4	3.93	2	0.103	0.0818	1.9954	2.952	-
Radical m.1	1.19	1	0.235	1.8599	-2.9961	2.923	-0.4274
Radical m.2	0.00	2	0.760	0.7583	4.3022	2.920	-0.4279
Radical m.3	18.52	2	0.000	0.2460	3.9157	3.024	-0.4339
Radical m.4	12.61	2	0.005	0.0818	1.9954	2.952	-0.4284
Cation n	-	-	1.000	-0.1002	7.0033	2.281	-
Radical n	-	-	1.000	-0.1002	7.0033	2.281	-0.4195
Cation o.1	0.00	1	0.789	0.4089	6.6060	2.283	-
Cation o.2	3.27	1	0.211	1.9227	-3.6347	2.281	-
Radical o.1	0.00	1	0.791	0.4089	6.6060	2.283	-0.4198
Radical o.2	3.29	1	0.209	1.9227	-3.6347	2.281	-0.4195
Cation r	-	-	1.000	1.3241	-0.4108	2.830	-
Nitroxide r	-	-	1.000	1.3241	-0.4108	2.830	-0.4252
Cation p	-	-	1.000	4.6521	-1.1516	2.593	-
Nitroxide p	-	-	1.000	4.6521	-1.1516	2.593	-0.4157

Table S4. Conformational Populations of the Radicals and Cations for Nitroxides 1 - 10

Species	Relative free-energy (kJ mol ⁻¹)	Relative # Degenerate Conformations	Relative Mole fraction	Dipole (D)	Quadrupole (DA)	r
Cation 1.1	0.00	1	0.750	1.0422	0.6344	2.304
Cation 1.2	4.23	1	0.136	0.8971	2.8382	2.306
Cation 1.3	4.66	1	0.114	-0.2292	0.5996	2.309
Nitroxide 1.1	0.00	1	0.890	1.0422	0.6344	2.304
Nitroxide 1.2	5.33	1	0.106	0.8971	2.8382	2.306
Nitroxide 1.3	10.75	1	0.004	-0.2292	0.5996	2.309
Cation 3a	-	-	1.000	0.5980	3.8997	2.840
Nitroxide 3a	-	-	1.000	0.5980	3.8997	2.840
Cation 3b	-	-	1.000	5.7600	-12.6535	2.854
Nitroxide 3b	-	-	1.000	5.7600	-12.6535	2.854
Cation 3c	-	-	1.000	9.9267	-24.0280	2.856
Nitroxide 3c	-	-	1.000	9.9267	-24.0280	2.856
Cation 4a	-	-	1.000	0.4884	2.2741	2.284
Nitroxide 4a	-	-	1.000	0.4884	2.2741	2.284
Cation 4b.1	0.13	1	0.486	2.7843	-7.6320	2.283
Cation 4b.2	0.00	1	0.514	1.4166	6.8182	2.283
Radical 4b.1	0.00	1	0.538	2.7843	-7.6320	2.283
Radical 4b.2	0.37	1	0.462	1.4166	6.8182	2.283
Cation 4c.1	2.81	1	0.164	1.9705	11.4072	2.282
Cation 4c.2	1.08	1	0.329	2.9104	1.3280	2.282
Cation 4c.3	0.00	1	0.508	3.9128	-10.0200	2.282
Radical 4c.1	1.97	1	0.187	1.9705	11.4072	2.282
Radical 4c.2	0.00	1	0.414	2.9104	1.3280	2.282
Radical 4c.3	0.09	1	0.399	3.9128	-10.0200	2.282
Cation 4d.1	0.00	1	0.550	-0.1005	7.0581	2.282
Cation 4d.2	0.50	1	0.450	1.2945	-3.9199	2.282
Radical 4d.1	0.00	1	0.513	-0.1005	7.0581	2.282
Radical 4d.2	0.12	1	0.487	1.2945	-3.9199	2.282
Cation 4e.1	0.15	1	0.485	0.7091	-1.5597	2.283

Cation 4e.2	0.00	1	0.515	-0.5217	8.5571	2.282
Radical 4e.1	0.00	1	0.516	0.7091	-1.5597	2.283
Radical 4e.2	0.16	1	0.484	-0.5217	8.5571	2.282
Cation 4f.1	0.00	1	0.652	0.7129	-4.5185	2.281
Cation 4f.2	5.00	4	0.348	0.4611	1.1126	2.282
Radical 4f.1	0.00	1	0.643	0.7129	-4.5185	2.281
Radical 4f.2	4.90	4	0.357	0.4611	1.1126	2.282
Cation 4g	-	-	1.000	2.4293	-2.8375	2.282
Nitroxide 4g	-	-	1.000	2.4293	-2.8375	2.282
Cation 4h	-	-	1.000	3.6031	-5.0163	2.280
Nitroxide 4h	-	-	1.000	3.6031	-5.0163	2.280
Cation 4j	-	-	1.000	5.6017	-12.2917	2.261
Nitroxide 4j	-	-	1.000	5.6017	-12.2917	2.261
Cation 4k	-	-	1.000	-0.4558	4.1589	2.283
Nitroxide 4k	-	-	1.000	-0.4558	4.1589	2.283
Cation 7	-	-	1.000	0.5056	5.4279	2.279
Nitroxide 7	-	-	1.000	0.5056	5.4279	2.279
Cation 8	-	-	1.000	0.8731	2.0407	2.919
Radical 8	-	-	1.000	0.8731	2.0407	2.919
Cation 9.1	5.32	1	0.055	1.2896	-1.8701	2.916
Cation 9.2	0.00	2	0.945	-0.6312	0.6578	2.950
Radical 9.1	0.00	1	0.776	1.2896	-1.8701	2.916
Radical 9.2	4.80	2	0.224	-0.6312	0.6578	2.950
Cation 10	-	-	1.000	0.4929	2.4489	3.032
Radical 10	-	-	1.000	0.4929	2.4489	3.032

Table S5. Total energies of all cations

Species	S (J/mol K)	Thermal Correction	ZPVE	M06-2X/ 6-31+G(d,p)	UMP2/ 6-31+G(d)	UMP2/ GTMP2Large	URCCSD(T)/ 6-31+G(d)	G _{gas} (ONIOM)	ΔG _{solv} (PCM)	G _{sol} (ONIOM)
TEMPO cat	428.43	0.012720	0.265792	-483.266593	-481.853581	-482.419218	-482.011711	-482.648703	-0.054676	-482.703380
Cation a.1	449.31	0.013545	0.245943	-557.243799	-555.706656	-556.326165	-555.862949	-556.594035	-0.059585	-556.653620
Cation a.2	456.67	0.013766	0.245267	-557.246193	-555.709461	-556.328625	-555.865405	-556.597437	-0.059186	-556.656624
Cation b.1	452.95	0.014006	0.269942	-558.456409	-556.883762	-557.530503	-557.046988	-557.790674	-0.060971	-557.851645
Cation b.2	454.47	0.014076	0.269807	-558.458749	-556.886349	-557.532538	-557.049433	-557.792803	-0.059521	-557.852324
Cation b.3	449.24	0.013884	0.270323	-558.463875	-556.891788	-557.536435	-557.054652	-557.795563	-0.058581	-557.854144
Cation c.1	469.15	0.014597	0.263333	-612.539771	-610.859607	-611.540058	-611.029230	-611.833308	-0.055155	-611.888463
Cation c.2	476.52	0.014840	0.262767	-612.540435	-610.860562	-611.540827	-611.029996	-611.835048	-0.054629	-611.889677
Cation d.1	460.02	0.014257	0.275412	-596.516099	-594.846528	-595.517198	-595.017351	-595.798875	-0.058071	-595.856945
Cation d.2	455.76	0.014134	0.275715	-596.522195	-594.853511	-595.523493	-595.024089	-595.804260	-0.055728	-595.859989
Cation e.1	490.05	0.016041	0.303940	-672.964798	-671.107054	-671.881149	-671.290279	-672.185976	-0.054326	-672.240302
Cation e.2	490.08	0.016042	0.303939	-672.964798	-671.107049	-671.881146	-671.290276	-672.185978	-0.054326	-672.240304
Cation e.3	493.36	0.016216	0.303439	-672.956775	-671.098861	-671.873735	-671.282579	-672.179758	-0.060047	-672.239805
Cation f	505.05	0.016284	0.292628	-785.060784	-782.983378	-783.837285	-783.173845	-784.199778	-0.064366	-784.264143
Cation g.1 CORE	556.25	0.018543	0.308810	-1146.248343	-1143.740641	-1144.706944	-1143.937153	-	-	-
Cation g.2 CORE	560.73	0.018610	0.308694	-1146.248140	-1143.740788	-1144.707054	-1143.937432	-	-	-
Cation g.1	678.86	0.023580	0.389720	-1377.216253	-1374.062233	-1375.249228	-	-1375.551942	-0.049418	-1375.601360
Cation g.2	682.66	0.023653	0.389708	-1377.218728	-1374.063505	-1375.249477	-	-1375.552693	-0.0469156	-1375.599608
Cation h.1	493.83	0.015499	0.268776	-646.787670	-645.035018	-645.735029	-645.203865	-646.042788	-0.059425	-646.102213
Cation h.2	491.10	0.015440	0.269029	-646.785882	-645.033609	-645.734011	-645.202097	-646.040906	-0.059776	-646.100682
Cation h.3	490.64	0.015324	0.269159	-646.790996	-645.038930	-645.738130	-645.207077	-646.044617	-0.057848	-646.102465
Cation h.4	497.75	0.015600	0.268718	-646.788473	-645.036171	-645.736039	-645.204546	-646.043727	-0.057306	-646.101033
Cation i	469.13	0.014170	0.255683	-3056.549860	-3053.638010	-3054.616208	-3053.656829	-3054.747903	-0.057290	-3054.805193
Cation k.1	528.92	0.017106	0.308352	-673.860834	-671.966609	-672.718365	-672.164887	-673.046593	-0.050645	-673.097238
Cation k.2	527.31	0.017223	0.308064	-673.858903	-671.964116	-672.716559	-672.162578	-673.044962	-0.049800	-673.094762

Cation k.3	525.30	0.017145	0.308316	-673.859481	-671.964661	-672.717471	-672.162872	-673.045220	-0.050406	-673.095625
Cation k.4	526.78	0.017222	0.308132	-673.860044	-671.965248	-672.717995	-672.163138	-673.045699	-0.050485	-673.096184
Cation k.5	534.38	0.017333	0.308034	-673.859698	-671.965860	-672.717808	-672.163941	-673.046551	-0.049003	-673.095555
Cation l.1	541.64	0.017889	0.313883	-749.135599	-747.085480	-747.910975	-747.290896	-748.269712	-0.050358	-748.320070
Cation l.2	541.87	0.017880	0.313942	-749.134205	-747.084008	-747.909798	-747.289554	-748.268641	-0.050661	-748.319302
Cation l.3	537.49	0.017713	0.314147	-749.136710	-747.087319	-747.911957	-747.292320	-748.269720	-0.050485	-748.320205
Cation l.4	536.83	0.017681	0.31425	-749.135223	-747.085769	-747.910747	-747.290922	-748.268516	-0.050756	-748.319273
Cation l.5	546.47	0.018007	0.313778	-749.134709	-747.085047	-747.910416	-747.289993	-748.269220	-0.049545	-748.318765
Cation l.6	545.91	0.017996	0.313708	-749.135503	-747.085905	-747.910988	-747.290881	-748.269838	-0.049497	-748.319335
Cation m.1	503.24	0.015731	0.280879	-671.776220	-669.953588	-670.703932	-670.128912	-671.016314	-0.058501	-671.074815
Cation m.2	495.70	0.015613	0.281834	-671.755431	-669.955563	-670.705971	-670.131138	-671.016912	-0.057943	-671.074855
Cation m.3	498.61	0.015705	0.281006	-671.779406	-669.955836	-670.706713	-670.130903	-671.018211	-0.055521	-671.073732
Cation m.4	485.29	0.015365	0.281323	-671.779466	-669.954931	-670.705913	-670.130288	-671.016211	-0.057147	-671.073357
Cation n	485.92	0.015217	0.238381	-611.392623	-609.745022	-610.407272	-609.903377	-610.706078	-0.055378	-610.761455
Cation o.1	476.94	0.014734	0.226496	-631.256995	-629.590666	-630.270521	-629.743615	-630.575269	-0.053306	-630.628575
Cation o.2	477.54	0.014744	0.226453	-631.254455	-629.588752	-630.267905	-629.741584	-630.572636	-0.054692	-630.627329
Cation p	451.17	0.013484	0.221926	-593.144327	-591.576678	-592.224529	-591.721345	-592.505062	-0.060318	-592.565379
Cation r	426.54	0.012532	0.241620	-519.147633	-517.703648	-518.294347	-517.852483	-518.538683	-0.058326	-518.597009

Unless otherwise noted units are in Hartree.

Table S4. Total energies of all radicals

Species	S (J/mol K)	Thermal Correction	ZPVE	M06-2X/ 6-31+G(d,p)	UMP2/ 6-31+G(d)	UMP2/ GTMP2Large	URCCSD(T)/ 6-31+G(d)	G _{gas} (ONIOM)	ΔG _{soln} (PCM)	G _{sol} (ONIOM)
TEMPO	431.72	0.012692	0.264452	-483.523430	-482.091358	-482.662112	-482.254390	-482.902210	0.003139	-482.899071
Radical a.1	453.93	0.013544	0.244951	-557.515374	-555.958683	-556.582603	-556.120363	-556.861348	0.002215	-556.859132
Radical a.2	465.13	0.013882	0.244031	-557.514687	-555.958467	-556.582219	-556.119395	-556.862065	0.002199	-556.859866
Radical b.1	456.30	0.013973	0.268846	-558.719728	-557.128223	-557.779472	-557.296448	-558.050119	0.000876	-558.049243
Radical b.2	456.70	0.013996	0.268749	-558.719955	-557.128674	-557.779728	-557.296701	-558.050297	0.000908	-558.049388
Radical b.3	452.02	0.013807	0.269163	-558.718638	-557.131557	-557.782483	-557.295481	-558.048192	0.000096	-558.048096
Radical c.1	474.55	0.014682	0.262108	-612.801745	-611.102604	-611.787817	-611.277681	-612.092243	0.002598	-612.089646
Radical c.2	486.98	0.015046	0.261279	-612.800219	-611.101534	-611.786658	-611.275970	-612.092320	0.002231	-612.090089
Radical d.1	462.76	0.014205	0.274326	-596.780184	-595.091723	-595.766954	-595.267578	-596.059079	0.002789	-596.056290
Radical d.2	461.57	0.014178	0.274416	-596.780625	-595.092913	-595.767731	-595.268693	-596.059581	0.002805	-596.056776
Radical e.1	496.98	0.016193	0.302449	-673.216545	-671.339755	-672.119298	-671.528230	-672.435469	0.000526	-672.434943
Radical e.2	496.54	0.016152	0.302527	-673.215738	-671.338877	-672.118585	-671.527606	-672.434924	0.000175	-672.434749
Radical e.3	494.85	0.016066	0.302539	-673.214984	-671.338015	-672.117707	-671.526929	-672.434113	-0.000080	-672.434193
Radical f	509.52	0.016288	0.291583	-785.329605	-783.232349	-784.090807	-783.428419	-784.464422	-0.000956	-784.465378
Radical g.1 CORE	564.57	0.018555	0.307579	-1146.510014	-1143.983119	-1144.955711	-1144.185033	-	-	-
Radical g.2 CORE	567.82	0.018613	0.307654	-1146.511337	-1143.984683	-1144.956269	-1144.186648	-	-	-
Radical g.1	671.74	0.023462	0.388791	-1377.479301	-1374.306733	-1375.499284	-	-1375.811607	0.007028	-1375.804579
Radical g.2	683.77	0.023607	0.388693	-1377.477625	-1374.30354	-1375.494756	-	-1375.160104	-1375.808449	-1375.801087
Radical h.1	497.46	0.015494	0.267665	-647.054002	-645.283219	-645.988019	-645.456044	-646.305253	0.003331	-646.301922
Radical h.2	494.63	0.015398	0.268047	-647.053811	-645.283181	-645.988173	-645.455869	-646.304661	0.003554	-646.301107
Radical h.3	490.57	0.015260	0.268133	-647.052400	-645.282100	-645.986686	-645.454178	-646.302157	0.003442	-646.298714
Radical h.4	506.07	0.015740	0.267364	-647.048776	-645.278782	-645.983416	-645.450710	-646.300785	0.003522	-646.297263
Radical i	473.98	0.014203	0.254500	-3056.817038	-3053.885594	-3054.868219	-3053.909489	-3055.010659	0.004223	-3055.006436
Radical k.1	526.70	0.017018	0.307079	-674.115454	-672.201161	-672.958689	-672.404862	-673.297419	0.005769	-673.291650
Radical k.2	530.62	0.017202	0.306723	-674.116581	-672.202035	-672.959660	-672.405616	-673.298887	0.006837	-673.292050

Radical k.3	530.38	0.017151	0.307030	-674.118491	-672.204501	-672.962160	-672.407809	-673.300832	0.007155	-673.293676
Radical k.4	544.26	0.017581	0.306232	-674.110812	-672.197078	-672.955065	-672.400349	-673.295643	0.006119	-673.289524
Radical k.5	541.96	0.017487	0.306496	-674.113241	-672.200253	-672.957472	-672.403087	-673.297182	0.006725	-673.290457
Radical l.1	546.74	0.017901	0.312759	-749.396272	-747.327177	-748.157518	-747.537601	-748.526923	0.006868	-748.520054
Radical l.2	547.81	0.017918	0.312736	-749.395442	-747.326190	-748.156724	-747.536798	-748.526441	0.007092	-748.519349
Radical l.3	543.05	0.017753	0.312961	-749.394607	-747.326050	-748.155849	-747.536216	-748.524523	0.006837	-748.517686
Radical l.4	542.66	0.017737	0.313020	-749.394326	-747.325423	-748.155546	-747.535809	-748.524353	0.007283	-748.517070
Radical l.5	557.37	0.018198	0.312317	-749.391122	-747.322750	-748.152984	-747.532393	-748.522962	0.007028	-748.515934
Radical l.6	557.20	0.018196	0.312285	-749.391354	-747.323029	-748.153075	-747.532670	-748.523064	0.007012	-748.516053
Radical m.1	505.27	0.015728	0.279727	-672.040085	-670.197952	-670.953201	-670.378596	-671.276257	0.001482	-671.274775
Radical m.2	500.84	0.015666	0.279614	-672.041310	-670.198594	-670.954085	-670.379326	-671.276900	0.001673	-671.275227
Radical m.3	510.66	0.015909	0.279585	-672.034132	-670.192036	-670.947250	-670.371903	-671.270102	0.001928	-671.268174
Radical m.4	489.44	0.015369	0.280113	-672.038122	-670.194241	-670.950087	-670.375028	-671.271461	0.001036	-671.270426
Radical n	494.53	0.015366	0.237289	-611.655798	-609.989544	-610.656448	-610.152393	-610.965637	0.000446	-610.965191
Radical o.1	492.24	0.014994	0.225378	-631.523393	-629.838095	-630.522877	-629.995296	-630.838441	0.003394	-630.835047
Radical o.2	491.50	0.014950	0.225460	-631.522224	-629.837178	-630.521505	-629.994284	-630.836852	0.003060	-630.833793
Radical p	459.64	0.013577	0.221115	-593.424034	-591.836311	-592.487712	-591.986800	-592.779717	0.001514	-592.778203
Radical r	430.73	0.012547	0.240548	-519.411999	-517.949150	-518.544381	-518.102971	-518.799206	0.002518	-518.796688

Unless otherwise noted units are in Hartree.

Table S5. Total energies of all radicals and cations

Species	S (J/mol K)	Thermal Correction	ZPVE	M06-2X/ 6-31+G(d,p)	UMP2/ 6-31+G(d)	UMP2/ GTMP2Large	URCCSD(T)/ 6-31+G(d)	G _{gas} (ONIOM)	ΔG _{solv} (PCM)	G _{sol} (ONIOM)
Cation 1.1	480.89	0.014837	0.250935	-632.484204	-630.790540	-631.490270	-630.949204	-0.056764	-631.786052	-631.842816
Cation 1.2	477.70	0.014765	0.251000	-632.484033	-630.789722	-631.489627	-630.948569	-0.055967	-631.785237	-631.841204
Nitroxide 1.1	495.60	0.015107	0.249484	-632.746599	-631.033624	-631.738155	-631.197114	0.002008	-632.045584	-632.043576
Nitroxide 1.2	493.10	0.015014	0.249517	-632.744731	-631.031082	-631.735821	-631.194913	0.001801	-632.043366	-632.041566
Cation 4b.1	534.45	0.017364	0.274045	-784.864481	-782.778884	-783.599808	-	-0.049943	-783.369091	-783.419034
Cation 4b.2	533.91	0.017355	0.274081	-784.865344	-782.779818	-783.600617	-	-0.049274	-783.369811	-783.419086
Radical 4b.1	550.15	0.017570	0.272921	-785.129356	-783.024462	-783.850602	-	0.005291	-783.622585	-783.617295
Radical 4b.2	549.07	0.017552	0.272973	-785.129449	-783.024492	-783.850664	-	0.005339	-783.622491	-783.617152
Cation 4c.1	599.30	0.020398	0.288802	-973.370530	-970.875821	-971.881522	-	-0.051394	-971.640378	-971.691772
Cation 4c.2	600.14	0.020414	0.288800	-973.370055	-970.875509	-971.881430	-	-0.052063	-971.640367	-971.692430
Cation 4c.3	602.86	0.020453	0.288767	-973.368533	-970.874827	-971.880709	-	-0.052892	-971.639950	-971.692842
Radical 4c.1	614.84	0.020599	0.287736	-973.638367	-971.124586	-972.135032	-	0.003681	-971.896517	-971.892836
Radical 4c.2	618.23	0.020632	0.287741	-973.638338	-971.124512	-972.135323	-	0.003570	-971.897156	-971.893587
Radical 4c.3	617.98	0.020643	0.287756	-973.637058	-971.123971	-972.134786	-	0.003012	-971.896564	-971.893552
Cation 4d.1	493.85	0.015670	0.263059	-671.550885	-669.715132	-670.433126	-669.889467	-0.049258	-670.761333	-670.810591
Cation 4d.2	493.86	0.015673	0.263068	-671.549364	-669.713656	-670.431699	-669.887995	-0.050501	-670.759899	-670.810401
Radical 4d.1	510.42	0.015949	0.261661	-671.808714	-669.954339	-670.677281	-670.133008	0.003697	-671.016791	-671.013094
Radical 4d.2	509.83	0.015937	0.261686	-671.808560	-669.954266	-670.677104	-670.132921	0.003474	-671.016521	-671.013047
Cation 4e.1	522.94	0.017061	0.291839	-710.833128	-708.871719	-709.635346	-709.063333	-0.044669	-709.982204	-710.026872
Cation 4e.2	523.41	0.017061	0.291870	-710.834166	-708.872756	-709.636215	-709.064126	-0.044079	-709.982851	-710.026930
Radical 4e.1	539.92	0.017278	0.290468	-711.090085	-709.109836	-709.878561	-709.305748	0.007474	-710.236768	-710.229294
Radical 4e.2	540.01	0.017271	0.290512	-711.090061	-709.109717	-709.878281	-709.305414	0.007012	-710.236247	-710.229235

Cation 4f.1	567.52	0.019656	0.324990	-825.313491	-823.064584	-823.957381	-	-0.041705	-823.677182	-823.718886
Cation 4f.2	582.20	0.019929	0.324475	-825.310085	-823.063149	-823.953344	-	-0.041928	-823.675055	-823.716983
Radical 4f.1	581.22	0.019813	0.323738	-825.567494	-823.299854	-824.197339	-	0.007283	-823.919791	-823.912508
Radical 4f.2	593.83	0.020051	0.323196	-825.565874	-823.300126	-824.195046	-	0.008590	-823.919235	-823.910645
Cation 9.1	489.15	0.015418	0.297185	-597.741958	-596.044180	-596.735284	-596.224691	-0.054103	-597.015011	-597.069114
Cation 9.2	479.37	0.015109	0.297711	-597.747325	-596.050022	-596.739960	-596.230223	-0.052987	-597.018152	-597.071139
Radical 9.1	487.58	0.015509	0.298338	-598.001615	-596.284637	-596.980738	-596.470085	0.004223	-597.270794	-597.266571
Radical 9.2	479.22	0.015224	0.298900	-598.001483	-596.284537	-596.980023	-596.469833	0.003857	-597.268599	-597.264743

Optimised Gas-phase structures for all the species in this study

Note: Because of standard molecular reorientation, the dipole/quadrupoles of the Model species may not correspond with those listed in Table S3 and S4. Values given in these tables were found using separate single point energy calculations (run on these optimised structures).

Cation TEMPO

1\1\GINC-R43\FOpt\RM062X\6-31+G(d,p)\C9H18N1O1(1+)\ROOT\17-Nov-2015\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\TEMPO_rad.freq\1,1\C,-3.1885117 461,0.7292222402,-0.1527989793\N,-2.9999212228,-0.6594351796,-0.7661812384\C,-2.1020686494,-1.74881 87313,-0.1768783922\C,-0.8271032731,-1.0803092014,0.3641456646\C,-1.0875509624,0.1597794628,1.2120 239452\C,-1.8291300187,1.2051886194,0.3863541132\C,-3.7140540309,1.6456965322,-1.2520691813\C,-4.2 458501434,0.5698932296,0.9580208447\C,-2.9277249084,-2.4365857545,0.9288065381\C,-1.7920181186,-2. 7382272587,-1.2946682797\O,-3.6125549133,-0.9185131268,-1.7456850161\H,-0.1833938838,-0.8172904039,- 0.4842065688\H,-0.2981759552,-1.8494408009,0.9356739856\H,-0.1318371867,0.5755985433,1.5405998985\ H,-1.6396711617,-0.0911445069,2.1237030953\H,-1.2056044239,1.5142441307,-0.4615507761\H,-2.0322989 148,2.1058770216,0.9741082698\H,-3.0552019652,1.6474683884,-2.1242078981\H,-3.7395746241,2.6578228 03,-0.8417337096\H,-4.7230608955,1.3760617692,-1.5673592303\H,-3.863042209,0.0766933194,1.85004900 99\H,-5.1288845526,0.0385399667,0.5931612197\H,-4.5525254131,1.5812462909,1.2365964646\H,-3.024682 5895,-1.8355002344,1.8314680023\H,-2.3897543035,-3.3517644092,1.1886618248\H,-3.9194193117,-2.7200 99146,0.566355202\H,-1.3505296341,-2.2406762295,-2.1619894524\H,-2.676239215,-3.2924827693,-1.61272 40216\H,-1.0620355312,-3.4493093558,-0.9010774244\Version=ES64L-G09RevD.01\State=1-A\HF=-483.26 65929\RMSD=4.259e-09\RMSF=1.910e-05\Dipole=0.0860746,0.0344802,0.3352123\Quadrupole=-0.9631267, 4.4530206,-3.4898939,-2.9374227,-0.188231,0.0071713\PG=CS [SG(C1H2N1O1),X(C8H16)]\@

Cation a.1

1\1\GINC-R206\FOpt\RM062X\6-31+G(d,p)\C9H16N1O2(1+)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideA.freq\1,1\C,-1.36270416 1,0.2926292976,0.0667096981\C,-1.2667457384,-1.0098047762,-0.74872888\C,0,-1.7688975728,-0.40375879 01\C,1.2667457384,-1.0098047762,-0.74872888\C,1.362704161,0.2926292976,0.0667096981\N,0,1.00264614 36,0.0137064406\O,0,-2.184833747,-0.0118373361\C,-1.6367005071,0.0071255119,1.5575791284\C,-2.40098 19701,1.2502719807,-0.5040175941\H,-1.280917248,-0.7785044612,-1.8204308692\H,2.1399609825,-1.6213 142607,-0.5094141014\H,1.280917248,-0.7785044612,-1.8204308692\H,2.1399609825,-1.6213142607,-0.509 4141014\C,2.4009819701,1.2502719807,-0.5040175941\C,1.6367005071,0.0071255119,1.5575791284\H,-1.05 34608039,-0.8287853687,1.9440984503\H,-2.6933162489,-0.2641381009,1.6266839752\H,-1.4753071203,0.8 974645603,2.1707243415\H,-2.1317283771,1.5855217176,-1.5089989399\H,-2.5515386106,2.1198945427,0.1 372154249\H,-3.3434597117,0.7013882569,-0.5675123445\H,2.1317283771,1.5855217176,-1.5089989399\H, 3.3434597117,0.7013882569,-0.5675123445\H,2.5515386106,2.1198945427,0.1372154249\H,1.0534608039,- 0.8287853687,1.9440984503\H,1.4753071203,0.8974645603,2.1707243415\H,2.6933162489,-0.2641381009,1. 6266839752\O,0,-2.8357501178,0.1547431072\Version=ES64L-G09RevD.01\State=1-A\HF=-557.2437991\ RMSD=3.184e-09\RMSF=1.264e-05\Dipole=0,1.2239249,-0.2320106\Quadrupole=9.4724916,-9.6707347,0.1 982431,0,0,1.6442208\PG=CS [SG(C1N1O2),X(C8H16)]\@

Cation a.21 1\1\GINC-R118\FOpt\RM062X\6-31+G(d,p)\C9H16N1O2(1+)\ROOT\28-Nov-2017\0\#M062X\6- 31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\CatA.freq\1,1\C,-1.4720269874, -0.7374273605,1.5269506098\C,-2.8802480497,-0.9647130355,0.9948968429\C,-3.5368209385,0.2000966181,0 .2670652523\C,-3.0256575453,1.5844485049,0.6720119598\N,-1.503899024,1.5855088564,0.6362655555\C,- 0.6628248679,0.3237981661,0.7782342741\O,-3.4470164828,-2.0145445263,1.1426644245\C,-3.3675187502, 1.9221800576,2.1397566798\C,-3.518341881,2.6774570468,-0.2719876231\C,0.6194771343,0.6958336626,1. 5169708598\C,-0.3641359348,-0.0949666885,-0.6777004047\O,-0.9461324973,2.6186120555,0.4907617654\ H,-0.9305723005,-1.6858662512,1.4668918759\H,-1.5389120286,-0.4894312607,2.5932398981\H,-4.6116166 989,0.1607178184,0.4659909891\H,-3.418815292,0.0467420507,-0.8125146897\H,-3.0421993168,1.15376479 91,2.8440132719\H,-4.4564400716,1.9941969455,2.2001520889\H,-2.9391970177,2.8859143253,2.42418698 2\H,-3.1567359356,2.5127415159,-1.2908550026\H,-3.21725924,3.6706131899,0.0625426248\H,-4.60971735 25,2.6331538173,-0.2855207797\H,0.4002297095,1.1259174528,2.4982593373\H,1.2311739843,1.393803188 2,0.9446131836\H,1.1912487112,-0.2228185089,1.6667013616\H,-1.2586907825,-0.3826388181,-1.23383491 42\H,0.293709303,-0.9662577418,-0.6253630333\H,0.1583101533,0.7030741203,-1.2099933899\Version=ES 64L-G09RevD.01\State=1-A\HF=-557.2461932\RMSD=7.937e-09\RMSF=3.348e-05\Dipole=0.6513127,1.206 7431,-0.1695756\Quadrupole=5.4777972,-5.8727628,0.3949656,-8.6569715,0.613586,1.2326388\PG=C01 [X(C9H16N1O2)]\@

Cation b.1

1\1\GINC-R2629\FOpt\RM062X\6-31+G(d,p)\C9H18N1O2(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=402653184\NitroxideC.1.freq\1,1\C,-0.375290 875,-1.3554753575,0.1004807035\C,1.0821577441,-1.2458160629,-0.3653000608\C,1.8132850155,0.,0.13104 05492\C,1.0821577441,1.2458160629,-0.3653000608\C,-0.375290875,1.3554753575,0.1004807035\N,-1.0587 527311,0.,-0.1072338917\O,-2.204991383,0.,-0.4009360226\C,-0.4997904045,-1.6627863464,1.6076302365\C,- 1.1533113663,-2.3862085549,-0.7117304777\H,1.1091573462,-1.2615853392,-1.4636968323\H,1.6015125097,- 2.1443539699,-0.0177877377\H,1.1091573462,1.2615853392,-1.4636968323\H,1.6015125097,2.1443539699,- 0.0177877377\C,-1.1533113663,2.3862085549,-0.7117304777\C,-0.4997904045,1.6627863464,1.6076302365\ H,0.1553559852,-1.0550414527,2.2301483646\H,-0.2068132971,-2.7083409249,1.7320869404\H,-1.53364633 68,-1.5577456129,1.9468157729\H,-1.2218349923,-2.099400228,-1.7643350783\H,-2.1575487597,-2.5478131 998,-0.3178179374\H,-0.60203443,-3.3273131739,-0.6498165863\H,-1.2218349923,2.099400228,-1.76433507 83\H,-0.60203443,3.3273131739,-0.6498165863\H,-2.1575487597,2.5478131998,-0.3178179374\H,0.1553559 852,1.0550414527,2.2301483646\H,-1.5336463368,1.5577456129,1.9468157729\H,-0.2068132971,2.7083409 249,1.7320869404\O,3.1590559865,0.,-0.2635952776\H,1.8530110936,0.,1.2255580398\H,3.2360857776,0.,-1.2 268580138\Version=ES64L-G09RevD.01\State=1-A\HF=-558.4564086\RMSD=2.296e-09\RMSE=4.976e-06\ Dipole=-0.8491717,0.,-0.1409338\Quadrupole=-7.1612742,6.881325,0.2799492,0.,-3.7677814,0.\PG=CS [SG(C1H2N1O2),X(C8H16)]\@

Cation b.2

1\1\GINC-R1519\FOpt\RM062X\6-31+G(d,p)\C9H18N1O2(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=402653184\NitroxideC.2.freq\1,1\C,-0.363143 7294,-1.3442956211,0.1094969427\C,1.0977554404,-1.2252229877,-0.335910303\C,1.820338835,0.01950606 61,0.1613697877\C,1.0798366558,1.261484317,-0.3369482999\C,-0.3838245099,1.3617392486,0.1116675973 \N,-1.0540844502,0.0037130878,-0.1108734688\O,-2.1937589912,-0.0041331771,-0.429067558\C,-0.5103414 27,-1.6518594758,1.614579566\C,-1.1180677289,-2.3825790143,-0.7148232859\H,1.1555408985,-1.23129340 65,-1.4312309269\H,1.6189057717,-2.1208897733,0.0157048382\H,1.1338855552,1.2650770209,-1.43229620 52\H,1.5753605446,2.1747768759,0.0108074286\C,-1.1557244298,2.3902028923,-0.7093128354\C,-0.532237 8757,1.6641972094,1.6176133789\H,0.1327135486,-1.0405806465,2.2462714926\H,-0.213601384,-2.6958128 204,1.7432625259\H,-1.5496216729,-1.5523053702,1.9386179592\H,-1.1706526781,-2.0964357544,-1.76840 90075\H,-2.1270786306,-2.5535308176,-0.3373641024\H,-0.5584623226,-3.3180747497,-0.6440628363\H,-1. 2046884821,2.1061898274,-1.7636413424\H,-0.6123793477,3.3350548306,-0.6361023528\H,-2.1673253508,2.5 434527156,-0.3309794705\H,0.1181587892,1.0587010371,2.2474680976\H,-1.5697056579,1.5504988163,1.9 428055707\H,-0.2498806182,2.711835236,1.749184565\O,3.1080527938,-0.0489884663,-0.3989683173\H,1.8 767754117,0.0154384968,1.259508118\H,3.7075050426,0.5726844031,0.030972444\Version=ES64L-G09Re vD.01\State=1-A\HF=-558.4587492\RMSD=8.372e-09\RMSE=1.437e-05\Dipole=-0.4389027,0.3954982,0.717 1369\Quadrupole=-2.646132,6.2548872,-3.6087552,3.226526,2.4866534,0.0406346\PG=C01 [X(C9H18N1O2)]\ @

Cation b.3

1\1\GINC-R111\FOpt\RM062X\6-31+G(d,p)\C9H18N1O2(1+)\ROOT\29-Apr-2016\0\#M062X/6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=normanmaxdisk=402653184\CatC.3.freq\1,1\C,-0.0243265189,0. 0517895181,0.0303495806\C,0.0519418945,0.0483479968,1.5661860014\C,1.4543709877,0.0076030576,2.16 09268066\C,2.2146188102,-1.2046426631,1.6223715348\C,2.3077446057,-1.3070021536,0.0902315871\N,0.9 381658628,-1.001080134,-0.5104366101\O,0.6246677468,-1.5841737485,-1.4924645663\C,0.4094803265,1.3 897294804,-0.6090660337\C,-1.4245207715,-0.3241137242,-0.4480679135\H,-0.5100798207,-0.8143768145, 1.9422565315\H,-0.4654603526,0.9490869678,1.9091908602\H,1.7374933165,-2.1141652097,2.0069642932\ H,3.2435882053,-1.20430186,1.9967506708\C,2.6880535312,-2.7209648762,-0.3421386096\C,3.2786655758, -0.2840419799,-0.540039484\H,1.3378035689,1.7759279218,-0.1964618932\H,-0.3844660562,2.1047037388, -0.3775292282\H,0.4725237772,1.2917970639,-1.6961344283\H,-1.6909873949,-1.3438648712,-0.157505544 5\H,-1.5302162921,-0.2202251732,-1.5285832387\H,-2.1242058406,0.3626257415,0.0339224222\H,1.922582 657,-3.4491988937,-0.0610601773\H,3.6129809524,-2.9793666171,0.1787202951\H,2.8683792136,-2.787027 7896,-1.4157474996\H,3.1319703655,0.7241218608,-0.1610105085\H,3.2044286089,-0.3061776181,-1.63058 23798\H,4.2844717879,-0.611091075,-0.2627878234\H,1.3459542079,-0.1169754694,3.2447427203\O,2.1110 037911,1.2300515573,1.8719797634\H,2.7280850587,1.4587574245,2.5767063072\Version=ES64L-G09Rev D.01\State=1-A\HF=-558.463875\RMSD=8.964e-09\RMSE=1.074e-05\Dipole=0.1610078,-0.2401385,0.52349 93\Quadrupole=3.2803652,-3.3738368,0.0934717,-2.8270572,2.1292019,0.7684384\PG=C01 [X(C9H18N1O2)]\ @

Cation c.1

1\1\GINC-R170\FOpt\RM062X\6-31+G(d,p)\C9H17N2O2(1+)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideB.1.freq\1,1\C,-1.354040 6302,0.2910595418,0.0485935033\C,-1.2384218497,-0.9737488223,-0.8221816937\C,0.0170822775,-1.72204 97875,-0.482775937\C,1.2853698397,-0.9817882927,-0.7695862077\C,1.3718831432,0.3144947128,0.062971 4206\N,0.0035165864,1.0118631811,0.0196626671\O,-0.0057265039,2.1952346895,0.006127714\C,-1.624787 1331,-0.0656080235,1.522791499\C,-2.3999143849,1.2618813685,-0.4822323413\H,-1.2242599106,-0.690538 0408,-1.8814579181\H,-2.1284093216,-1.5795910023,-0.6418185371\H,1.3432254487,-0.7304028885,-1.8356 194727\H,2.1540522226,-1.5947615042,-0.5151457442\C,2.3997415149,1.2876197904,-0.4992998448\C,1.65 06606308,0.0162149875,1.5490323569\H,-1.0315445038,-0.9144886362,1.8632697845\H,-2.6784299748,-0.3 504148996,1.5799247743\H,-1.4689371276,0.7948689569,2.178781886\H,-2.1370120772,1.6373253502,-1.47 45308092\H,-2.5544041279,2.1064607134,0.1908301981\H,-3.3387689391,0.7091491711,-0.5630861776\H,2. 1240503776,1.6338651782,-1.4988397843\H,3.3456336141,0.7458065845,-0.5746615563\H,2.5479705957,2. 1505719912,0.1512890741\H,1.0776150301,-0.8335096224,1.9190031056\H,1.4731957599,0.8953869565,2.1 739641193\H,2.7117877124,-0.237391755,1.6160391976\N,0.0940712595,-2.8563698962,0.094195269\O,-1.1 404469257,-3.3941092755,0.3659836922\H,-0.9478526029,-4.2692407267,0.7287357621\Version=ES64L-G0 9RevD.01\State=1-A\HF=-612.5397711\RMSD=9.894e-09\RMSE=1.846e-05\Dipole=0.0761396,0.5988534,0. 1001257\Quadrupole=3.9726204,-0.0373741,-3.9352463,1.8378574,-0.3701641,-1.9127442\PG=C01 [X(C9H1 7N2O2)]\@

Cation c.2

1\1\GINC-R51\FOpt\RM062X\6-31+G(d,p)\C9H17N2O2(1+)\ROOT\29-Nov-2017\0\#M062X\6-31+G(d,p) S CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\RadC2.freq\1,1\C,-1.6170450992,-0.627911 8604,1.7158845717\C,-2.9972679143,-0.8216474038,1.1563441959\C,-3.7003379019,0.3458128709,0.513531 5605\C,-3.0412975287,1.7055579219,0.7630231605\N,-1.5315000571,1.581914215,0.5998624219\C,-0.76955 8597,0.2813057968,0.8217386871\N,-3.4917617196,-1.9950526532,1.1907850054\C,-3.2272347156,2.188167 7956,2.2187855135\C,-3.5308704294,2.7616997484,-0.2233002614\C,0.5759647181,0.6260077997,1.4510241 735\C,-0.6030786358,-0.2953648008,-0.599102554\O,-0.9191902961,2.5446821745,0.2859150675\H,-1.11583 1207,-1.5975249916,1.7787278021\H,-1.6449012617,-0.2213033874,2.7331903335\H,-4.7276497275,0.40617 64294,0.8902217948\H,-3.7976394739,0.1601406181,-0.563992705\H,-2.9540418284,1.434768727,2.9586458 958\H,-4.2914675126,2.4066889695,2.3381846805\H,-2.6645782456,3.1071866703,2.3990102124\H,-3.25525 98415,2.5032526965,-1.2494443772\H,-3.1459098053,3.7536343104,0.0150637644\H,-4.6211076536,2.78787 76035,-0.1593135485\H,0.4451525316,1.1414322898,2.4067137907\H,1.1895417035,1.2388192122,0.790162 7823\H,1.1014022694,-0.313205045,1.6383464516\H,-1.5588538068,-0.5132506114,-1.081280776\H,-0.0569 648517,-1.2366783964,-0.4970357367\H,-0.0198351962,0.3843897303,-1.2241915851\O,-4.7443099983,-2.02 64918459,0.6259989786\H,-5.0305279175,-2.944904584,0.7199306998\Version=ES64L-G09RevD.01\State= 1-A\HF=-612.5404354\RMSD=4.450e-09\RMSE=3.542e-06\Dipole=0.4077817,0.6334546,0.0045023\Quadrup ole=3.9959444,1.1492574,-5.1452018,-0.7878242,0.1609747,1.3125631\PG=C01 [X(C9H17N2O2)]\@

Cation d.1

1\1\GINC-R126\FOpt\RM062X\6-31+G(d,p)\C10H18N1O2(1+)\ROOT\19-Jun-2017\0\#M062X\6-31+G** S CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610612736\NitroxideD.1.freq\1,1\C,0.142927976 2,0.5211271855,-1.3585923094\C,0.5115257293,-0.9657574521,-1.2560469683\C,-0.0048644807,-1.62608204 54,0.\C,0.5115257293,-0.9657574521,1.2560469683\C,0.1429279762,0.5211271855,1.3585923094\N,0.41108 30962,1.1817129785,0.\O,0.8071895382,2.2965607253,0.\C,-1.35696224,0.7361573114,-1.6445694588\C,0.99 32434358,1.2467271732,-2.394842199\H,1.6031018351,-1.0756324877,-1.2858906232\H,0.1126347393,-1.46 56427951,-2.1439097572\H,1.6031018351,-1.0756324877,1.2858906232\H,0.1126347393,-1.4656427951,2.14 39097572\C,0.9932434358,1.2467271732,2.394842199\C,-1.35696224,0.7361573114,1.6445694588\H,-1.9996 753298,0.099623262,-1.0380021139\H,-1.5095245591,0.4711334451,-2.694043139\H,-1.6405218412,1.78405 66444,-1.5160911991\H,2.0511870875,1.2451014677,-2.1201028489\H,0.66431939,2.2751122674,-2.5502895 22\H,0.8852691309,0.7032189512,-3.3364341652\H,2.0511870875,1.2451014677,2.1201028489\H,0.8852691 309,0.7032189512,3.3364341652\H,0.66431939,2.2751122674,2.550289522\H,-1.9996753298,0.099623262,1. 0380021139\H,-1.6405218412,1.7840566444,1.5160911991\H,-1.5095245591,0.4711334451,2.694043139\O,0.0 643417849,-3.0316868322,0.\C,-1.2314971777,-2.449017622,0.\H,-1.7931417345,-2.5767035765,-0.92361837 68\H,-1.7931417345,-2.5767035765,0.9236183768\Version=ES64L-G09RevE.01\State=1-A\HF=-596.516099 2\RMSD=7.458e-09\RMSE=1.377e-05\Dipole=-0.4724217,1.2098194,0.\Quadrupole=-0.4045955,-7.2753881,7.6 799836,3.0096789,0.,0.\PG=CS [SG(C2N1O2),X(C8H18)]\@

Cation d.2

1\1\GINC-R140\FOpt\RM062X\6-31+G(d,p)\C10H18N1O2(1+)\ROOT\19-Jun-2017\0\#M062X\6-31+G** S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610612736\NitroxideD.2.freq\1,1\C,0.137113525
2,-0.5048768342,-1.3548337404\C,-0.9933553108,0.5353819429,-1.2590225256\C,-0.9246829742,1.36365344
48,0\C,-0.9933553108,0.5353819429,1.2590225256\C,0.1371135252,-0.5048768342,1.3548337404\N,0.26562
8807,-1.2046991797,0\O,0.5306677672,-2.3586650251,0\C,1.5080427688,0.1490989161,-1.6305570915\C,-0.1
660157178,-1.5756727839,-2.3958735875\H,-1.9632875383,0.0263052516,-1.3093769822\H,-0.9083613214,1.1
765333775,-2.1415130469\H,-1.9632875383,0.0263052516,1.3093769822\H,-0.9083613214,1.1765333775,2.1
415130469\C,-0.1660157178,-1.5756727839,2.3958735875\C,1.5080427688,0.1490989161,1.6305570915\H,1.
6735795026,1.0481039051,-1.0398953541\H,1.498282107,0.4379214875,-2.6848470173\H,2.3213544229,-0.5
667198401,-1.4842652019\H,-1.0485914204,-2.162815466,-2.1285545674\H,0.6785472039,-2.2488509965,-2.
549522595\H,-0.370384025,-1.0599011973,-3.3370937179\H,-1.0485914204,-2.162815466,2.1285545674\H,-
0.370384025,-1.0599011973,3.3370937179\H,0.6785472039,-2.2488509965,2.549522595\H,1.6735795026,1.0
481039051,1.0398953541\H,2.3213544229,-0.5667198401,1.4842652019\H,1.498282107,0.4379214875,2.684
8470173\C,-1.3402659964,2.7739899789,0\O,0.0381548292,2.4103941284,0\H,-1.6968855276,3.2234006388,0
.9233315536\H,-1.6968855276,3.2234006388,-0.9233315536\Version=ES64L-G09RevE.01\State=1-A\HF=-5
96.522195\RMSD=6.296e-09\RMSF=1.640e-05\Dipole=-0.4636862,-0.5022883,0\Quadrupole=-2.3948317,-3.
1861004,5.5809321,-4.4701458,0,0\PG=CS [SG(C2N1O2),X(C8H18)]\@

Cation e.1

1\1\GINC-R2456\FOpt\RM062X\6-31+G(d,p)\C10H20N1O3(1+)\ROOT\19-Jun-2017\0\#M062X\6-31+G** S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610612736\CationE.1ii.freq\1,1\C,-0.0126374304,0
.0058393822,0.0276634435\C,0.0119449172,-0.0561798744,1.5617090728\C,1.4024970415,-0.0532586055,2.
2109775921\C,2.2274910379,-1.2064224985,1.6513655748\C,2.3756089579,-1.2492526107,0.1218969224\N,
1.0198561949,-0.9745855314,-0.5218541763\O,0.777189157,-1.5172432101,-1.5463004675\C,0.3724219181,
1.3837372885,-0.5546379638\C,-1.3755772851,-0.4219823829,-0.5130201805\H,-0.5241013633,-0.95902797
68,1.8802266235\H,-0.5629096507,0.7998957712,1.9293719228\H,1.7813581031,-2.1513985925,1.98529329
86\H,3.2423918326,-1.1594314477,2.0596635765\C,2.8258682556,-2.632827288,-0.3424245007\C,3.3299318
493,-0.170123859,-0.4369371666\H,1.286135389,1.7828573715,-0.1224701063\H,-0.4496949892,2.05866894
37,-0.3014469206\H,0.4453987465,1.3301368307,-1.6441785432\H,-1.5994778374,-1.4630614469,-0.265180
209\H,-1.4499872445,-0.2862959642,-1.5925775415\H,-2.12467747,0.211908452,-0.0330108667\H,2.077617
6869,-3.3977755335,-0.1177864159\H,3.7387088651,-2.8753919707,0.2065724004\H,3.0506281541,-2.65361
73203,-1.4093228291\H,3.1375455833,0.8168365898,-0.0244479479\H,3.2919501632,-0.1557192869,-1.5294
102923\H,4.3364194507,-0.4724348045,-0.1355377069\C,1.2562024773,-0.2107770247,3.7279657137\O,2.09
0751556,1.1563630485,1.9524121192\O,0.6078159794,0.9702112253,4.1582799577\H,0.6691822577,-1.1056
253241,3.9711042149\H,2.2568186052,-0.3016536157,4.1696561428\H,1.7734442519,1.811701496,2.594626
5188\H,0.6157154263,1.0395664399,5.1194616668\Version=ES64L-G09RevE.01\State=1-A\HF=-672.96479
75\RMSD=6.985e-09\RMSF=1.012e-05\Dipole=-0.0932204,-0.5588957,0.1618982\Quadrupole=-2.1678876,-4.9
602659,7.1281535,-4.0510083,0.1385113,1.2480334\PG=C01 [X(C10H20N1O3)]\@

Cation e.2

1\1\GINC-R195\FOpt\RM062X\6-31+G(d,p)\C10H20N1O3(1+)\ROOT\20-Jun-2017\0\#M062X\6-31+G** S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610612736\CationE.1iii.freq\1,1\C,0.6107295106,
1.4195373554,0.0392124004\C,-0.7822969963,1.0699183093,-0.5038783586\C,-1.3297250631,-0.3083150455,-
0.1089168219\C,-0.3422738192,-1.3888269986,-0.5344939031\C,1.0931516861,-1.2362941063,-0.005980734
8\N,1.5311820973,0.2176987745,-0.1547372694\O,2.67479817,0.4273903879,-0.3804210111\C,0.6398122837,1
.7244446185,1.5531599748\C,1.2203549159,2.5861886949,-0.7355158937\H,-0.7539807509,1.1376025446,-1.5
986671103\H,-1.4698473997,1.847608313,-0.1560698862\H,-0.3088656063,-1.4214023014,-1.6305587669\H,
-0.6983222263,-2.3642979272,-0.187184651\C,2.0655758051,-2.0880773607,-0.8192766713\C,1.2363481179,
-1.5642694182,1.4971302298\H,0.1240445637,0.972211126,2.1439838638\H,0.1173831901,2.6766502371,1.6
791783281\H,1.6698595133,1.8533944427,1.8961854855\H,1.3785463337,2.3334664076,-1.7874259096\H,2.
163510136,2.9194007687,-0.3009715963\H,0.5068382699,3.411930292,-0.6863767227\H,2.1198858032,-1.75
70008999,-1.8599157906\H,1.6857199497,-3.1122945275,-0.8053981699\H,3.068115197,-2.0874224769,-0.3
901570922\H,0.4724446658,-1.0887550929,2.1067060123\H,2.2389354607,-1.3082281214,1.8498483693\H,1.1
118967182,-2.6470666512,1.5825895741\C,-2.6772898886,-0.5380510894,-0.8008675695\O,-1.5242945681,-
0.4053158722,1.2898351204\O,-3.549254872,0.4194829218,-0.2324575952\H,-2.5844290285,-0.4060617547,
-1.8864214268\H,-3.0120897689,-1.5610993374,-0.5866905218\H,-2.3790781198,0.008503773,1.4915472416
\H,-4.4635032802,0.2492180146,-0.485246127\Version=ES64L-G09RevE.01\State=1-A\HF=-672.9647976\R
MSD=4.659e-09\RMSF=6.056e-06\Dipole=0.0597636,-0.1655936,-0.5627063\Quadrupole=6.3523579,0.46821
91,-6.820577,0.4228083,3.3703052,1.7245898\PG=C01 [X(C10H20N1O3)]\@

Cation e.3

1\1\GINC-R142\FOpt\RM062X\6-31+G(d,p)\C10H20N1O3(1+)\ROOT\19-Jun-2017\0\#M062X\6-31+G** S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610612736\CationE.1iv.freq\1,1\C,-0.0250996669,0
.0221863147,0.017948932\C,0.0083377383,-0.0006457001,1.5518302795\C,1.3865602407,0.0069296442,2.20
68766759\C,2.2209560488,-1.1523881389,1.6580313447\C,2.3674790369,-1.2230699004,0.1285135417\N,1.0
077126584,-0.9658335062,-0.5157851868\O,0.7645861104,-1.5307119834,-1.5277142027\C,0.3448298036,1.
3910617961,-0.5962678081\C,-1.3891895349,-0.4269150981,-0.5027516325\H,-0.5272518516,-0.8915136958,1
.9011178116\H,-0.5593902129,0.8649423471,1.9041686564\H,1.779175275,-2.0940406787,2.0064674104\H,
3.2388734863,-1.1172962474,2.0656447267\C,2.8231096878,-2.6140347052,-0.3081016926\C,3.3107775252,
-0.1531636124,-0.4625219931\H,1.2369545229,1.825756158,-0.1533469631\H,-0.497113438,2.0535219182,-
0.3785581608\H,0.442572454,1.3105926264,-1.6822025439\H,-1.6021051884,-1.4650856641,-0.2339498368\
H,-1.4738961531,-0.3111102768,-1.5838727403\H,-2.139240498,0.2090828927,-0.0270773263\H,2.08326285
45,-3.3782561868,-0.0554002165\H,3.7444170572,-2.8381126474,0.2347605184\H,3.0344737002,-2.6595670
378,-1.3769306517\H,3.0775122802,0.8516533858,-0.1196117349\H,3.2988160259,-0.1970716081,-1.554749
4621\H,4.3182213995,-0.4117355446,-0.1248594153\C,1.2192136672,-0.1404425304,3.727908126\O,1.98127
51857,1.2711285721,1.9270734096\O,0.3451717238,0.8232631739,4.2468654517\H,0.7869513293,-1.116471
8894,3.9680075042\H,2.2147617107,-0.0921035619,4.1986489975\H,2.816403953,1.3539679887,2.40845224
54\H,0.7478965488,1.6985781743,4.1897517375\Version=ES64L-G09RevE.01\State=1-A\HF=-672.956775\
RMSD=9.770e-09\RMSF=1.035e-05\Dipole=0.8901494,-0.3937473,-0.7687415\Quadrupole=3.3828342,-0.996
2875,-2.3865467,-1.5536091,5.4389916,1.3658676\PG=C01 [X(C10H20N1O3)]\@

Cation f

1\1\GINC-R1020\FOpt\RM062X\6-31+G(d,p)\C11H18N1O4(1+)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p)
INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=536870912\NitroxideF.2.freq\1,1\C,0.7603017
407,3.1204906374,-1.0611790525\C,-0.7143443807,2.7270925298,-1.1419100746\C,1.6320382253,1.8822406
154,-0.9453730608\C,1.2897541197,0.9296719686,0.2131765782\C,-1.2412224263,1.8644038453,0.01498914
15\N,-0.2259473786,0.7589159949,0.3006116231\O,0.9817324556,3.9821730203,0.056996192\C,1.16571279
77,4.0365975465,-2.2311857658\H,-0.8716066123,2.1873191636,-2.0838994007\H,-1.3383517112,3.6273765
049,-1.1818294214\H,2.677436507,2.1780039924,-0.8105477323\H,1.5687970915,1.3313518348,-1.89233082
82\C,1.7263692602,1.4664225517,1.595130791\C,1.8909856373,-0.4536070647,-0.0253960847\C,-2.5549581
333,1.1865789069,-0.3693262222\C,-1.4140542088,2.6315903043,1.3449192948\O,-0.6391448099,-0.283963
2868,0.67798729\H,1.4335752696,2.4997294469,1.7657634653\H,2.8185393025,1.4176095075,1.6085659571
\H,1.3477397164,0.8205325324,2.3914248568\H,1.4616318846,-0.934127759,-0.9087622232\H,1.763415237
3,-1.108255787,0.8372129935\H,2.9612708469,-0.3158108485,-0.1966076516\H,-2.424369808,0.4966590973,
-1.2074572444\H,-3.246523231,1.9739799554,-0.6783095649\H,-2.998490545,0.6512947416,0.4707573614\H,-
0.5422454988,3.2193620492,1.621172264\H,-1.6846655491,1.9408283942,2.1476064654\H,-2.2501869979,3.
3195926033,1.1921454247\C,0.9520762935,5.2946973159,-0.3533522262\O,0.9212512113,6.2179734361,0.3
857679527\O,0.9449413998,5.3380593495,-1.7010860284\H,0.5485551023,3.9121491077,-3.1219648658\H,2.2
243071918,3.9256077923,-2.488310204\Version=ES64L-G09RevD.01\State=1-A\HF=-785.0607843\RMSD=
7.162e-09\RMSF=1.566e-05\Dipole=-0.3914631,-3.0762654,-0.6152291\Quadrupole=8.2741426,-10.1848252,
1.9106826,-3.4038423,-1.5949481,-4.4964881\PG=C01 [X(C11H18N1O4)]\@

Cation g.1 CORE

1\1\GINC-R217\Freq\RM062X\6-31+G(d,p)\C10H20N1O4S1(1+)\ROOT\25-Aug-2017\0\#M062X\6-31+G**
SCF=Tight guess=read IOP(2/17=4) INT(Grid=Ultrafine) geom=check Freq=norman maxdisk=2147483648\
CationG.1.a1b2.Methyl.freq\1,1\C,0.6846293655,-0.0421265,-0.1471449388\C,1.7485621576,-1.1263887501,
0.003748351\C,1.1890922871,1.0479669872,-1.0772176156\C,2.4538301983,1.7497333163,-0.565379769\C,3.0
582349702,-0.6127306415,0.6110023592\N,3.4517554868,0.6868326647,-0.0947402391\H,1.9350602549,-1.5
733097889,-0.980307869\H,1.3977025115,-1.9320193353,0.6566428837\H,0.4235069258,1.819028266,-1.207
0757014\H,1.3815723939,0.6091214818,-2.0633050794\C,2.1899542476,2.6484817363,0.6607256428\C,3.13
07374632,2.5529996512,-1.671769457\C,4.1984427302,-1.6052835707,0.406504707\C,2.9193805274,-0.2589
663643,2.1076579791\O,4.6040607448,0.9108242207,-0.2427263842\H,1.5821261509,2.1703772666,1.42773
0278\H,1.6439118675,3.5202665706,0.291398471\H,3.1281665647,2.997593231,1.099675452\H,3.477925019
8,1.9065739393,-2.4819111904\H,3.9690733653,3.1415105031,-1.2971402186\H,2.3823560518,3.237283497
6,-2.0781100599\H,4.4237854584,-1.7443301047,-0.6540022197\H,3.8667058523,-2.563543307,0.812592585
7\H,5.1054619548,-1.3019523002,0.9309990976\H,2.0194822722,0.3099346786,2.338067466\H,3.801649365
8,0.2747417488,2.4704689522\H,2.8537504273,-1.2114844853,2.6395234924\H,0.3939676034,0.3644469696,
0.8281034622\O,-0.4894421084,-0.567603275,-0.7726747293\S,-1.3245258736,-1.65667294,0.1407918129\O,
-0.8096392847,-2.9739551745,-0.1640270941\O,-1.2840539233,-1.1629392742,1.5059334762\C,-2.92176040
79,-1.4302616341,-0.5867494203\H,-2.8407300741,-1.6435088233,-1.6524106117\H,-3.2481478907,-0.40915

50162,-0.3954816101\H,-3.5790846561,-2.1515154443,-0.0981422612\\Version=ES64L-G09RevE.01\State=1-A\HF=-1146.2483429\RMSD=3.984e-09\RMSF=6.312e-06\ZeroPoint=0.3088097\Thermal=0.3264087\Dipole=1.6181314,2.0761658,-0.5505366\ PG=C01 [X(C10H20N1O4S1)]\@

Cation g.2 CORE

1\1\GINC-R216\Freq\RM062X\6-31+G(d,p)\C10H20N1O4S1(1+)\ROOT\25-Aug-2017\0\#M062X\6-31+G**
SCF=Tight guess=read IOP(2/17=4) INT(Grid=Ultrafine) geom=check Freq=norman maxdisk=2147483648\
CationG.1.Methyl.freq\1,1\C,-1.0259447729,0.1636797655,0.1420280865\C,-1.6847344494,1.3874480519,-0.4701532421\C,-1.5747998319,-1.1055776725,-0.4953629754\C,-3.0807099905,-1.2885175161,-0.2800268005\C,-3.2063642229,1.4207084127,-0.2721497388\N,-3.78112,0.0368400661,-0.5974795122\H,-1.4476015778,1.4171424483,-1.5403929585\H,-1.2795090211,2.2979767507,-0.0183695945\H,-1.0734818548,-1.9817475973,-0.0729373539\H,-1.3521725578,-1.0802384895,-1.5690776702\C,-3.4395498856,-1.6189057922,1.1842788073\C,-3.6589504803,-2.3448295998,-1.2159387343\C,-3.8703003261,2.421901838,-1.2122928052\C,-3.612510706,1.7100366282,1.18854835\O,-4.8602244383,-0.0095031401,-1.0804270543\H,-2.9339818273,-0.9850916608,1.9116000575\H,-3.1087367556,-2.6466635475,1.3538681333\H,-4.5201286399,-1.5762342337,1.3434858397\H,-3.5594450657,-2.0503325187,-2.2639148248\H,-4.7069562111,-2.5560458663,-0.9995729531\H,-3.0823427989,-3.2598079481,-1.0622371783\H,-3.736361311,2.1386905064,-2.2595411948\H,-3.38091026,3.3857399995,-1.0541308181\H,-4.9347019589,2.5369853625,-1.0041261396\H,-3.0512573208,1.1298301019,1.9200700831\H,-4.6840609585,1.552995205,1.3365596607\H,-3.3972985338,2.7672744472,1.3630358465\H,-1.1714840436,0.1593166258,1.2296912958\O,0.3759320239,0.2658212735,-0.132535122\N,1.3059960222,-0.3078842639,1.099784828\O,1.1268530474,0.5846378073,2.2256848136\O,0.989402257,-1.7167658661,1.2455421658\C,2.8871212436,-0.0768946669,0.3417764886\H,2.9255870612,-0.6803954373,-0.5641855239\H,3.6211532762,-0.4223115755,1.0718174244\H,3.0154448688,0.9850821017,0.1355603135\\Version=ES64L-G09RevE.01\State=1-A\HF=-1146.24814\RMSD=1.863e-09\RMSF=3.309e-06\ZeroPoint=0.308694\Thermal=0.32636\Dipole=-2.002986,0.5564826,-1.5086872\ PG=C01 [X(C10H20N1O4S1)]\@

Cation g.1

1\1\GINC-R289\FOpt\RM062X\6-31+G(d,p)\C16H24N1O4S1(1+)\ROOT\10-Aug-2017\0\#M062X\6-31+G**
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2684354560\CationG.1.a1b2.freq\1,1\C,1.3592998695,0.013747547,0.2000386889\C,2.0030519728,-0.785641445,-0.9259105726\C,1.8035424472,1.4657877319,0.1284799009\C,3.320912314,1.6509403959,0.258877102\C,3.5332313351,-0.8036641817,-0.8718036919\N,4.0274449005,0.6268734112,-0.6371925091\H,1.6667485718,-0.363423149,-1.880696113\H,1.6621421707,-1.824220745,-0.8825595975\H,1.3359269639,2.0430139065,0.9325606026\H,1.4564259531,1.8897828356,-0.821101449\C,3.8351622235,1.3800248248,1.6881662439\C,3.7565090184,3.0377114913,-0.2041376893\C,4.1388405448,-1.2851837718,-2.1861027945\C,4.0771211557,-1.6405889352,0.3052176628\O,5.047690118,0.9506848691,-1.1415008502\H,3.4274194059,0.4714481852,2.1298494013\H,3.508753817,2.2267823574,2.2971982102\H,4.9273880516,1.3443599391,1.7137271698\H,3.5517348023,3.1876068771,-1.2673054396\H,4.8142559611,3.2219741367,-0.0120820958\H,3.1697300716,3.7652282278,0.361438435\H,3.8967781388,-0.609320972,-3.0103499246\H,3.6968044177,-2.2599884874,-2.404222491\H,5.2214886348,-1.4020087129,-2.122123991\H,3.5667906465,-1.4462621808,1.2477209872\H,5.1537589956,-1.4968418789,0.4283679183\H,3.8981822487,-2.6860315309,0.0417162668\H,1.6003643179,-0.4198415879,1.1790421646\O,-0.0535746018,0.0192861919,0.0199245292\N,-0.8990370461,-1.1874136804,0.7619534696\O,-2.1626581104,-1.1863915951,0.0759850228\O,-0.0170782677,-2.3427190133,0.7920742538\C,-1.0779786448,-0.5571788724,2.4006903694\C,-0.2881135847,-1.0723937867,3.424852919\C,-0.4388353404,-0.5515380759,4.7080563512\C,-1.3648211998,0.4634626789,4.9708991752\C,-2.146526882,0.9555650961,3.9146464358\C,-2.0161094272,0.450404654,2.6282471294\C,-1.5563742745,0.9930013107,6.3665992568\H,0.400851055,-1.8867422018,3.2225637777\H,0.1586112856,-0.9534734666,5.5210999609\H,-2.8777457945,1.7345651404,4.1106053521\H,-2.6371268697,0.812246785,1.8144749286\H,-0.6987561785,0.7637188383,7.001917674\H,-2.4423183883,0.5400172793,6.8230828016\H,-1.7063767985,2.0752845592,6.3609442133\\Version=ES64L-G09RevE.01\State=1-A\HF=-1377.2162532\RMSD=4.714e-09\RMSF=3.740e-06\Dipole=4.1323916,1.8517876,-0.0991034\Quadrupole=3.3162219,-10.7081598,7.3919379,-5.0695334,-23.3786255,1.9014119\PG=C01 [X(C16H24N1O4S1)]\@

Cation g.2

1\1\GINC-R227\Freq\RM062X\6-31+G(d,p)\C16H24N1O4S1(1+)\ROOT\21-Jun-2017\0\#M062X\6-31+G**
SCF=Tight guess=read IOP(2/17=4) INT(Grid=Ultrafine) geom=check Freq=norman maxdisk=2684354560\
NitroxideG.1.a1.freq\1,1\C,1.0257732601,-0.0746962701,0.1887112413\C,1.7191038959,-0.7628535528,-0.9743998268\C,1.5569891536,1.3425844441,0.3545365109\C,3.0558513294,1.3973822534,0.6662188198\C,3.2385356335,-0.880475362,-0.7936586192\N,3.7871955723,0.4654895687,-0.3056638175\H,1.4942276202,-0.2107187213,-1.8947728843\H,1.327613618,-1.7773318357,-1.0967844223\H,1.0312868727,1.8401892831,1.1752117101\H,1.3460421364,1.9024566185,-0.5647781703\C,3.3906630494,0.8828975918,2.0821744712\C,3.62

34202664,2.7987517389,0.4665898928\C,3.9359085789,-1.2055576449,-2.1107031355\C,3.6328965516,-1.9095688302,0.2869024174\O,4.868754062,0.7813865512,-0.6672779754\H,2.8867691234,-0.0480312772,2.3382752328\H,3.0386692995,1.6510442289,2.7753424234\H,4.4697702305,0.7697134773,2.215061778\H,3.5424164872,3.1196097035,-0.5752280022\H,4.6641912247,2.8704270019,0.7851921933\H,3.0255988731,3.476576922,1.0800578158\H,3.8085349427,-0.4022141862,-2.8409348429\H,3.4649971908,-2.1069127641,-2.5097183247\H,4.9999813867,-1.4028385712,-1.9748166215\H,3.048322122,-1.8247060232,1.2021081175\H,4.698570293,-1.8447882502,0.5215863517\H,3.439315078,-2.8952411207,-0.1437105028\H,1.1579730403,-0.6594798443,1.1078844132\O,-0.366336461,-0.0218915506,-0.1305442468\S,-1.3314293856,-0.2467190172,1.1929807843\O,-1.1363070697,-1.6212890045,1.6101073079\O,-1.0157732783,0.8386779127,2.1064896091\C,-2.9009189824,-0.0215531835,0.4467229943\C,-3.453761516,1.2565119422,0.4155467265\C,-4.6968657713,1.4216187143,-0.1832278181\C,-5.3821547371,0.3335587613,-0.7388886565\C,-4.7942630067,-0.9374622156,-0.6847433986\C,-3.5532085796,-1.1294208383,-0.0912811949\C,-6.7451372417,0.5165554464,-1.3494862353\H,-2.9266260105,2.0920111446,0.8642973918\H,-5.1478678627,2.4089037703,-0.2133688341\H,-5.321564019,-1.7881268025,-1.1062735856\H,-3.1012696997,-2.1139101831,-0.028967653\H,-6.8871886431,1.5387765596,-1.7056795091\H,-7.5214076204,0.3108873198,-0.6051252974\H,-6.8987810076,-0.168383905,-2.1862346279\\Version=ES64L-G09RevE.01\State=1-A\HF=-1377.2187284\RMSD=3.492e-09\RMSF=8.793e-06\ZeroPoint=0.389714\Thermal=0.4124173\Dipole=3.5926529,0.4375473,-1.502409\PG=C01 [X(C16H24N1O4S1)]\@

Cation h.1

1\1\GINC-R144\FOpt\RM062X\6-31+G(d,p)\C9H17N4O1(1+)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=402653184\NitroxideH.1.freq\1,1\C,0.6738755754,2.8702173567,-0.7784449591\C,-0.7782512891,2.4017198303,-0.8947541256\C,1.5908306068,1.6553050931,-0.7383956087\C,1.3226287613,0.6950032051,0.4259715368\C,-1.253268927,1.5081849797,0.2587347986\N,-0.1844159446,0.4439774352,0.5193975206\H,-0.8881162664,1.8661811865,-1.8454881194\H,-1.4633585841,3.2566688048,-0.9267591611\H,2.6345423897,1.9745650898,-0.6597857681\H,1.4924220219,1.1209403104,-1.6910735547\C,1.7383825716,1.2756996409,1.7939282219\C,1.9966603111,-0.6551244307,0.2014948563\C,-2.5460052293,0.7786509345,-0.0942335588\C,-1.4206211161,2.2758464432,1.5864285848\O,-0.5462156832,-0.6292902096,0.8614750231\H,1.4147458852,2.304669898,1.945058003\H,2.8310338095,1.2601652863,1.8136546688\H,1.3759378611,0.6509913127,2.6144986922\H,1.5931058741,-1.1635433778,-0.6779078307\H,1.9051339552,-1.3097314686,1.0691243903\H,3.0570478842,-0.4603745556,0.0253186631\H,-2.4050909163,0.0981930785,-0.9379354455\H,-3.2757327611,1.5373253232,-0.3864004561\H,-2.9480394645,0.2218029129,0.753184679\H,-0.586516162,2.9386711846,1.812904507\H,-1.5814956516,1.5887349321,2.4212499543\H,-2.318629905,2.8890336871,1.4756628155\N,1.075960785,3.6264954412,-1.9726807124\H,0.8121165986,3.488112474,0.1202185404\N,0.5898508081,4.7700402401,-2.0225635598\N,0.2032722015,5.8187879613,-2.161172596\\Version=ES64L-G09RevD.01\State=1-A\HF=-646.7876699\RMSD=5.684e-09\RMSF=1.726e-05\Dipole=-0.3352495,-1.2644943,1.3862127\Quadrupole=5.5020932,-2.4931667,-3.0089265,-2.8461873,1.6945435,0.4083144\PG=C01 [X(C9H17N4O1)]\@

Cation h.2

1\1\GINC-R135\FOpt\RM062X\6-31+G(d,p)\C9H17N4O1(1+)\ROOT\19-Jun-2017\0\#M062X\6-31+G** SC F=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610612736\CationH.1.ii.freq\1,1\C,1.2128804741,-0.4934068579,-0.0003536188\C,0.8527080437,0.9007506849,-0.5134335007\C,0.1621665744,-1.4981276462,-0.4727804042\C,-1.2640517254,-1.1902513154,0.0026943467\C,-0.5146527294,1.413091821,-0.04142342\N,-1.5471397224,0.2972530972,-0.2269623984\H,0.8714850219,0.8985649114,-1.6117883386\H,1.599272667,1.6283724428,-0.1797388204\H,0.4107601457,-2.5004087376,-0.1097677608\H,0.1693389339,-1.5406300176,-1.570451929\C,-1.4531884581,-1.4277404287,1.5154765068\C,-2.3028592236,-1.9792417396,-0.7884112973\C,-0.9822767894,2.608340931,-0.8661551332\C,-0.5349927917,1.761985568,1.4614216469\O,-2.6501922569,0.6098303973,-0.5189260583\H,-0.6469624609,-1.0192909352,2.1234041936\H,-1.4650262531,-2.5115030836,1.6565060307\H,-2.4117779543,-1.0310437115,1.8598336086\H,-2.2997025296,-1.7004304442,-1.8453733644\H,-3.308945707,-1.8519118526,-0.3867380464\H,-2.0318721683,-3.0348878034,-0.7131351527\H,-1.1373186571,2.3375853234,-1.9138039015\H,-0.1909729554,3.3602280194,-0.8215106501\H,-1.898488238,3.0478883969,-0.4697728382\H,-0.0637471704,1.0067418855,2.0890696193\H,-1.554665594,1.9464837804,1.8093752157\H,0.0322963822,2.6900581525,1.5683572614\N,2.5683469224,-0.8904631818,-0.4056898972\H,1.2709098086,-0.4916184952,1.090871238\N,2.7274041432,-0.9571023424,-1.6371097876\N,2.9825742683,-1.0490068186,-2.7316133501\\Version=ES64L-G09RevE.01\State=1-A\HF=-646.7858824\RMSD=9.833e-09\RMSF=6.222e-06\Dipole=-1.7383365,0.5151164,0.8700977\Quadrupole=-4.4179994,6.9261219,-2.5081225,3.5360269,-1.2704526,0.1887655\PG=C01 [X(C9H17N4O1)]\@

Cation h.3

1\1\GINC-R163\FOpt\RM062X\6-31+G(d,p)\C9H17N4O1(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramanmaxdisk=402653184\NitroxideH.2.freq\1,1\C,0.8169189 654,2.8543263919,-0.7678035592\C,-0.6630875098,2.4687518005,-0.8454721486\C,1.6788491961,1.6007851 548,-0.6794981022\C,1.3400545733,0.6166121001,0.4529705872\C,-1.1864153986,1.5593342681,0.27900216 34\N,-0.1748088397,0.4414237771,0.5214998823\H,-0.8326555768,1.9686615935,-1.8066715226\H,-1.29729 09469,3.3625920935,-0.8466456483\H,2.7287069226,1.88009143,-0.5507669272\H,1.599796,1.069205254,-1. 6346693202\C,1.7726661182,1.1024801538,1.8544994822\C,1.9426399613,-0.7584085628,0.1723409737\C,- 2.5042703898,0.9024584962,-0.1257748837\C,-1.3520288411,2.2727534465,1.6384734869\O,-0.5938446013, -0.6199144812,0.837628444\H,1.4923242533,2.1338141677,2.0537485766\H,2.8642443235,1.0434063433,1.8 695905688\H,1.384767993,0.433482059,2.6272982084\H,1.5171981391,-1.2106116493,-0.727607326\H,1.81 31552172,-1.4413223118,1.0126600648\H,3.0130377315,-0.6132326108,0.0086836326\H,-2.3793606241,0.24 71299925,-0.9919169041\H,-3.1939681037,1.7040249903,-0.4006313308\H,-2.9473111461,0.3341423657,0.6 926745657\H,-0.464511776,2.8225588994,1.9430843886\H,-1.6407833701,1.5556743058,2.4114349673\H,-2. 1723165591,2.9848920986,1.5125639475\N,1.1386374954,3.7344764349,0.3739159905\H,1.0770009762,3.36 35205639,-1.7047592119\N,0.7254654989,4.8983906793,0.2271683266\N,0.3857903179,5.9710107555,0.182 1686278\Version=ES64L-G09RevD.01\State=1-A\HF=-646.7909957\RMSD=5.819e-09\RMSF=1.030e-05\Di pole=-0.2566844,-1.197414,-0.3888902\Quadrupole=4.2707026,-2.9567685,-1.3139341,-3.0582848,-0.300239, -1.2623138\PG=C01 [X(C9H17N4O1)]\@

Cation h.4

1\1\GINC-R51\FOpt\RM062X\6-31+G(d,p)\C9H17N4O1(1+)\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) S CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\CatH1.freq\1,1\C,0.2287428683,-1.2800856 908,-0.7218952769\C,1.3088006502,-0.520319673,0.0753348413\C,0.7591288554,0.7255725939,0.790342201 \C,-0.477198679,1.365552052,0.1603335512\N,-1.5354867009,0.2871621335,-0.0190366407\C,-1.189012244 9,-1.1863121361,-0.1547527976\C,-0.2248927521,1.9176972867,-1.2580995151\C,-1.0701234952,2.44658103 66,1.061801943\C,-2.2193809116,-1.819235743,-1.0869225593\C,-1.3169540039,-1.7579454467,1.274039903 1\O,-2.6734859095,0.6100495435,-0.0540598409\H,0.4820433056,-2.3449906781,-0.7581497284\H,0.215014 6017,-0.9427932392,-1.7632326515\H,1.5298206729,1.5001655745,0.8347602334\H,0.5397399423,0.462529 6564,1.8292628385\H,0.2191796539,1.1863528023,-1.9347826595\H,0.4769248344,2.7486624956,-1.149429 2776\H,-1.150059042,2.3029880024,-1.6931343862\H,-1.3791457147,2.03177661,2.0251717054\H,-1.919604 9315,2.9449332067,0.5937822886\H,-0.2904930765,3.1894435108,1.2440503213\H,-2.2279934077,-1.327462 4508,-2.063783268\H,-3.2228402603,-1.7911714262,-0.6610362926\H,-1.9358534418,-2.8640586672,-1.2314 021356\H,-0.5780967559,-1.3573797672,1.9681315169\H,-1.1406492352,-2.8338928263,1.1934541242\H,-2. 3278309627,-1.5989491954,1.6570839888\N,1.8873069913,-1.3446331591,1.1549082557\H,2.0965016895,-0. 2254608986,-0.6290380053\N,2.6996971957,-2.1948515864,0.7482405743\N,3.4448502644,-2.9941939208,0. 4766967487\Version=ES64L-G09RevD.01\State=1-A\HF=-646.7884733\RMSD=9.553e-09\RMSF=5.137e-06 \Dipole=-1.1195884,0.9764234,-0.7100811\Quadrupole=-2.2583314,5.6318056,-3.3734742,3.0110928,-0.9573 54,0.5962079\PG=C01 [X(C9H17N4O1)]\@

Cation i

1\1\GINC-R86\FOpt\RM062X\Gen\C9H17Br1N1O1(1+)\ROOT\05-Dec-2016\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2684354560\CatJ.New.1.freq\1,1\C,0.1079760128,-1.351800 8824,1.3946857034\C,-0.1890766683,-1.2461847942,-0.1114670482\C,0.393489014,0,-0.7608496351\C,-0.18 90766683,1.2461847942,-0.1114670482\C,0.1079760128,1.3518008824,1.3946857034\N,-0.1895510945,0,-2.0 451522092\O,-0.640473739,0,3.1392689431\C,1.5904908554,-1.6545129725,1.6942649839\C,-0.7876643322,- 2.3890163444,2.064430211\H,-1.274148681,-1.2571673489,-0.2691654413\H,0.2115042942,-2.1523067248,- 0.5756078035\H,-1.274148681,1.2571673489,-0.2691654413\H,0.2115042942,2.1523067248,-0.5756078035\ C,-0.7876643322,2.3890163444,2.064430211\C,1.5904908554,1.6545129725,1.6942649839\H,2.2840154388,- 1.0487562881,1.1126579712\H,1.7501657637,-2.7015703225,1.4245604236\H,1.8084669918,-1.5426841375, 2.7596059213\H,-1.8421321676,-2.1071811006,2.006702777\H,-0.5163585845,-2.5522182838,3.1083274188\ H,-0.6554341678,-3.3282164104,1.5223526709\H,-1.8421321676,2.1071811006,2.006702777\H,-0.655434167 8,3.3282164104,1.5223526709\H,-0.5163585845,2.5522182838,3.1083274188\H,2.2840154388,1.0487562881, 1.1126579712\H,1.8084669918,1.5426841375,2.7596059213\H,1.7501657637,2.7015703225,1.4245604236\Br,- 0.0425240414,0,-2.6564491145\H,1.4845603483,0,-0.7286779799\Version=ES64L-G09RevE.01\State=1-A\ HF=-3056.5498603\RMSD=7.903e-09\RMSF=5.275e-06\Dipole=0.4064171,0,2.5050966\Quadrupole=-3.6707 733,5.504596,-1.8338227,0,1.1501882,0\PG=CS [SG(C1H1Br1N1O1),X(C8H16)]\@

Cation k.1

1\1\GINC-R424\Freq\RM062X\6-31+G(d,p)\C12H20N1O2(1+)\ROOT\28-Apr-2016\0\#N Geom=AllCheck G uess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\NitroxideK.2.freq\1,1\C,0.4323795726,

2.6182104066,-0.9071150798\C,-0.9752807662,2.0406717002,-0.9711010762\C,1.4421280701,1.4936066289,-0.6654759499\C,1.1968519551,0.6479265511,0.594766096\C,-1.4198999742,1.2348283238,0.2610768482\N,-0.2877056549,0.3025122742,0.6813992461\H,-1.0495998964,1.399176755,-1.856735157\H,-1.6986439482,2.8520850795,-1.0937291661\H,2.4591080886,1.8887886947,-0.5762517854\H,1.4431523618,0.8352184807,-1.5423263066\C,1.5338093591,1.3853562913,1.9102342569\C,1.9649547172,-0.6704361432,0.5257169544\C,-2.6281716492,0.3607586707,-0.0688867096\C,-1.7235360758,2.1052984968,1.5016943564\O,-0.581929672,-0.7405757249,1.1591047421\H,1.092480269,2.3779453922,1.9673864171\H,2.6220511422,1.4933259135,1.9274646035\H,1.2399819553,0.7801807235,2.7720304828\H,1.6214168704,-1.2948685898,-0.3034544196\H,1.8921840835,-1.2363827939,1.455027507\H,3.0153020524,-0.4233797415,0.3547375627\H,-2.3878910307,-0.3919474477,-0.8246851527\H,-3.3994633217,1.0190488964,-0.4754978197\H,-3.0300817064,-0.1342194041,0.8157449151\H,-0.9422911636,2.8311046999,1.7132771019\H,-1.9192850285,1.4712794259,2.3705446029\H,-2.6390553813,2.6548401328,1.2668981166\O,0.4550173829,3.5985758866,0.1085742685\H,0.6550934119,3.079946841,-1.8801983109\C,1.5016077684,4.5591629628,-0.0127763375\C,1.6141340062,5.2824052502,1.2517101486\C,1.7190239104,5.8807511136,2.2923259531\H,1.2738089187,5.2512860298,-0.8335270241\H,2.4580532847,4.0674572706,-0.2371994767\H,1.8121360887,6.425340953,3.2073555916\Version=ES64L-G09RevD.01\State=1-A\HF=-673.8608339\RMSD=3.779e-10\RMSF=3.563e-06\ZeroPoint=0.3083522\Thermal=0.3245144\Dipole=-0.1135996,-1.0258872,-0.5012205\PG=C01 [X(C12H20N1O2)]\@

Cation k.2

1\GINC-R99\Freq\RM062X\6-31+G(d,p)\C12H20N1O2(1+)\ROOT\19-Jun-2017\0\#M062X\6-31+G** SCF=Tight guess=read IOP(2/17=4) INT(Grid=Ultrafine) geom=check Freq=norman maxdisk=1610612736\NitroxideK.3.freq\1,1\C,-0.8477019938,-0.7582589275,0.1225350519\C,0.1415806349,-1.4070471685,-0.8431598143\C,-0.7514709429,0.7576582105,-0.0000762237\C,0.6388194404,1.3332798964,0.2991878779\C,1.6060692923,-1.0293584181,-0.5995173422\N,1.6904773003,0.4891414632,-0.4263016534\H,-0.1514838049,-1.1270094888,-1.8622986757\H,0.0717500517,-2.496627613,-0.7732712064\H,-1.4530166974,1.23790317,0.689379784\H,-1.0583039573,1.0365574525,-1.0152613267\C,1.0064349981,1.2626822249,1.7961982764\C,0.7749612109,2.7654828784,-0.2081508946\C,2.4919746382,-1.4009858854,-1.78423405\C,2.1704320389,-1.6408046547,0.7000245278\O,2.6506108107,1.0424140178,-0.841821792\H,0.7839414685,0.2984765823,2.2514939015\H,0.3991012516,2.0208351167,2.2970306342\H,2.0587155996,1.5117127279,1.9565545017\H,0.6844793759,2.8150512595,-1.2962860463\H,1.7177528392,3.2224847479,0.0954140953\H,-0.0450338841,3.3405692895,0.2280270583\H,2.2087672735,-0.8501161871,-2.6848104194\H,2.3419642889,-2.4658739119,-1.9754803389\H,3.5496058946,-1.2316948053,-1.5771289914\H,1.4942349352,-1.5524224428,1.5492805486\H,3.1427086152,-1.2092310207,0.9522154312\H,2.3126936279,-2.7053264443,0.497517343\O,-2.1570697496,-1.1272904076,-0.2466405546\H,-0.6477064922,-1.0773277874,1.155833704\C,-2.785448307,-2.0739441576,0.6076418967\C,-2.0255069491,-3.324744065,0.7564550338\C,-1.4092569406,-4.3513661986,0.9071737488\H,-3.7574392901,-2.2780819057,0.1549307148\H,-2.9540539663,-1.63303841,1.5995687611\H,-0.8969926111,-5.2805691375,1.0373664388\Version=ES64L-G09RevE.01\State=1-A\HF=-673.8589033\RMSD=2.109e-09\RMSF=4.848e-06\ZeroPoint=0.3080633\Thermal=0.3243417\Dipole=1.2540033,0.7003785,0.4010355\PG=C01 [X(C12H20N1O2)]\@

Cation k.3

1\GINC-R105\FOpt\RM062X\6-31+G(d,p)\C12H20N1O2(1+)\ROOT\19-Jun-2017\0\#M062X\6-31+G** SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610612736\NitroxideK.3i.freq\1,1\C,-0.6620434225,-0.8126116559,0.6197969166\C,0.2858853963,-1.598760634,-0.2862669083\C,-0.7434239139,0.6269791934,0.1363708751\C,0.5957209377,1.3709271051,0.1508519208\C,1.7174506654,-1.0507930866,-0.309112641\N,1.6613697537,0.4702522563,-0.4795569668\H,-0.1274635312,-1.607537489,-1.3027667164\H,0.3701114001,-2.6397068763,0.044795899\H,-1.4354306653,1.1900313944,0.7701424537\H,-1.160050872,0.6308720931,-0.8780145715\C,1.0992499053,1.6797394133,1.5764143099\C,0.5365778286,2.6522589041,-0.6750374858\C,2.5182165895,-1.6086395306,-1.4818602503\C,2.468775956,-1.2996506875,1.0161007759\O,2.5260187738,0.9879884667,-1.0997733856\H,1.0246212431,0.8309806862,2.2547965269\H,0.4572762946,2.476014275,1.9615337133\H,2.1273131351,2.0510506148,1.5590767056\H,0.3461982432,2.440300178,-1.7303047034\H,1.4494703918,3.242488597,-0.5856774106\H,-0.2976099364,3.2436995616,-0.2908391373\H,2.091894903,-1.3019073256,-2.4405050928\H,2.4658890707,-2.6978542947,-1.4181089613\H,3.5668146903,-1.310541243,-1.443241472\H,1.8722068955,-1.0740149181,1.899163222\H,3.4084448883,-0.7419182455,1.0482079617\H,2.7055034882,-2.366473801,1.0368613501\O,-1.978377635,-1.30196085,0.5569405735\H,-0.3109494464,-0.8548647955,1.6607588492\C,-2.1717450437,-2.6392291977,1.00568212\C,-1.5198801066,-2.9276640668,2.2909036346\C,-0.9730764898,-3.1808136723,3.3364242592\H,-1.8206343542,-3.352781976,0.2487957639\H,-3.2527685205,-2.7586561276,1.099346438\H,-0.5255865125,-3.4200222652,4.2773914341\Version=ES64L-G09RevE.01\State=1-A\HF=-673.8594813\RMSD=9.872e-09\RMSF=2.021e-05\Dipole=1.3342669,0.5932406,-0.25

30716\Quadrupole=-3.8329246,5.5495156,-1.716591,0.8022228,-0.7708697,-1.7129015\PG=C01 [X(C12H20N1O2)]\@

Cation k.4

1\1\GINC-R51\FOpt\RM062X\6-31+G(d,p)\C12H20N1O2(1+)\ROOT\03-Dec-2017\0\#M062X\6-31+G(d,p)
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\CatK5.freq\1,1\C,0.2565263066,-1.064650
4637,-1.0867239068\C,1.2983858866,0.0341314248,-0.8308518975\C,0.7220056985,1.2237752603,-0.039386
3678\C,-0.7999307779,1.3795214905,-0.0320723977\N,-1.4411370132,0.0375691507,0.2954070141\C,-0.735
0303539,-1.282432004,0.0552526783\C,-1.3773590058,1.7702688162,-1.4088398396\C,-1.252061659,2.3724
43307,1.0382151797\C,-1.7909490298,-2.3260829156,-0.2949390841\C,-0.0591113348,-1.6137339454,1.4042
25789\O,-2.5340025966,0.0314179339,0.7507193318\H,0.7633649928,-2.0194938238,-1.2508285048\H,-0.29
83129385,-0.8559063723,-2.0071494333\H,1.1283803105,2.1654488967,-0.4188591361\H,1.0802967066,1.13
4126147,0.9902223415\H,-1.0430378707,1.1184601621,-2.2169231559\H,-1.0214627392,2.7818383279,-1.62
02061846\H,-2.4694175985,1.7890422547,-1.3807811038\H,-0.9785032935,2.025471456,2.0384477589\H,-2.
3271282658,2.5507595307,0.998625398\H,-0.7364559401,3.3170982439,0.8518397588\H,-2.3479177903,-2.0
434518804,-1.1928280957\H,-2.4896281684,-2.4909235922,0.525868207\H,-1.2669370595,-3.2632540238,-0.
496199788\H,0.6607292312,-0.859922244,1.7228826248\H,0.498171436,-2.5420667194,1.2510455873\H,-0.8
181828285,-1.7676836964,2.1748190113\O,2.3871283408,-0.4082043507,-0.0423199765\H,1.6766742689,0.3
718742991,-1.8060578847\C,2.9603409315,-2.7139433999,-0.4897808013\C,2.7170120851,-3.8870509016,-0.
3445325454\H,2.5317489424,-4.9320579603,-0.2150937762\C,3.3051175543,-1.2936339938,-0.6689072055\
H,4.2742241566,-1.1040450947,-0.2011069128\H,3.3955794157,-1.0607793197,-1.7383226825\Version=ES6
4L-G09RevD.01\State=1-A\HF=-673.8600437\RMSD=7.977e-09\RMSE=4.699e-06\Dipole=-1.0339323,0.623
0916,-0.4047642\Quadrupole=-1.4119025,8.2475917,-6.8356892,-4.0520609,-2.2066502,-1.0653384\PG=C01
[X(C12H20N1O2)]\@

Cation k.5

1\1\GINC-R51\FOpt\RM062X\6-31+G(d,p)\C12H20N1O2(1+)\ROOT\03-Dec-2017\0\#M062X\6-31+G(d,p)
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\CatK3.freq\1,1\C,-0.6773280693,0.993645
0484,0.0029483343\C,-1.0730295018,-0.2565705366,0.8039385489\C,0.0874034477,-1.2521811982,0.982598
71\C,1.1149119743,-1.2635071168,-0.1506490036\N,1.621633968,0.1568955111,-0.3369209686\C,0.8001876
111,1.3776372269,0.0481481926\C,0.5033808533,-1.648376949,-1.5154865761\C,2.319818386,-2.143442543
1,0.1725757985\C,1.1285010103,2.4873184694,-0.9481004637\C,1.2878657704,1.7531788479,1.4630861666\
O,2.6989346957,0.3209716542,-0.7994558561\H,-1.2445519581,1.8578484262,0.3603273893\H,-0.98276272
15,0.8426844047,-1.0367151578\H,-0.3232941196,-2.2655335783,1.0379676745\H,0.60584205,-1.085327371
7,1.9321772801\H,-0.3894849829,-1.0747030998,-1.7627552374\H,0.2063746003,-2.6972333357,-1.4335759
782\H,1.2505163429,-1.5590847604,-2.3077958339\H,2.8423179963,-1.7895860496,1.0658734576\H,3.02284
6001,-2.1929597754,-0.6596242324\H,1.9477331398,-3.1510678575,0.370253316\H,0.911921605,2.17389659
12,-1.9730303966\H,2.1703378122,2.8018568739,-0.8789930015\H,0.4917677738,3.3423583017,-0.71085725
03\H,1.0586776604,0.9953000153,2.2134922352\H,0.764382144,2.6720323199,1.739580493\H,2.3617607727,1
.9543705735,1.4617943766\O,-2.1394728329,-0.8335114325,0.0750260536\H,-1.4296196128,0.0387163639,1.7
990514816\C,-3.7652188365,-0.7374303518,1.8450372377\C,-4.3289355069,-0.0569975923,2.6658592039\H,
-4.8500097948,0.5368360884,3.3858718786\C,-3.0727591947,-1.5725584976,0.8551407857\H,-2.5810213317,-
2.413881381,1.3636902718\H,-3.7883671519,-1.9841832893,0.1410410698\Version=ES64L-G09RevD.01\St
ate=1-A\HF=-673.8596984\RMSD=7.910e-09\RMSE=1.004e-05\Dipole=1.3409147,0.2513542,0.0763792\Qua
drupole=0.5162517,3.8876934,-4.4039451,0.5892241,-5.3388129,2.0977984\PG=C01 [X(C12H20N1O2)]\@

Cation l.1 1\1\GINC-R136\FOpt\RM062X\6-31+G(d,p)\C12H20N1O3(1+)\ROOT\20-Jul-2017\0\#M062X\6-3
1+G** SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483648\CatL.1iii.freq\1,1\C,-0.50185
61153,-0.0172980785,0.8969292446\C,-0.044040377,-1.2579830851,0.1492242114\C,-0.0612057822,1.23165
40366,0.1409087858\C,1.4594372489,1.3570635777,0.0032816489\C,1.4797341595,-1.3530298044,-0.001221
7733\N,2.0191786368,0.0075733524,-0.4563426212\H,-0.5151411657,-1.269810804,-0.8408494216\H,-0.371
9578448,-2.1607341442,0.673945029\H,-0.4078775432,2.1273042685,0.6642945082\H,-0.5247468542,1.2205
718818,-0.85326165\C,2.1549816438,1.6710976305,1.344810486\C,1.8480644057,2.3919267981,-1.04775414
6\C,1.8747368729,-2.3766824774,-1.0611920178\C,2.1964140668,-1.6612805585,1.3301722579\O,2.9613956
336,0.0138016661,-1.1721137117\H,1.7952831935,1.0625183366,2.1732421411\H,1.9182851884,2.71327216
96,1.5732615862\H,3.240601467,1.5780004869,1.2570386567\H,1.5019876693,2.1022381813,-2.0433465692\
H,2.9248358853,2.5636547175,-1.0771197227\H,1.3556499347,3.3278032341,-0.7741876044\H,1.517278564
8,-2.0857216207,-2.0523401146\H,1.3973687752,-3.3212675307,-0.7904403034\H,2.9533948679,-2.5333189
806,-1.0996966244\H,1.843938057,-1.0543222304,2.1631312979\H,3.2792853806,-1.552901977,1.227619495
8\H,1.980856574,-2.7078484015,1.5598778199\O,-1.9204876248,-0.0805020025,0.9491631567\H,-0.1225816

958,0.0014928457,1.9240982126\C,-2.5049031041,0.7224626969,1.8878962436\O,-1.8502447883,1.4491182136,2.5973736874\C,-3.9730368269,0.5649095195,1.8902293403\C,-4.708113956,1.2712888544,2.749013201\H,-4.3986117094,-0.1358650012,1.1806186969\H,-4.2334580588,1.9596539194,3.4423592913\H,-5.787674779,1.1754303097,2.7775372808\Version=ES64L-G09RevE.01\State=1-A\HF=-749.1355991\RMSD=4.546e-09\RMSF=6.149e-06\Dipole=1.5477218,-0.6276759,-0.9284169\Quadrupole=10.6943642,-1.0835901,-9.610774,-2.7545236,-5.881555,-0.0879059\PG=C01 [X(C12H20N1O3)]\@

Cation I.2

1\1\GINC-R119\FOpt\RM062X\6-31+G(d,p)\C12H20N1O3(1+)\ROOT\20-Jul-2017\0\#M062X/6-31+G** SC F=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483648\CatL.iv.freq\1,1\C,-0.4879620677,-0.0455493626,0.8998917578\C,-0.0226405303,-1.279239624,0.1453415108\C,-0.0627092931,1.2096693811,0.1453883167\C,1.456164046,1.3503853895,0.0037100352\C,1.5018019157,-1.359437769,-0.0102268569\N,2.0269301829,0.0077473779,-0.4625182585\H,-0.4959218731,-1.2914450386,-0.8437291555\H,-0.3400673394,-2.1869733393,0.6679566923\H,-0.4159525605,2.1008271279,0.6719987749\H,-0.5291939445,1.1968078912,-0.8473773149\C,2.152271504,1.6667043124,1.3444783494\C,1.8319324453,2.3924011597,-1.0448947076\C,1.902657754,-2.3758604293,-1.0749689632\C,2.2260427836,-1.6654082053,1.3175222495\O,2.9664455007,0.0250534309,-1.1816510477\H,1.7983397451,1.0543701513,2.1726592722\H,1.9086228357,2.7067518755,1.5754147051\H,3.2383601482,1.581522179,1.2544097892\H,1.4855246016,2.1030665991,-2.0404799715\H,2.9070079818,2.574054779,-1.0768030021\H,1.331853118,3.3227270049,-0.7663388846\H,1.538503298,-2.0855248738,-2.0638708657\H,1.436051178,-3.3260853933,-0.8051720746\H,2.9826458617,-2.5215963688,-1.1182338258\H,1.8742817452,-1.0617997969,2.15318064\H,3.3077159974,-1.5502640182,1.2098702808\H,2.0179613568,-2.7136392446,1.546576587\O,-1.9055686552,-0.1209943694,0.9629710753\H,-0.1002692635,-0.0279012515,1.9237546539\C,-2.4840221421,0.6780122539,1.9090718423\O,-1.8228307375,1.4049460551,2.6122034061\C,-3.9539329586,0.5562157689,1.9685932709\C,-4.6603609045,-0.2522682725,1.1785190739\H,-4.4130965802,1.1893107804,2.7199694347\H,-4.1810233859,-0.8782939043,0.4331305946\H,-5.7403117631,-0.3045822561,1.2628226159\Version=ES64L-G09RevE.01\State=1-A\HF=-749.134205\RMSD=4.025e-09\RMSF=9.621e-06\Dipole=1.5760963,-0.7465756,-1.0966678\Quadrupole=11.4634318,-0.6245939,-10.8388379,0.7597343,-2.1390777,-1.5460794\PG=C01 [X(C12H20N1O3)]\@

Cation I.3

1\1\GINC-R376\FOpt\RM062X\6-31+G(d,p)\C12H20N1O3(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=536870912\NitroxideL.2i.freq\1,1\C,0.7094063469,2.5781650325,-0.7193739094\C,-0.7642971354,2.1991464716,-0.8239504578\C,1.5756533597,1.3365913819,-0.5826236639\C,1.2039388519,0.3706682368,0.5559763276\C,-1.3139354298,1.3208675765,0.3098870117\N,-0.3140222139,0.2015882792,0.592317879\H,-0.9050865941,1.6734541052,-1.7759882453\H,-1.3797207477,3.1019734317,-0.8685841525\H,2.6198328803,1.6238985407,-0.4261557505\H,1.5305767415,0.7908637574,-1.5320628065\C,1.6035636586,0.8841008982,1.9565537076\C,1.8086829688,-1.010798012,0.3172816068\C,-2.6305654442,0.664473002,-0.097126067\C,-1.4943666206,2.0729015382,1.6464054707\O,-0.7424541717,-0.8561256658,0.9083861981\H,1.3207055825,1.9201082148,2.1244902831\H,2.6939098851,0.8195944609,2.0024986264\H,1.1915821358,0.2375167186,2.7359147353\H,1.4039241091,-1.4781474641,-0.5843916451\H,1.6560888307,-1.6781269522,1.1662800154\H,2.8832155993,-0.8718388787,0.1767513509\H,-2.4980033789,-0.0126055015,-0.9451459185\H,-3.3078485074,1.4653156132,-0.4027279037\H,-3.0908623465,0.1196175341,0.7279574331\H,-0.6122167983,2.6340135225,1.9451953775\H,-1.7917793009,1.3811263868,2.4390094465\H,-2.3114604135,2.7818794831,1.4872889376\O,0.9806212345,3.4360220716,0.3935138896\H,0.9844765403,3.1095068476,-1.6353890537\C,0.6006957358,4.7423204293,0.2401885669\O,0.0274050223,5.1260523059,-0.7484826137\C,0.9733835114,5.5502074422,1.420251639\C,0.6490778637,6.8427782836,1.4614280732\H,1.5157833861,5.0529133893,2.2175859601\H,0.1147605372,7.3007160174,0.6338457549\H,0.9132643213,7.4637615012,2.3100338969\Version=ES64L-G09RevD.01\State=1-A\HF=-749.1367095\RMSD=9.218e-09\RMSF=6.133e-06\Dipole=0.0349404,-1.6156026,0.531713\Quadrupole=-0.1612192,6.5636371,-6.4024179,-0.2730402,0.9086749,7.0540553\PG=C01 [X(C12H20N1O3)]\@

Cation I.4

1\1\GINC-R374\FOpt\RM062X\6-31+G(d,p)\C12H20N1O3(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=536870912\NitroxideL.2ii.freq\1,1\C,0.5986418156,2.6131407932,-0.6641556618\C,-0.8396415871,2.1399150377,-0.851537259\C,1.5341861521,1.4262753839,-0.5012077066\C,1.166918031,0.4174406791,0.601544761\C,-1.3897218126,1.2128041844,0.2419008427\N,-0.3370715745,0.1525434827,0.5581902743\H,-0.892341664,1.6183318517,-1.8148106646\H,-1.5117870057,2.9991985765,-0.9218936807\H,2.5489855405,1.7749324654,-0.2867815421\H,1.5720054386,0.896368559,-1.4598249826\C,1.458569448,0.9277139807,2.0290452796\C,1.871368395,-0.9176348495,0.3729401275\C,-2.6410249753,0.482801493,-0.2391859634\C,-1.6837529113,1.9334691799,1.5757806813\O,-0.712215984

7,-0.9358182466,0.8351901751\H,1.0750669175,1.9293951141,2.2060147203\H,2.5472703433,0.9569646647,2.1249217026\H,1.0694378579,0.228951864,2.7743373662\H,1.5459616405,-1.3908950907,-0.5573127291\H,1.7170067185,-1.6108097783,1.2005762425\H,2.9407427252,-0.7083618785,0.2932169792\H,-2.4245052437,-0.1721090832,-1.0873387406\H,-3.350854203,1.2448125891,-0.5691097963\H,-3.1069942324,-0.1017188293,0.5550324953\H,-0.8598112434,2.5539947634,1.9208473114\H,-1.9672192363,1.2131068205,2.3478066476\H,-2.5418639719,2.5837363093,1.384666606\O,0.7622359794,3.4647774928,0.4750060976\H,0.8848052634,3.1767353597,-1.5572659545\C,0.2762837407,4.7353908846,0.3349357549\O,-0.3089446343,5.0865685903,-0.6588713267\C,0.5272516987,5.5941778775,1.5121523492\C,1.2818757407,5.2306065605,2.5491178539\H,0.057296964,6.5696979361,1.4473805265\H,1.7700196818,4.2615984544,2.5851831822\H,1.4458401879,5.9054468078,3.3820380313\Version=ES64L-G09RevD.01\State=1-A\HF=-749.1352228\RMSD=3.855e-09\RMSF=8.011e-06\Dipole=0.2307852,-1.7897624,0.5283003\Quadrupole=2.1285672,1.2250615,-3.3536287,0.7750145,1.6743739,8.0165999\PG=C01 [X(C12H20N1O3)]\@\

Cation I.5

1\1\GINC-R166\FOpt\UM062X\6-31+G(d,p)\C12H20N1O3(2)\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\RadL1.freq\0,2\C,-0.1106290447,0.6112446313,1.0451305375\C,0.6115067558,-0.4740402528,0.2381560476\C,-0.3023979531,-1.2027336905,-0.7478426815\C,-1.7653177524,-1.2923208639,-0.3016141415\N,-2.2548033771,0.0792178024,-0.0125764576\C,-1.358705883,1.1986825268,0.3770437998\C,-1.9382240476,-2.1650486601,0.9509006345\C,-2.6027729011,-1.86728875,-1.4449752791\C,-2.1028717286,2.0738835049,1.3866227499\C,-1.0139622071,2.0308989157,-0.8675917359\O,-3.5054516718,0.3022942197,-0.096227009\H,0.5922609847,1.4197199877,1.268245621\H,-0.4024954345,0.1896021948,2.0131104803\H,0.073952455,-2.2147082271,-0.9295055962\H,-0.2633291798,-0.6756842457,-1.7064978676\H,-1.3101506533,-1.8279071145,1.7801459842\H,-1.6756319237,-3.2030514798,0.7225280538\H,-2.9824456529,-2.1308804734,1.2731607667\H,-2.5568337722,-1.2119013164,-2.3194765553\H,-3.6468240412,-1.9640313319,-1.1454258156\H,-2.2129951691,-2.8523737093,-1.7185310812\H,-2.4414441062,1.4756974765,2.2374258695\H,-2.9765645802,2.536747797,0.9263884671\H,-1.4288583279,2.8560595885,1.7486110855\H,-0.4004423209,1.4748215111,-1.5800668478\H,-0.4563911638,2.9251804911,-0.5705881876\H,-1.9388201652,2.3423697422,-1.3611528734\O,1.6651911197,0.0950797045,-0.5693097311\H,1.08280061,-1.172716795,0.934580579\C,2.8039483481,0.4177064611,0.0708121214\O,2.9731291348,0.2599799764,1.2588023301\C,3.803707811,0.985259343,-0.8721616817\C,4.9974909872,1.3682932256,-0.4240594116\H,3.5096831348,1.0648656265,-1.9134696728\H,5.2405982753,1.265883571,0.6296945707\H,5.745453441,1.7846186126,-1.089807072\Version=ES64L-G09RevD.01\State=2-A\HF=-749.3911219\S2=0.755238\S2-1=0.\S2A=0.750018\RMSD=4.667e-09\RMSF=6.793e-06\Dipole=1.0490068,-0.1320037,-0.4997303\Quadrupole=-5.4155795,5.0012405,0.4143391,4.7020335,-5.5341644,-0.2057908\PG=C01 [X(C12H20N1O3)]\@\

Cation I.6

1\1\GINC-R170\FOpt\UM062X\6-31+G(d,p)\C12H20N1O3(2)\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\RadL4.freq\0,2\C,-0.35234564,-0.8822953034,-0.5519071225\C,0.7005537199,-0.3295525292,0.4070936696\C,1.2463942233,-1.3820776586,1.3807939454\C,0.2623013044,-2.5095954547,1.7111598248\N,-0.2207213419,-3.1129981626,0.443046145\C,-0.2424439934,-2.3821359504,-0.8500858663\C,-0.9426868278,-2.0057876964,2.5204318682\C,0.9932310553,-3.5926878006,2.5064299794\C,-1.4787600608,-2.8300278193,-1.6306832549\C,1.0232152389,-2.7270051425,-1.6490078799\O,-0.6445015623,-4.3133352392,0.4688389833\H,-0.2945211698,-0.3259200616,-1.4931173984\H,-1.3459636794,-0.6913550629,-0.1325073599\H,1.5612951778,-0.8981867296,2.3093720579\H,2.143448079,-1.8259503274,0.9342956215\H,-1.4596393221,-1.1804749773,2.0228529251\H,-0.6117083756,-1.6572055412,3.5037535825\H,-1.6533353148,-2.8252068973,2.6585464102\H,1.8019862095,-4.0245821774,1.9099916566\H,0.3078917157,-4.3943204414,2.7839923798\H,1.4177945018,-3.149932639,3.4122703844\H,-2.384825115,-2.675662782,-1.0375777355\H,-1.4132675602,-3.8891171735,-1.8821075011\H,-1.5530733937,-2.2448125765,-2.5522892095\H,1.9296305767,-2.3562670305,-1.1657128835\H,0.966445045,-2.2773088496,-2.6455854359\H,1.0956953433,-3.81289632,-1.7562228485\O,1.78327552,0.1816914001,-0.402793832\H,0.2895777813,0.5196516568,0.9611929613\C,2.6334926637,1.0281914877,0.2057721899\O,2.5296593434,1.3646193039,1.3636869417\C,3.6940807714,1.4858660519,-0.7305898416\C,4.6335903228,2.3299048004,-0.3093159359\H,3.6563368405,1.1012702438,-1.7444098911\H,4.6244416,2.6839612907,0.7175878444\H,5.4185063232,2.6799321088,-0.9706553747\Version=ES64L-G09RevD.01\State=2-A\HF=-749.3913538\S2=0.755241\S2-1=0.\S2A=0.750018\RMSD=9.447e-09\RMSF=1.000e-05\Dipole=0.4456935,0.9382995,-0.5644039\Quadrupole=4.7981923,-8.1549147,3.3567225,-1.6737626,-2.7514454,-3.6926495\PG=C01 [X(C12H20N1O3)]\@\

Cation m.1

1\1\GINC-R207\FOpt\RM062X\6-31+G(d,p)\C10H18N1O3(1+)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideM. li.freq\1,1\C,-2.12546

56685,-0.014579322,0.8558054535\C,-1.5991954293,1.2402973021,0.1550985852\C,-1.5532834069,-1.2513888651,0.158938051\C,-1.949885506,-1.3675831077,-1.3202258109\C,-1.9997465603,1.3372430813,-1.3243882029\N,-1.7241178897,-0.011577261,-1.9908354023\H,-0.5065196745,1.2660871141,0.2381690608\H,-1.9802895895,2.1471497412,0.6365870206\H,-1.9007702591,-2.1701632025,0.6432439714\H,-0.4604006735,-1.2366521044,0.2420333551\C,-3.4435519831,-1.6978092272,-1.5169384606\C,-1.083659222,-2.3882348431,-2.0515242662\C,-1.1716922429,2.3868725593,-2.0588821955\C,-3.504559029,1.6115868815,-1.5220289154\O,-1.3517835239,-0.0064449936,-3.1142608047\H,-4.1056335417,-1.1043655584,-0.8880895397\H,-3.5651608608,-2.7475208106,-1.237835197\H,-3.7364355158,-1.5903834563,-2.564616815\H,-0.0331672849,-2.0865927772,-2.0666274629\H,-1.4229499005,-2.5579318634,-3.0742063205\H,-1.1605482642,-3.329279048,-1.5019913485\H,-0.1107948905,2.1241116954,-2.0731195368\H,-1.2832430661,3.3261307779,-1.5122446318\H,-1.516954051,2.5407986189,-3.0820609404\H,-4.1443581557,0.9960714382,-0.8913338673\H,-3.7932219636,1.4902347053,-2.5693581136\H,-3.6647904794,2.656952762,-1.2461344642\H,-3.2186014173,-0.0347428881,0.8632093272\C,-1.729020044,-0.00519274,2.3245444891\O,-2.508605756,-0.0191628565,3.2369758039\O,-0.3927051942,0.0207096889,2.4704768112\H,-0.1832689562,0.0257985591,3.4192903672\Version=ES64L-G09RevD.01\State=1-A\HF=-671.7762197\RMSD=9.320e-09\RMSF=1.131e-05\Dipole=0.1560536,0.0009079,-1.6092203\Quadrupole=-3.4124825,6.0549881,-2.6425056,-0.1649621,7.6374867,0.1327561\PG=C01 [X(C10H18N1O3)]\@

Cation m.2

1\1\GINC-R37\FOpt\RM062X\Gen\C10H18N1O3(1+)\ROOT\15-Dec-2016\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2952790016\CatM.1ii.freq\1,1\C,1.2744212382,0.0645178258,0.2938626141\C,0.5668052539,1.2860486056,-0.2781462444\C,0.6200694368,-1.2138657506,-0.235728512\C,-0.8687162389,-1.3401691345,0.1176811303\C,-0.9240311346,1.3650243102,0.0732819549\N,-1.5582103112,-0.0055715387,-0.1727249951\H,0.6865078156,1.2915922087,-1.3684588682\H,1.0312739611,2.2090928845,0.0830948483\H,1.1178294929,-2.1008104661,0.1684819665\H,0.7319473001,-1.2520480626,-1.3273707317\C,-1.1037223791,-1.6235382287,1.6151393661\C,-1.5553998164,-2.4039877969,-0.733217501\C,-1.6537967448,2.3705791675,-0.811893569\C,-1.1746470326,1.6878793083,1.5606591937\O,-2.6712670183,-0.0362550589,-0.5736152467\H,-0.5009865724,-0.9992435847,2.2742941213\H,-0.8158782345,-2.6654533443,1.7816839932\H,-2.1606970121,-1.5187852144,1.8766362833\H,-1.54811202,-2.1379204101,-1.7941550366\H,-2.5843031921,-2.584439958,-0.4168154064\H,-0.9895992217,-3.331369848,-0.6107245621\H,-1.6337041668,2.070132685,-1.8634040791\H,-1.1253277581,3.3232462654,-0.7212272928\H,-2.6894477397,2.5196869242,-0.5011576284\H,-0.552036623,1.108026132,2.2416649764\H,-2.2281009612,1.554547066,1.823396362\H,-0.9244912998,2.7443760822,1.6927217659\H,1.2524747527,0.0667361726,1.3915807903\C,2.7463590066,0.1022219298,-0.0928989521\O,3.2629473443,0.9934513602,-0.7123867546\O,3.3890411883,-0.9881173855,0.3474150049\H,4.3288186869,-0.921243146,0.0946910092\Version=ES64L-G09RevE.01\State=1-A\HF=-671.7554313\RMSD=9.595e-09\RMSF=1.765e-06\Dipole=-1.3408884,-0.4933552,0.5890922\Quadrupole=1.695878,3.1044064,-4.8002844,-4.8268662,0.879436,1.6126733\PG=C01 [X(C10H18N1O3)]\@

Cation m.3

1\1\GINC-R206\FOpt\RM062X\6-31+G(d,p)\C10H18N1O3(1+)\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\CatM2.freq\1,1\C,0.1514360794,-1.4032963034,0.6181533138\C,0.5229681464,0.063925213,0.290318391\C,0.065703298,1.0622938709,1.3637715992\C,-1.1746990712,0.6490626261,2.1556253734\N,-0.9384492108,-0.7383318059,2.7308631295\C,0.0327561447,-1.7265055415,2.1099540808\C,-2.4351248336,0.5011512316,1.2780989561\C,-1.4370432871,1.5945881755,3.3257795285\C,-0.5225274756,-3.1302888699,2.3377414475\C,1.349760644,-1.5224710692,2.8900412126\O,-1.5336545769,-1.0593397731,3.7022774223\H,0.903707283,-2.0839646296,0.2077651185\H,-0.7874433495,-1.6739752192,0.1271844473\H,-0.1728788014,2.0241406373,0.9001944852\H,0.8894229773,1.26296563,2.0547092888\H,-2.2887264594,-0.1584200582,0.4213865929\H,-2.6724733396,1.4993352976,0.9010646688\H,-3.2809464486,0.1466519701,1.8718511612\H,-0.5961082674,1.6000108526,4.0246497373\H,-2.3510744815,1.3359687317,3.8611905729\H,-1.5479972959,2.6016689059,2.9179341247\H,-1.5180157784,-3.2405948422,1.8985412323\H,-0.5672969284,-3.3818733703,3.3977177214\H,0.1498993855,-3.8356297869,1.8445105043\H,1.7832202082,-0.5292268704,2.7647545808\H,2.0627925656,-2.2501562722,2.4923086594\H,1.1974110281,-1.7330066685,3.9512069059\C,2.0294129232,0.1858742668,0.0841243667\H,0.0662086593,0.3016794094,-0.6748662881\O,2.7946210626,0.7072708064,0.8555400028\O,2.4015473527,-0.3967116207,-1.0599638394\H,3.3641818474,-0.3099949234,-1.1608084986\Version=ES64L-G09RevD.01\State=1-A\HF=-671.7794056\RMSD=8.550e-09\RMSF=5.429e-06\Dipole=-1.1239453,-0.4550241,0.1053217\Quadrupole=0.4977672,1.2388834,-1.7366506,-6.1401249,-4.8147392,-0.8491039\PG=C01 [X(C10H18N1O3)]\@

Cation m.4

1\1\GINC-R1028\FOpt\RM062X\6-31+G(d,p)\C10H18N1O3(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideM.2i.freq\1,1\C,-2.06185 23961,-0.1866537344,0.7992380744\C,-1.5590944397,1.0912705542,0.1241064687\C,-1.5520554809,-1.4295 635982,0.0707044207\C,-1.7276719799,-1.477354828,-1.4605591888\C,-1.904337378,1.2159865881,-1.36813 75235\N,-1.4973912844,-0.0874378331,-2.0513320908\H,-0.469081475,1.1353538383,0.2303102137\H,-1.96 56929255,1.9773552447,0.6192522771\H,-2.0407719795,-2.3245749932,0.4660426751\H,-0.481435055,-1.52 20337986,0.2822111535\C,-3.1376597192,-1.9008862662,-1.9305410373\C,-0.687493772,-2.4078899616,-2.0 838841652\C,-1.114427682,2.3459573466,-2.0196236146\C,-3.4099519357,1.3959977356,-1.644347307\O,-1. 0123040523,-0.0197997004,-3.1293664364\H,-3.9455977659,-1.374314393,-1.4307753533\H,-3.2351804064,- 2.958576717,-1.6728072205\H,-3.2214392585,-1.8014437457,-3.0159804239\H,0.328951787,-2.0334432135,- 1.9355283309\H,-0.8613119022,-2.5643818607,-3.1488755127\H,-0.774246457,-3.3707147377,-1.574769429 4\H,-0.0373075212,2.1680390962,-1.965058328\H,-1.3390128855,3.2600576363,-1.4653125657\H,-1.397861 1696,2.4974974568,-3.061900881\H,-4.0424967821,0.6547055991,-1.1595900426\H,-3.6060845392,1.386641 537,-2.719733934\H,-3.6808066145,2.3794234548,-1.2517095288\C,-3.5580401804,-0.2135514355,1.0680768 569\H,-1.6210399054,-0.1977422872,1.804868387\O,-4.2760273414,-1.1623852264,0.8743946038\O,-3.9820 576987,0.9434405239,1.5937589118\H,-4.9189998038,0.8532617189,1.8357188721\Version=ES64L-G09Rev D.01\State=1-A\HF=-671.7794657\RMSD=6.131e-09\RMSF=8.820e-06\Dipole=0.7119111,0.5001952,-0.4548 467\Quadrupole=-1.8287157,2.5551593,-0.7264437,-4.3874975,-1.5237349,2.099963\PG=C01 [X(C10H18N1 O3)]\@

Cation n

1\1\GINC-R261\FOpt\RM062X\6-31+G(d,p)\C9H15N2O2(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideN.2.freq\1,1\C,-0.562526 889,-1.0571413556,-0.5566637091\C,0.1708666515,0.1050318056,-1.1917017405\N,0.6669149475,0.7968058 518,0.0539549135\C,0.1945236372,0.1603130965,1.3407578536\C,-0.5604852675,-1.0116209897,0.77678347 93\O,1.3553216034,1.753081308,0.0322814338\C,-0.7400127632,1.1124649078,-1.9169417842\C,1.38988828 25,-0.2811735977,-2.0373167314\C,-0.6847850462,1.189252096,2.0664217111\C,1.4377612148,-0.21919199 51,2.1550960241\H,-1.0493895485,-1.7091311029,1.4490253754\H,-1.5864131784,1.4074385351,-1.2915803 29\H,-1.1197046464,0.6080684368,-2.8066942796\H,-0.1613513987,1.9932356349,-2.2053186246\H,2.05429 43238,-0.9580318989,-1.4940567852\H,1.9369829908,0.6140295634,-2.3409016025\H,1.0099283897,-0.7916 176323,-2.9244639041\H,-1.541002442,1.4863757022,1.4566502666\H,-0.0946032709,2.0682718699,2.33596 13184\H,-1.056662468,0.722702375,2.9816058912\H,2.0823674755,-0.9067643462,1.6024274954\H,1.10107 89238,-0.7160053046,3.0679144107\H,1.9989588291,0.6764449017,2.4311168364\C,-1.2141484829,-2.05151 16795,-1.4779319659\N,-1.6867113066,-3.1882670413,-0.9248721998\O,-1.2989940948,-1.7855963387,-2.66 54621409\H,-1.495039611,-3.4669388252,0.0233710218\H,-2.1180868557,-3.861783977,-1.5435122343\Vers ion=ES64L-G09RevD.01\State=1-A\HF=-611.392623\RMSD=7.531e-09\RMSF=3.006e-06\Dipole=0.3444924,- 0.0308107,1.9253841\Quadrupole=-4.6125804,4.5533547,0.0592256,4.0390638,-1.6616371,-1.3910689\PG=C 01 [X(C9H15N2O2)]\@

Cation o.1

1\1\GINC-R286\FOpt\RM062X\6-31+G(d,p)\C9H14N1O3(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideO.2.freq\1,1\C,-0.542256 4129,-1.0486908042,-0.5912110528\C,0.1715361116,0.1267955312,-1.2134195172\N,0.6117283752,0.832455 5028,0.0485869594\C,0.1932355021,0.1332165389,1.3261980458\C,-0.5312374636,-1.0459012654,0.7420859 885\O,1.2259119065,1.8376323609,0.0434752921\C,-0.7377089237,1.0905098658,-1.989246279\C,1.4357693 546,-0.2374711552,-2.0048397334\C,-0.7042253204,1.1013085213,2.1093062044\C,1.4718969356,-0.228304 3437,2.0944319675\H,-0.9886784456,-1.8017727152,1.3716810588\H,-1.6115536367,1.3784963497,-1.39946 30477\H,-1.0745031513,0.5603747623,-2.8825768314\H,-0.1767723142,1.9796661041,-2.2858861478\H,2.09 68902739,-0.887341617,-1.4260697311\H,1.9678794272,0.6692994363,-2.301264182\H,1.1084096642,-0.773 3623051,-2.8982424317\H,-1.5845252671,1.389455047,1.5300147569\H,-0.1396363849,1.9905850718,2.3989 200932\H,-1.0380340291,0.5870934003,3.0134895978\H,2.1241820396,-0.8765536937,1.5046577962\H,1.17 56597386,-0.7654924965,2.9983482212\H,2.0084345509,0.6781053811,2.3842536019\C,-1.1709724206,-2.06 75444416,-1.4745363846\O,-1.7608316532,-3.041050497,-0.7834841542\O,-1.1326315349,-1.9908973435,-2. 6780346795\H,-2.1539769218,-3.6774011951,-1.4039454115\Version=ES64L-G09RevD.01\State=1-A\HF=-6 31.2569953\RMSD=5.151e-09\RMSF=1.068e-05\Dipole=0.3233358,0.5143818,1.3155785\Quadrupole=-2.584 4122,0.6280283,1.956384,3.1478367,0.7151407,1.0970082\PG=C01 [X(C9H14N1O3)]\@

Cation o.2

1\1\GINC-R286\FOpt\RM062X\6-31+G(d,p)\C9H14N1O3(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramanmaxdisk=402653184\NitroxideO.2.freq\1,1\C,-0.5422564

129,-1.0486908042,-0.5912110528\C,0.1715361116,0.1267955312,-1.2134195172\N,0.6117283752,0.8324555
028,0.0485869594\C,0.1932355021,0.1332165389,1.3261980458\C,-0.5312374636,-1.0459012654,0.74208598
85\O,1.2259119065,1.8376323609,0.0434752921\C,-0.7377089237,1.0905098658,-1.989246279\C,1.43576935
46,-0.2374711552,-2.0048397334\C,-0.7042253204,1.1013085213,2.1093062044\C,1.4718969356,-0.2283043
437,2.0944319675\H,-0.9886784456,-1.8017727152,1.3716810588\H,-1.6115536367,1.3784963497,-1.399463
0477\H,-1.0745031513,0.5603747623,-2.8825768314\H,-0.1767723142,1.9796661041,-2.2858861478\H,2.096
8902739,-0.887341617,-1.4260697311\H,1.9678794272,0.6692994363,-2.301264182\H,1.1084096642,-0.7733
623051,-2.8982424317\H,-1.5845252671,1.389455047,1.5300147569\H,-0.1396363849,1.9905850718,2.39892
00932\H,-1.0380340291,0.5870934003,3.0134895978\H,2.1241820396,-0.8765536937,1.5046577962\H,1.175
6597386,-0.7654924965,2.9983482212\H,2.0084345509,0.6781053811,2.3842536019\C,-1.1709724206,-2.067
5444416,-1.4745363846\O,-1.7608316532,-3.041050497,-0.7834841542\O,-1.1326315349,-1.9908973435,-2.6
780346795\H,-2.1539769218,-3.6774011951,-1.4039454115\Version=ES64L-G09RevD.01\State=1-A\HF=-63
1.2569953\RMSD=5.151e-09\RMSF=1.068e-05\Dipole=0.3233358,0.5143818,1.3155785\Quadrupole=-2.5844
122,0.6280283,1.956384,3.1478367,0.7151407,1.0970082\PG=C01 [X(C9H14N1O3)]\@

Cation p

1\1\GINC-R2550\FOpt\RM062X\6-31+G(d,p)\C8H14N1O3(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p)
INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideP.freq\1,1\O,-1.8446505
87,-0.2058139605,0.6660435443\C,-2.3995842995,0.8674212814,0.0757981725\C,-1.062951348,-1.10520269
46,-0.102723638\C,-1.7127280664,-1.43096363,-1.4532542558\C,-2.1061952493,1.1523808658,-1.413176528
1\N,-1.7412522534,-0.1084434386,-2.1621807781\H,-1.0003671736,-2.0264387041,0.4792665355\H,-0.04795
89855,-0.7120652445,-0.2395943595\C,-3.1869632464,-1.8581271174,-1.3107410171\C,-0.8899751177,-2.42
11588155,-2.25888376\C,-0.8914954754,2.0974861599,-1.5113010685\C,-3.3445296686,1.7417197036,-2.102
3668833\O,-1.4791946699,-0.0288188871,-3.311895195\H,-3.7939253703,-1.1436614998,-0.7505517801\H,-3.1
924040865,-2.8024507256,-0.7600277023\H,-3.6283155169,-2.0247846979,-2.2959553668\H,0.134245619,-2.
0691334735,-2.408765012\H,-1.3434444908,-2.6143857295,-3.2322694209\H,-0.857942514,-3.3619598241,-1.7
048446188\H,0.0036472688,1.6691077192,-1.0526224058\H,-1.1550434189,3.0093235387,-0.9715480746\H,-
0.6926450917,2.3425015587,-2.5562430358\H,-4.1890230404,1.0487175667,-2.0727157314\H,-3.1067294502,1
.9998944968,-3.1356024708\H,-3.6218726504,2.6409039829,-1.5514448293\O,-3.0718111171,1.6364315692,
0.6913196797\Version=ES64L-G09RevD.01\State=1-A\HF=-593.144327\RMSD=8.408e-09\RMSF=6.174e-0
6\Dipole=0.790291,-1.0953254,-1.4475608\Quadrupole=-0.3270145,8.5190188,-8.1920043,0.3850103,3.35853
57,-3.5536261\PG=C01 [X(C8H14N1O3)]\@

Cation r

1\1\GINC-R636\FOpt\RM062X\6-31+G(d,p)\C8H16N1O2(1+)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) I
NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\NitroxideR.freq\1,1\C,-0.74350397
92,-1.2513636205,-1.1559582288\C,0.0604220149,0.0569330412,-1.3344363122\N,-0.0048985198,0.7798115
358,0\C,0.0604220149,0.0569330412,1.3344363122\C,-0.7435039792,-1.2513636205,1.1559582288\O,-0.345
0410164,-1.9370053851,0\O,-0.1205387657,1.9592900967,0\C,-0.5487891896,0.9582583397,-2.3969041282\
C,1.5431556027,-0.2419213165,-1.6236997107\C,-0.5487891896,0.9582583397,2.3969041282\C,1.543155602
7,-0.2419213165,1.6236997107\H,-1.8211192651,-1.0330356884,1.1320323949\H,-0.5330625004,-1.8901226
563,2.0168690551\H,-1.5532981182,1.2917658934,-2.1242915667\H,-0.6176808299,0.3762886543,-3.319531
8188\H,0.0752140613,1.8320997831,-2.5912490108\H,1.9143706856,-1.0793644454,-1.0349354112\H,2.1682
451647,0.6409023658,-1.4660144397\H,1.6033105051,-0.5120534738,-2.6810675109\H,-1.5532981182,1.291
7658934,2.1242915667\H,0.0752140613,1.8320997831,2.5912490108\H,-0.6176808299,0.3762886543,3.3195
318188\H,1.9143706856,-1.0793644454,1.0349354112\H,1.6033105051,-0.5120534738,2.6810675109\H,2.16
82451647,0.6409023658,1.4660144397\H,-0.5330625004,-1.8901226563,-2.0168690551\H,-1.8211192651,-1.
0330356884,-1.1320323949\Version=ES64L-G09RevD.01\State=1-A\HF=-519.1476329\RMSD=3.558e-09\R
MSF=2.184e-05\Dipole=-0.0258837,0.2877731,0\Quadrupole=-1.5044411,-7.066058,8.5704991,0.4834515,0.,
0\PG=CS [SG(N1O2),X(C8H16)]\@

Nitroxide TEMPO

1\1\GINC-R3523\FOpt\UM062X\6-31+G(d,p)\C9H18N1O1(2)\ROOT\18-Nov-2014\0\#M062X/6-31+G(d,p) I
NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramanmaxdisk=268435456\TEMPO.freq\0,2\C,-3.1795695774,
0.6943840806,-0.1543978295\N,-3.0111091496,-0.6645227138,-0.7474070193\C,-2.1216419643,-1.71861663
51,-0.1778452386\C,-0.8388983908,-1.0785296864,0.3680998261\C,-1.098476247,0.1548451927,1.22687578
15\C,-1.835785072,1.1952442897,0.3901943528\C,-3.6560721161,1.6204220309,-1.274930014\C,-4.2509331
437,0.638971433,0.9459956346\C,-2.8804531409,-2.4869222357,0.9156209616\C,-1.7714822058,-2.6780921
076,-1.3166991768\O,-3.9914971532,-1.0875822902,-1.4441355913\H,-0.2044304603,-0.7887816971,-0.4802
770318\H,-0.2927318602,-1.8456082837,0.9290419387\H,-0.1493419719,0.5675071656,1.5834918306\H,-1.6

779759482,-0.1079021929,2.1199763312\H,-1.1988640854,1.4793971645,-0.4582368735\H,-2.0258390315,2.107392652,0.9674537094\H,-2.9604672147,1.5864125622,-2.1183802738\H,-3.7017280578,2.6464577713,-0.8968153984\H,-4.6440264258,1.3242459484,-1.6301073411\H,-3.9056557026,0.1110272116,1.8382430558\H,-5.1406851559,0.1331938842,0.5613572075\H,-4.5251846193,1.6569024339,1.2404806744\H,-3.0283905726,-1.8899049507,1.8187997648\H,-2.3155619019,-3.3829709303,1.1915076377\H,-3.858031528,-2.7923787955,0.5329290769\H,-1.3312005709,-2.1297411036,-2.154490572\H,-2.6612429111,-3.1982355339,-1.6740528207\H,-1.0451436066,-3.4128794674,-0.9556946844\Version=ES64L-G09RevD.01\State=2-A\HF=-483.5234304\S2=0.754861\S2-1=0.\S2A=0.750014\RMSD=3.991e-09\RMSF=5.988e-06\Dipole=0.8207978,0.3514986,0.8605761\Quadrupole=-0.7073146,2.3702525,-1.6629378,-1.6385592,-2.2349817,-0.9337956\PG=CS [SG(C1H2N1O1),X(C8H16)]\@

Nitroxide a.1

1\1\GINC-R278\FOpt\UM062X\6-31+G(d,p)\C9H16N1O2(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) IN T(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideA.freq\0,2\C,-1.3187957309,0.3009776879,0.0750811002\C,-1.259589816,-1.0121361435,-0.7292009159\C,0,-1.7811958418,-0.4090697062\C,1.259589816,-1.0121361435,-0.7292009159\C,1.3187957309,0.3009776879,0.0750811002\N,0,0.9982434561,-0.0057462148\O,0,2.2136398464,0.3765496069\C,-1.6718551148,0.0192537297,1.5432392741\C,-2.3645390133,1.2314130453,-0.5387719223\H,-1.2601460071,-0.7743625699,-1.8005153755\H,-2.1350123447,-1.6244194913,-0.4993872046\H,1.2601460071,-0.7743625699,-1.8005153755\H,2.1350123447,-1.6244194913,-0.4993872046\C,2.3645390133,1.2314130453,-0.5387719223\C,1.6718551148,0.0192537297,1.5432392741\H,-1.0760505469,-0.7938403115,1.9652033632\H,-2.7248207509,-0.2698578378,1.6132195077\H,-1.5168955981,0.9252915936,2.1351980238\H,-2.064032564,1.5328460807,-1.5461861299\H,-2.4846744012,2.1290319144,0.0690559643\H,-3.3215753138,0.7046260658,-0.5964164959\H,2.064032564,1.5328460807,-1.5461861299\H,3.3215753138,0.7046260658,-0.5964164959\H,2.4846744012,2.1290319144,0.0690559643\H,1.0760505469,-0.7938403115,1.9652033632\H,1.5168955981,0.9252915936,2.1351980238\H,2.7248207509,-0.2698578378,1.6132195077\O,0,-2.8820049853,0.0978979259\Version=ES64L-G09RevD.01\State=2-A\HF=-557.5153744\S2=0.75482\S2-1=0.\S2A=0.750014\RMSD=7.589e-09\RMSF=1.033e-05\Dipole=0,0.0414782,-0.4648758\Quadrupole=7.4005147,-11.8728859,4.4723712,0,0,0.8636565\PG=CS [SG(C1N1O2),X(C8H16)]\@

Nitroxide a.2

1\1\GINC-R74\FOpt\UM062X\6-31+G(d,p)\C9H16N1O2(2)\ROOT\29-Nov-2017\0\#M062X\6-31+G(d,p) SC F=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\CatA.freq\0,2\C,-1.4625347252,-0.7375558797,1.4900744844\C,-2.8758024434,-0.9613306347,0.991032749\C,-3.5360695893,0.2132946756,0.2977936234\C,-2.9951014137,1.5864870986,0.7156348353\N,-1.5113520648,1.5734631688,0.6394344877\C,-0.6822563285,0.3440421209,0.7322964533\O,-3.4456812132,-2.0197509637,1.1381442089\C,-3.4125610067,1.9363684317,2.1517047217\C,-3.5169505626,2.6517507174,-0.249154447\C,0.5942952474,0.6819165627,1.5031144219\C,-0.324884553,-0.1187793976,-0.6879533826\O,-0.9125731154,2.6860443961,0.4856589694\H,-0.927504867,-1.6909120013,1.4494629794\H,-1.5371491185,-0.4606722327,2.5504354157\H,-4.6137778645,0.1585404261,0.4776302281\H,-3.3871148418,0.0737187121,-0.7815213646\H,-3.1277451819,1.1554442071,2.8632557145\H,-4.4979456096,2.0657053985,2.2057290129\H,-2.9312494607,2.871331104,2.4503945157\H,-3.1460928049,2.4657142884,-1.2612237265\H,-3.1879377587,3.6448614949,0.0582669458\H,-4.6105198071,2.6212287017,-0.2608283084\H,0.3495173173,1.102983443,2.4825103337\H,1.1926963889,1.4118721113,0.9571108508\H,1.1801752083,-0.2309691683,1.6457621263\H,-1.2066483339,-0.4481537887,-1.2458668944\H,0.3806410074,-0.954236518,-0.6436256073\H,0.141497495,0.7075035256,-1.2308733468\Version=ES64L-G09RevD.01\State=2-A\HF=-557.5146868\S2=0.755176\S2-1=0.\S2A=0.750017\RMSD=6.422e-09\RMSF=1.053e-05\Dipole=0.0391388,0.0723491,-0.0104077\Quadrupole=3.4763119,-8.2208402,4.7445283,-8.8424425,1.1325733,1.8855547\PG=C01 [X(C9H16N1O2)]\@

Nitroxide b.1

1\1\GINC-R528\FOpt\UM062X\6-31+G(d,p)\C9H18N1O2(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) IN T(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideC.1.freq\0,2\C,-0.3836850378,-1.31685687,0.1034860503\C,1.078658559,-1.2390403912,-0.3512729132\C,1.8094932373,0,0.1478912042\C,1.078658559,1.2390403912,-0.3512729132\C,-0.3836850378,1.31685687,0.1034860503\N,-1.0509439019,0,-0.1136323162\O,-2.3210412895,0,-0.0062087419\C,-0.4962050344,-1.7090833693,1.585619771\C,-1.1295157341,-2.3473431125,-0.7464793418\H,1.1084308709,-1.2317884582,-1.4513615864\H,1.6019533994,-2.1413651324,-0.0165665744\H,1.1084308709,1.2317884582,-1.4513615864\H,1.6019533994,2.1413651324,-0.0165665744\C,-1.1295157341,2.3473431125,-0.7464793418\C,-0.4962050344,1.7090833693,1.585619771\H,0.1305148306,-1.0911234964,2.2329347517\H,-0.186206421,-2.75097455,1.7118507051\H,-1.5365295803,-1.6106390251,1.9070567402\H,-1.157484974,-2.0297460221,-1.7927652564\H,-2.1550041612,-2.4678766642,-0.3947048139\H,-0.6107296467,-3.3086179541,-0.6826617795\H,-1.157484974,2.0297460221,-1.7927652564\H,

-0.6107296467,3.3086179541,-0.6826617795\H,-2.1550041612,2.4678766642,-0.3947048139\H,0.1305148306,1.0911234964,2.2329347517\H,-1.5365295803,1.6106390251,1.9070567402\H,-0.186206421,2.75097455,1.7118507051\O,3.169485622,0,-0.2524756964\H,1.8497610181,0,1.2425851298\H,3.2083712523,0,-1.2171010761\Version=ES64L-G09RevD.01\State=2-A\HF=-558.7197282\S2=0.754858\S2-1=0.\S2A=0.750014\RMSD=6.797e-09\RMSF=1.301e-05\Dipole=0.5494301,0,-0.2279559\Quadrupole=-9.8122808,5.1255375,4.6867432,0,-3.3644438,0.\PG=CS [SG(C1H2N1O2),X(C8H16)]\@

Nitroxide b.2

1\1\GINC-R834\FOpt\UM062X\6-31+G(d,p)\C9H18N1O2(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) IN T(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=402653184\NitroxideC.2.freq\0,2\C,-0.3726851232,-1.3129526657,0.1121948395\C,1.0925215088,-1.2287347546,-0.3284884277\C,1.8088432945,0.006425193,0.1852372811\C,1.0832911648,1.2430851687,-0.3282726149\C,-0.3830008264,1.3212813844,0.1140085064\N,-1.0446333893,0.0022975627,-0.1023253885\O,-2.3148843524,-0.0007950123,0.0024397111\C,-0.5036419513,-1.7149110082,1.5903070226\C,-1.1045583275,-2.3402318411,-0.7536953702\H,1.149023007,-1.209816656,-1.4244467581\H,1.6159363882,-2.129666856,0.0092387355\H,1.1381348201,1.2252012384,-1.4243563918\H,1.5886577424,2.1576731191,0.0095400763\C,-1.1218504134,2.3458100636,-0.7491975108\C,-0.5137071046,1.7199601576,1.5931143142\H,0.1065421845,-1.0931287743,2.2500153648\H,-0.1834298613,-2.753839657,1.7154245085\H,-1.5495865219,-1.6298814477,1.8969627707\H,-1.1173922775,-2.0170772442,-1.7984122627\H,-2.1345261977,-2.465227971,-0.4167280567\H,-0.5841468627,-3.3004827045,-0.6883767396\H,-1.1326144661,2.0253041715,-1.7947135263\H,-0.6097592555,3.3105168958,-0.6809741927\H,-2.1528197408,2.4615800787,-0.411967208\H,0.0975901114,1.0975581779,2.2510901247\H,-1.5592271945,1.6302709357,1.8997831538\H,-0.1982824303,2.7602395924,1.7211977978\O,3.1382821715,-0.059314224,-0.3077864006\H,1.8252678809,0.0021492014,1.2855568809\H,3.6269060225,0.7152578758,-0.0070302392\Version=ES64L-G09RevD.01\State=2-A\HF=-558.719955\S2=0.754867\S2-1=0.\S2A=0.750014\RMSD=5.344e-09\RMSF=6.782e-06\Dipole=0.8779104,0.4733964,0.4786435\Quadrupole=-6.2357911,5.0686079,1.1671832,3.771824,1.8561235,-0.047468\PG=C01 [X(C9H18N1O2)]\@

Nitroxide b.3

1\1\GINC-R97\FOpt\UM062X\6-31+G(d,p)\C9H18N1O2(2)\ROOT\30-Mar-2017\0\#M062X\6-31+G(d,p) IN T(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=134217728\NitroxideC.3.freq\0,2\C,-0.0091419961,-0.0056465011,-0.0063652219\C,-0.0179654346,-0.008454791,1.5269636177\C,1.3728079849,-0.0163107609,2.1468163005\C,2.1222063198,-1.2502307953,1.6628515991\C,2.2655042519,-1.3254450566,0.1380124854\N,0.9535262883,-1.0294019198,-0.5079912699\O,0.8781947893,-1.2954715461,-1.7522033034\C,0.3722670581,1.3734812666,-0.568305595\C,-1.3944721354,-0.3940684908,-0.5266218363\H,-0.5519159686,-0.9047099061,1.8773805063\H,-0.5787674667,0.8640597192,1.8793862387\H,1.5756994026,-2.1392963748,2.0123042478\H,3.1198730838,-1.282103661,2.1141274557\C,2.6598030918,-2.7464652981,-0.2691822514\C,3.3249173215,-0.3396937685,-0.3808340618\H,1.2891456966,1.7692013365,-0.1250912416\H,-0.4338275307,2.0854655743,-0.366258031\H,0.5104523216,1.2967813645,-1.6500966905\H,-1.6398387135,-1.4177017483,-0.2294589545\H,-1.4288959735,-0.3329058866,-1.615186175\H,-2.1405711997,0.2851801178,-0.1032768026\H,1.8662274138,-3.4520117334,-0.0069181381\H,3.5744809799,-3.0309176785,0.2597018747\H,2.8328790889,-2.8056187248,-1.3445616086\H,3.174534165,0.6752188593,-0.0052840912\H,3.2930307467,-0.3176094895,-1.473422605\H,4.3184593425,-0.6719163394,-0.0645550967\O,1.3130160738,0.0358370136,3.56226075\H,1.9174834594,0.8915013851,1.8653657548\H,0.8438683313,-0.7451963353,3.8814456817\Version=ES64L-G09RevD.01\State=2-A\HF=-558.7197281\S2=0.754857\S2-1=0.\S2A=0.750014\RMSD=8.426e-09\RMSF=9.337e-06\Dipole=-0.0552517,-0.0351196,0.5916151\Quadrupole=4.5241148,2.1282865,-6.6524013,-1.3450169,-2.854503,-6.2407982\PG=C01 [X(C9H18N1O2)]\@

Nitroxide c.1

1\1\GINC-R423\FOpt\UM062X\6-31+G(d,p)\C9H17N2O2(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) IN T(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=402653184\NitroxideB.1.freq\0,2\C,-1.3110055231,0.3022561111,0.0572258587\C,-1.2366146671,-0.9774899036,-0.7950754474\C,0.0149512226,-1.7349037025,-0.4695456208\C,1.2760004185,-0.97964904,-0.7508373258\C,1.3298842929,0.3225272589,0.0708438019\N,0.0041027667,1.0111483093,0.0117069056\O,-0.0059852062,2.2124187747,0.4368236239\C,-1.6668804941,-0.0421386751,1.5106024689\C,-2.3589753607,1.2480059491,-0.5277505314\H,-1.2037155394,-0.697666582,-1.8557154512\H,-2.1296126736,-1.5793166897,-0.6205829037\H,1.306965032,-0.7277261007,-1.8188407128\H,2.1506165418,-1.5914826325,-0.5135182672\C,2.3619932208,1.2708168394,-0.5384998239\C,1.6926468456,0.0276963394,1.5331904917\H,-1.061160012,-0.8669447377,1.8950122254\H,-2.716209718,-0.3476568639,1.5643750386\H,-1.5227607361,0.8389508568,2.1418503743\H,-2.0576329893,1.5839869137,-1.5240442235\H,-2.484799164,2.1247361004,0.1086327309\H,-3.313505037,0.7190239444,-0.605388091\H,2.0542219824,1.5774184239,-1.542337106\H,3.3252128836,0.755894255,-0.6054267451\H,2.4747011819,2.164461491,

0.0765677618\H,1.1025777355,-0.7952192588,1.9435367159\H,1.5318960716,0.9251964232,2.1365142249\H,2.7485546174,-0.2532749313,1.5955902102\N,0.1021182459,-2.8845691022,0.0754580322\O,-1.1490104384,-3.4445192346,0.3310730781\H,-0.9316755003,-4.3041905358,0.7085187067\Version=ES64L-G09RevD.01\State=2-A\HF=-612.8017448\S2=0.754836\S2-1=0.\S2A=0.750014\RMSD=5.078e-09\RMSF=1.839e-05\Dipole=-0.0134443,-0.8801805,-0.1900647\Quadrupole=2.9961636,-4.4287397,1.4325761,0.7789965,-0.3824438,-2.5178906\PG=C01 [X(C9H17N2O2)]\@

Nitroxide c.2

1\1\GINC-R51\FOpt\UM062X\6-31+G(d,p)\C9H17N2O2(2)\ROOT\29-Nov-2017\0\#M062X\6-31+G(d,p) SC F=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\RadC2.freq\0,2\C,-1.6116262246,-0.6339994046,1.6706739741\C,-3.0032682431,-0.8223722281,1.1420836122\C,-3.7058901012,0.3640461255,0.5403172384\C,-3.0071684183,1.7066061838,0.7967736817\N,-1.5452739166,1.5635659291,0.5691637417\C,-0.7897514963,0.2990132558,0.7699528435\N,-3.4968475272,-1.9979858502,1.1738401242\C,-3.2445110525,2.201078721,2.2326864014\C,-3.5430747691,2.7433588305,-0.1913330898\C,0.5374154563,0.6300131416,1.4514570574\C,-0.5401968833,-0.3361336495,-0.6039149834\O,-0.8874176782,2.5980542305,0.2260388441\H,-1.1162610333,-1.6062565124,1.7428278107\H,-1.6480855467,-0.2099156765,2.681526599\H,-4.7331889772,0.4112923773,0.9182411491\H,-3.7948981746,0.188519967,-0.5406382534\H,-2.9894283669,1.4440347428,2.9789169325\H,-4.2989382334,2.4636230029,2.3646686087\H,-2.6365932926,3.09166146,2.4138216377\H,-3.2785669957,2.4675873574,-1.2158510478\H,-3.1257595295,3.7292767785,0.0156830232\H,-4.633055867,2.7867992158,-0.1052534716\H,0.3624165457,1.1512082461,2.397486772\H,1.1465944659,1.2719244069,0.8143353608\H,1.0804109386,-0.2981143331,1.6537867355\H,-1.4779309346,-0.6321027993,-1.0845078462\H,0.0863077291,-1.2274658548,-0.4989592401\H,-0.0280932519,0.3835092325,-1.2479323516\O,-4.7806229302,-2.0206521358,0.6302674457\H,-5.0426556916,-2.9439947606,0.7172706903\Version=ES64L-G09RevD.01\State=2-A\HF=-612.8002191\S2=0.755191\S2-1=0.\S2A=0.750017\RMSD=4.917e-09\RMSF=7.000e-06\Dipole=-0.5032298,-0.7027126,0.3015833\Quadrupole=1.7329153,-2.0705375,0.3376223,-2.9325983,1.1326868,2.3199126\PG=C01 [X(C9H17N2O2)]\@

Nitroxide d.1

1\1\GINC-R223\FOpt\UM062X\6-31+G(d,p)\C10H18N1O2(2)\ROOT\30-Mar-2017\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\NitroxideD.1.freq\0,2\C,0.1422095189,0.5246296337,-1.3192096496\C,0.5133382902,-0.9630103042,-1.2507763816\C,0.0000666197,-1.6278677355,0.\C,0.5133382902,-0.9630103042,1.2507763816\C,0.1422095189,0.5246296337,1.3192096496\N,0.4103815175,1.1722925808,0.\O,0.389149575,2.446609149,0.\C,-1.3358040182,0.717074564,-1.6928457695\C,1.0232452436,1.2239944819,-2.3550259863\H,1.606654078,-1.0651577393,-1.261407079\H,0.1262890453,-1.4720356142,2.1398525761\C,1.0232452436,1.2239944819,2.3550259863\C,-1.3358040182,0.717074564,1.6928457695\H,-2.0014060803,0.1134733148,-1.0714916529\H,-1.4888139249,0.4247902962,-2.7365809484\H,-1.6049909105,1.7707632057,-1.5805536449\H,2.0718302799,1.194950043,-2.04576176\H,0.7265730251,2.2668462917,-2.4737679674\H,0.9242366006,0.7091775271,-3.3155455538\H,2.0718302799,1.194950043,2.04576176\H,0.9242366006,0.7091775271,3.3155455538\H,0.7265730251,2.2668462917,2.4737679674\H,-2.0014060803,0.1134733148,1.0714916529\H,-1.6049909105,1.7707632057,1.5805536449\H,-1.4888139249,0.4247902962,2.7365809484\O,0.0328805977,-3.0476064332,0.\C,-1.2431528766,-2.4168208059,0.\H,-1.8105138644,-2.5245340781,-0.9231609\H,-1.8105138644,-2.5245340781,0.9231609\Version=ES64L-G09RevD.01\State=2-A\HF=-596.7801838\S2=0.754858\S2-1=0.\S2A=0.750014\RMSD=2.754e-09\RMSF=8.168e-06\Dipole=-0.5732859,-0.3956209,0.\Quadrupole=4.26971,-10.8292594,6.5595494,1.3529096,0,0.\PG=CS [SG(C2N1O2),X(C8H18)]\@

Nitroxide d.2

1\1\GINC-R76\FOpt\UM062X\6-31+G(d,p)\C10H18N1O2(2)\ROOT\30-Mar-2017\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\NitroxideD.2.freq\0,2\C,0.1496836395,-0.5096769468,-1.316517917\C,-0.9648337268,0.545186611,-1.2565439647\C,-0.9142298626,1.3768892444,0.\C,-0.9648337268,0.545186611,1.2565439647\C,0.1496836395,-0.5096769468,1.316517917\N,0.2484386729,-1.2071893336,0.\O,0.9244591464,-2.2878541856,0.\C,1.5026732193,0.1286396465,-1.6692348217\C,-0.2065324837,-1.5665326027,-2.3626203681\H,-1.9395231589,0.0413450123,-1.2935881182\H,-0.8859231251,1.1904075262,-2.1381164348\H,-1.9395231589,0.0413450123,1.2935881182\H,-0.8859231251,1.1904075262,2.1381164348\C,-0.2065324837,-1.5665326027,2.3626203681\C,1.5026732193,0.1286396465,1.6692348217\H,1.7097777948,1.0145880564,-1.0669500944\H,1.493399455,0.4339650318,-2.7205332863\H,2.2982360435,-0.6079626558,-1.5267011855\H,-1.1026572362,-2.1171859634,-2.0620871881\H,0.6103564678,-2.278523976,-2.4862295172\H,-0.3992295608,-1.0711529253,-3.3192993664\H,-1.1026572362,-2.1171859634,2.0620871881\H,-0.3992295608,-1.0711529253,3.3192993664\H,0.6103564678,-2.278523976,2.4862295172\H,1.7097777948,1.0145880564,1.0669500944\H,2.2982360435,-0.6079626558,1.5267011855\H,1.493399455,0.4339650318,

2.7205332863\C,-1.3803761152,2.7698249725,0.\O,0.010975504,2.465947268,0.\H,-1.7552710011,3.2083392034,0.9228408774\H,-1.7552710011,3.2083392034,-0.9228408774\Version=ES64L-G09RevD.01\State=2-A\HF=-596.7806245\S2=0.754852\S2-1=0.\S2A=0.750014\RMSD=5.851e-09\RMSF=1.128e-05\Dipole=-1.0696962,0.8605077,0.\Quadrupole=1.6544791,-6.1508052,4.4963261,-1.3325119,0.,0.\PG=CS [SG(C2N1O2),X(C8H18)]\@

Nitroxide e.1

1\1\GINC-R241\FOpt\UM062X\6-31+G(d,p)\C10H20N1O3(2)\ROOT\30-Mar-2017\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\NitroxideE.1ii.freq\0,2\C,0.0238481095,-0.0060012694,0.0140794359\C,0.0225799414,-0.0322958308,1.5484154505\C,1.404320653,-0.0390794153,2.2108231169\C,2.2311869553,-1.1849447416,1.6412581145\C,2.3450988494,-1.2302131261,0.1101935815\N,1.0077675635,-0.9978185884,-0.5035099688\O,0.9091887816,-1.2855033516,-1.7416739082\C,0.3416433856,1.3837748891,-0.5608582972\C,-1.357445845,-0.4431859332,-0.4830320154\H,-0.5060806655,-0.9381176501,1.8745534251\H,-0.5554858445,0.8233022427,1.9159695947\H,1.7719957463,-2.123509874,1.9793666456\H,3.2437540265,-1.141608053,2.0595422013\C,2.7914631321,-2.6351254687,-0.3050681679\C,3.3518178783,-0.2043722944,-0.4353939824\H,1.267379934,1.7920125342,-0.1567577734\H,-0.4744070114,2.0712178485,-0.3138571466\H,0.4168215559,1.3087319802,-1.6493179169\H,-1.5603422159,-1.4783981864,-0.1931801378\H,-1.4159783432,-0.3716684129,-1.5698474845\H,-2.1193913812,0.2043430249,-0.0382342219\H,2.0304875714,-3.3748350487,-0.0390909522\H,3.7232213331,-2.8831972645,0.2128162395\H,2.9570295646,-2.6829424086,-1.3820287706\H,3.1624724939,0.7986523764,-0.0549092633\H,3.3009811297,-0.2046919247,-1.527787826\H,4.3627497925,-0.4962321621,-0.1322452046\C,1.2573168264,-0.2231589109,3.722709335\O,2.1051728206,1.1790303697,1.9932182969\O,0.5926495871,0.9353663544,4.2090139684\H,0.6798900841,-1.1298358992,3.9452750486\H,2.2594986587,-0.3114813318,4.1627992411\H,1.6844576766,1.8456304156,2.555659659\H,0.6461678426,0.9698727809,5.168806303\Version=ES64L-G09RevD.01\State=2-A\HF=-673.2165447\S2=0.754882\S2-1=0.\S2A=0.750014\RMSD=4.461e-09\RMSF=1.554e-05\Dipole=0.0074474,0.0848452,2.030203\Quadrupole=-1.0395322,-1.3532452,2.3927774,-2.0249545,-0.7205482,-2.5724408\PG=C01 [X(C10H20N1O3)]\@

Nitroxide e.2

1\1\GINC-R277\FOpt\UM062X\6-31+G(d,p)\C10H20N1O3(2)\ROOT\30-Mar-2017\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\NitroxideE.1iii.freq\0,2\C,0.0204427066,-0.0055469042,-0.0074140054\C,0.0241084871,-0.012994323,1.5283367192\C,1.4059758626,-0.0166670414,2.191626121\C,2.2269636122,-1.1703097677,1.6292097791\C,2.3401228156,-1.2304280689,0.0990135556\N,1.0000189908,-1.0072374915,-0.512825057\O,0.8946884508,-1.3114756783,-1.7462725664\C,0.3423669506,1.3773341542,-0.596369492\C,-1.3631568485,-0.4440267818,-0.496542368\H,-0.513498392,-0.9103763336,1.8655877582\H,-0.5491643488,0.8603884291,1.8668266969\H,1.7656136197,-2.1051026439,1.9761210258\H,3.2391339628,-1.1259502705,2.0479353287\C,2.7884074346,-2.6378871819,-0.3046949835\C,3.3427068483,-0.2065857429,-0.4573583125\H,1.2624064457,1.792536849,-0.1866955648\H,-0.4775520843,2.0667661718,-0.3679613401\H,0.4286932989,1.2877461232,-1.6828197866\H,-1.5684949708,-1.4758105158,-0.1962837083\H,-1.423481059,-0.3835112406,-1.5838260598\H,-2.1230435019,0.2107428079,-0.0584139972\H,2.0295474252,-3.3769497215,-0.0310832646\H,3.7212960673,-2.8791900767,0.214134808\H,2.9527793875,-2.6950544806,-1.3813821651\H,3.1541453347,0.7988958682,-0.0829450772\H,3.2885197356,-0.2143867861,-1.5495857581\H,4.3549989361,-0.4948251608,-0.1556524329\C,1.2699008604,-0.1877918197,3.7104440801\O,2.1016115942,1.2014825884,1.9625732962\O,0.6921685063,0.9688780873,4.2986052869\H,0.6958035872,-1.0906796228,3.9533461194\H,2.2705098636,-0.2794290355,4.1437006343\H,1.7478658184,1.8481116252,2.5915446935\H,-0.2678098546,0.9211284108,4.2351217246\Version=ES64L-G09RevD.01\State=2-A\HF=-673.2157384\S2=0.754876\S2-1=0.\S2A=0.750014\RMSD=5.995e-09\RMSF=8.736e-06\Dipole=-0.5440153,-0.0219224,1.2850663\Quadrupole=4.9608005,0.7439893,-5.7047898,-3.4946252,-4.0261861,-5.0450577\PG=C01 [X(C10H20N1O3)]\@

Nitroxide e.3

1\1\GINC-R290\FOpt\UM062X\6-31+G(d,p)\C10H20N1O3(2)\ROOT\30-Mar-2017\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\NitroxideE.1iv.freq\0,2\C,-0.0010674274,0.0054460623,0.0147878698\C,-0.0045702113,0.0004516362,1.5495347038\C,1.3630485069,-0.0042121351,2.2245178754\C,2.2053775735,-1.1429340696,1.659230644\C,2.3345357646,-1.1929315317,0.1294605672\N,1.0010636249,-0.9746787708,-0.4939761579\O,0.9184110928,-1.2645258454,-1.7325437978\C,0.2861723309,1.3955760974,-0.5754111324\C,-1.3730433235,-0.4663827319,-0.476829739\H,-0.5313086133,-0.8993043074,1.8919360116\H,-0.5811040329,0.8605465884,1.904903703\H,1.7504345196,-2.0831773031,1.9978561009\H,3.216707855,-1.1138843567,2.0896464906\C,2.8022871359,-2.594251971,-0.2741033076\C,3.3312729057,-0.1598518417,-0.4213298761\H,1.1812771472,1.8472318974,-0.1492459237\H,-0.559697637,2.05684

24101,-0.361255237\H,0.39359277,1.3067492874,-1.6600652002\H,-1.5530994925,-1.5031940979,-0.178006
245\H,-1.4338360335,-0.4047201201,-1.5641457818\H,-2.1485127058,0.1678379842,-0.0367244538\H,2.055
0196609,-3.3427886768,0.0046882367\H,3.7411369065,-2.8232143404,0.2399868022\H,2.961003048,-2.6506
176488,-1.3515403804\H,3.0761441993,0.8579387221,-0.1255597431\H,3.3351503025,-0.2199620656,-1.512
9686718\H,4.3382401366,-0.3910169843,-0.0568482898\C,1.2093801581,-0.1671986056,3.7426244422\O,1.9
628656169,1.2802948128,2.0048286515\O,0.4885840209,0.9016186762,4.3060185877\H,0.6644527659,-1.08
56460125,3.9804431332\H,2.2160881592,-0.2437426354,4.1891975135\H,2.8952357869,1.2353085466,2.255
4707209\H,0.8457729689,1.7154881094,3.9237876845\Version=ES64L-G09RevD.01\State=2-A\HF=-673.21
49837\S2=0.754882\S2-1=0.\S2A=0.750014\RMSD=6.156e-09\RMSF=7.567e-06\Dipole=0.9309411,0.045976
6,0.7264001\Quadrupole=6.5645353,2.8364344,-9.4009697,0.4926969,3.7159322,-4.3370943\PG=C01 [X(C10
H20N1O3)]\@

Nitroxide f

1\1\GINC-R2788\FOpt\UM062X\6-31+G(d,p)\C11H18N1O4(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p)
INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=536870912\NitroxideF.2.freq\0,2\C,0.7567387
732,3.1305593219,-1.0479859379\C,-0.7162593853,2.73991508,-1.1113528479\C,1.6275170175,1.895547892
4,-0.9144308736\C,1.2478122423,0.9358272535,0.2235570304\C,-1.2118052502,1.8404585259,0.0291167472
\N,-0.2295660032,0.7411469445,0.2488675827\O,0.9903599386,4.0330103788,0.0533736045\C,1.161987073
4,4.0190388529,-2.2353414047\H,-0.8608000061,2.2059002507,-2.0597716267\H,-1.3376509308,3.64340591
57,-1.1494198744\H,2.6728584545,2.1977802716,-0.7840364345\H,1.558090284,1.3559890486,-1.869052122
7\C,1.7314314294,1.438678849,1.5934286204\C,1.8786432073,-0.4299324396,-0.0599434167\C,-2.52785811
08,1.18826358,-0.4038884001\C,-1.4429222908,2.6100401301,1.3393764729\O,-0.6437763814,-0.239591864
2,0.9489257718\H,1.4286345141,2.4663216951,1.7935171727\H,2.8247529663,1.395768307,1.6285761364\H,1
.3316656351,0.7829059593,2.3714763046\H,1.4574320332,-0.8672195715,-0.9699402835\H,1.6955970602,-1.1
152760158,0.7681227668\H,2.9580976749,-0.3071805553,-0.1914955414\H,-2.3686849486,0.5340091142,-1.
2660266584\H,-3.2432229385,1.9696044189,-0.6780297974\H,-2.9444069773,0.5920021209,0.4084765249\H,-
0.5765833793,3.1977058023,1.6412915657\H,-1.6909430837,1.895276342,2.1286541647\H,-2.2871663523,3.
295120474,1.2114568682\C,0.9835863278,5.3143814376,-0.3841578986\O,0.9809396012,6.2747384695,0.31
92205646\O,0.9792813582,5.3415198167,-1.7371569888\H,0.5262409043,3.8842810775,-3.1116409336\H,2.
2142995427,3.8825431159,-2.5083668576\Version=ES64L-G09RevD.01\State=2-A\HF=-785.3296053\S2=0.
754857\S2-1=0.\S2A=0.750014\RMSD=5.624e-09\RMSF=1.102e-05\Dipole=0.3059295,-0.8635912,-1.465096
2\Quadrupole=9.3583678,-16.7643072,7.4059394,-5.8238671,-0.3630764,0.2102603\PG=C01 [X(C11H18N1O
4)]\@

Nitroxide g.1 CORE

1\1\GINC-R781\FOpt\UM062X\6-31+G(d,p)\C10H20N1O4S1(2)\ROOT\10-Aug-2017\0\#M062X\6-31+G**
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483648\NitroxideG.1.a1b2.Methyl.freq\0,2\
C,0.6765863954,-0.631554675,-0.2613417948\C,1.99295712,-1.2885148225,0.1082051489\C,0.9080877176,0.
4425073401,-1.3050482573\C,1.8509410342,1.5463816272,-0.807544088\C,2.9991063167,-0.290493563,0.69
34656018\N,3.0457697015,0.9373225424,-0.154666535\H,2.4053675663,-1.7411414171,-0.802246478\H,1.82
15282914,-2.0869730275,0.8365732014\H,-0.0425789578,0.899706015,-1.6017547473\H,1.3359926929,-0.03
63133355,-2.1941684008\C,1.150409288,2.4884487836,0.1850460475\C,2.3503332983,2.3575021639,-2.0046
159878\C,4.3973976942,-0.9099608945,0.669142486\C,2.6397804256,0.0946241483,2.13755952\O,4.008077
3504,1.7380522088,0.0824517564\H,0.6585474072,1.9523208801,1.0007692182\H,0.392523311,3.077344850
5,-0.3409897632\H,1.8884486607,3.1707138042,0.6147945956\H,2.9441580715,1.7260260873,-2.671225888
3\H,2.9719945675,3.1894324845,-1.6714360474\H,1.4918766094,2.7482334874,-2.5593729699\H,4.7152549
864,-1.0937729572,-0.3609549514\H,4.3775959183,-1.8617602106,1.2079502387\H,5.1206471189,-0.243922
0171,1.1414992817\H,1.5992314038,0.4109064724,2.2446443732\H,3.2907116396,0.9088293848,2.46695686
3\H,2.7922727614,-0.7682113244,2.7923783143\H,0.1811827179,-0.2245789752,0.627833098\O,-0.20241737
93,-1.6130792419,-0.8700240042\S,-1.2173423737,-2.426282383,0.0868402178\O,-1.5106860161,-3.6584497
384,-0.6058993829\O,-0.6869964271,-2.4257569163,1.4395878596\C,-2.65643836,-1.3787607621,0.03982952
12\H,-2.9971406753,-1.3211346058,-0.9933190102\H,-2.3865432127,-0.3961087341,0.4286774352\H,-3.4101
766641,-1.8460126792,0.6745435278\Version=ES64L-G09RevE.01\State=2-A\HF=-1146.5100138\S2=0.754
855\S2-1=0.\S2A=0.750014\RMSD=6.807e-09\RMSF=2.437e-06\Dipole=-1.1198003,1.1840279,-0.1387338\Q
uadrupole=6.0729231,-8.7680716,2.6951485,-12.1994633,0.1273454,-1.7190322\PG=C01 [X(C10H20N1O4S1)
\@

Nitroxide g.2 CORE

1\1\GINC-R2203\FOpt\UM062X\6-31+G(d,p)\C10H20N1O4S1(2)\ROOT\10-Aug-2017\0\#M062X\6-31+G**
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483648\NitroxideG.1.Methyl.freq\0,2\C,1.1

273126442,-0.3077768969,0.0242246295\C,2.0330592593,-0.870405198,-1.0515573013\C,1.4328313081,1.16
00237711,0.2543810627\C,2.8808227104,1.3907191826,0.7034735715\C,3.5186585653,-0.7555189919,-0.684
323313\N,3.809417152,0.6148678766,-0.1704480439\H,1.8396490103,-0.3170471794,-1.9792975517\H,1.793
2736006,-1.9231676655,-1.2333651871\H,0.7540848818,1.5722778013,1.0075188222\H,1.2530445024,1.689
7579043,-0.6898953224\C,3.0923501331,0.9840136143,2.1706754638\C,3.231035017,2.8701216734,0.53485
86465\C,4.3643839103,-0.9570445683,-1.9429844565\C,3.9247453255,-1.7971881646,0.3707743392\O,5.044
1485089,0.9125783109,-0.0674639677\H,2.7268148043,-0.0223152182,2.388525717\H,2.5566835188,1.6808
153391,2.8220583845\H,4.1588484238,1.028235305,2.4069178598\H,3.1917283311,3.1534315952,-0.520761
9621\H,4.235010342,3.0724042112,0.9101616271\H,2.5090579041,3.4753516042,1.0909909705\H,4.1699274
473,-0.1589606056,-2.6650030411\H,4.1073609024,-1.9177403577,-2.3992774716\H,5.4268469486,-0.94904
09784,-1.6965579442\H,3.2621231521,-1.8007153327,1.2395639496\H,4.9432198411,-1.5882892719,0.70856
80703\H,3.8995087204,-2.7965268752,-0.0741537387\H,1.2165407222,-0.8901297634,0.9491265992\O,-0.23
75314128,-0.4410813942,-0.46551711\S,-1.3234050709,-0.8506117512,0.657892909\O,-1.0862691233,-2.224
331446,1.0624698124\O,-1.3634074951,0.1875353474,1.6736014646\C,-2.7654800025,-0.7593696452,-0.370
3072162\H,-2.65005304,-1.4717712915,-1.1860405925\H,-2.8634295565,0.2622520739,-0.734672006\H,-3.60
85618858,-1.0296130146,0.2665623264\Version=ES64L-G09RevE.01\State=2-A\HF=-1146.5113366\S2=0.7
54856\S2-1=0.\S2A=0.750014\RMSD=3.195e-09\RMSF=2.518e-06\Dipole=-1.0635902,-0.0048081,-1.058331
7\Quadrupole=1.0317569,-1.0430645,0.0113076,-4.5888518,8.1375028,3.1160159\PG=C01 [X(C10H20N1O4
S1)]\@

Nitroxide g.1 1\1\GINC-R289FOpt\UM062X\6-31+G(d,p)\C16H24N1O4S1(2)\ROOT\20-Jun-2017\0\#M062
X\6-31+G(d,p) SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2684354560\A1 b2\0,2\C,1.266033
7865,-0.5659998733,0.1300726236\C,2.046113988,-0.8800336243,-1.1307332122\C,1.4017892944,0.9064427
571,0.4709435743\C,2.8580283826,1.3070913946,0.7328617931\C,3.5434487672,-0.5811006935,-0.97623483
24\N,3.7346123575,0.7575067326,-0.3419239792\H,1.6284729116,-0.2787132054,-1.9477545683\H,1.919864
5957,-1.9351166076,-1.3946041466\H,0.8067503376,1.1559490355,1.3572242467\H,1.0028033043,1.485200
01,-0.3714546325\C,3.3426695818,0.8027404835,2.102113313\C,2.9808042655,2.830943525,0.6848079137\
C,4.1924958777,-0.5230699435,-2.3600605692\C,4.2500350278,-1.6514994689,-0.1289876842\O,4.92294138
94,1.2166020132,-0.3711926443\H,3.1632609777,-0.266309687,2.2453907331\H,2.8131288391,1.340221959
2,2.8954084504\H,4.4149704369,0.9924308804,2.1987704308\H,2.7373304892,3.2011507439,-0.3149726641\
H,3.9965124349,3.1429182603,0.9313951068\H,2.2830580019,3.2703780127,1.4041359586\H,3.7765686642,
0.3043062668,-2.9417997964\H,3.9957561192,-1.4604666602,-2.8887235582\H,5.2701244558,-0.3785006274,-
2.2729906964\H,3.7445793946,-1.8385800684,0.8217924035\H,5.2747299384,-1.3303583583,0.0755646085\
H,4.2794765347,-2.5946207689,-0.682660922\H,1.6064345096,-1.2042752349,0.9528761463\O,-0.129531551
9,-0.8569481183,-0.1299123668\S,-0.9080582373,-1.7900629289,0.9346807849\O,-2.2428930998,-1.9121856
843,0.3975882292\O,-0.0835437049,-2.9502685275,1.2203596705\C,-0.9314110999,-0.7565018794,2.375790
0227\C,0.0263618998,-0.9422537614,3.3665361503\C,0.061496001,-0.0546231237,4.4402564719\C,-0.84793
14582,1.0031966964,4.5301682237\C,-1.8072950569,1.1562168436,3.5190019328\C,-1.8575775765,0.283106
0247,2.4395823204\C,-0.8254218143,1.9462955921,5.7046537309\H,0.721682618,-1.7732803932,3.29660540
03\H,0.805894927,-0.1887730936,5.2201438893\H,-2.5233794354,1.9710718638,3.5824428925\H,-2.5970780
104,0.3961122924,1.6527906489\H,0.1268532107,1.895307871,6.2367861133\H,-1.6203182978,1.692387354
1,6.4134616317\H,-0.9871139768,2.9786167187,5.3837418567\Version=ES64L-G09RevE.01\State=2-A\HF=
-1377.4793005\S2=0.75487\S2-1=0.\S2A=0.750014\RMSD=2.072e-09\RMSF=1.881e-06\Dipole=0.0802198,1.3
297672,1.5685961\Quadrupole=-10.5391232,-2.5257832,13.0649064,-15.8684006,-3.9653112,5.1377706\PG=
C01 [X(C16H24N1O4S1)]\@

Nitroxide g.2

1\1\GINC-R3117FOpt\UM062X\6-31+G(d,p)\C16H24N1O4S1(2)\ROOT\29-Apr-2016\0\#M062X\6-31+G(d,
p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=671088640\NitroxideG.1.freq\0,2\C,0.7924
557011,3.095549534,-0.6793485785\C,-0.631361586,2.7924709492,-1.0985548977\C,1.5931701108,1.811577
3628,-0.5736753657\C,1.0052074399,0.8380417005,0.4548526713\C,-1.3520443871,1.8722615948,-0.104517
7059\N,-0.4696891794,0.7238731751,0.2557016012\H,-0.5975005216,2.3142036108,-2.0856076775\H,-1.200
3833577,3.7227165897,-1.1975377726\H,2.6292316079,2.0372706663,-0.302157858\H,1.5980536866,1.3401
572257,-1.5647482185\C,1.2973522593,1.2883910103,1.8952511242\C,1.6009016827,-0.5529383835,0.23097
6542\C,-2.601494777,1.2927668188,-0.7702031494\C,-1.7612826318,2.6249780727,1.1718969431\O,-1.0388
693382,-0.2344269062,0.8735630643\H,1.0217150728,2.3298368151,2.0772924966\H,2.3676655253,1.18715
85823,2.0978853739\H,0.7441619994,0.6523188265,2.5913900086\H,1.3119522123,-0.9378923099,-0.75110
03748\H,1.2485617055,-1.2493402152,0.9930095651\H,2.6919613811,-0.4876357911,0.2784611311\H,-2.323
3316473,0.6610936292,-1.6185343216\H,-3.2299299889,2.1127460253,-1.1306443244\H,-3.1695725709,0.68
94150658,-0.0610323375\H,-0.9343418484,3.1832316748,1.6172109906\H,-2.1363078901,1.9085328686,1.90

75333185\H,-2.5578789295,3.3371381339,0.9361159955\H,0.8078579617,3.6605893201,0.2603664631\O,1.3676693686,3.9290284658,-1.7238905381\S,2.3127492022,5.1284392711,-1.1916915629\O,1.4726326558,6.1071411826,-0.5241365475\O,3.436210606,4.5423184759,-0.4796182852\C,2.8429980807,5.7549774236,-2.7544156436\C,3.9991390376,5.2393981744,-3.3308474351\C,4.4003608287,5.7302229403,-4.5690084529\C,3.6635733061,6.7230580885,-5.2246027415\C,2.5062170602,7.2205289207,-4.6136451225\C,2.0873511495,6.74443626,-3.3763732356\C,4.1244369301,7.27376781,-6.5488733528\H,4.570280647,4.477799534,-2.8098761518\H,5.3014714202,5.33928791,-5.0328546468\H,1.9285961214,7.9934868602,-5.1128715212\H,1.1985885181,7.1323051551,-2.889315857\H,4.737430747,6.5480180524,-7.0879486804\H,4.7282481113,8.1747521522,-6.3979775394\H,3.275226517,7.5457276767,-7.1803673924\Version=ES64L-G09RevD.01\State=2-A\HF=-1377.4776245\S2=0.754863\S2-1=0.\S2A=0.750014\RMSD=3.923e-09\RMSF=3.945e-06\Dipole=0.456008,0.7600506,-1.9871457\Quadrupole=1.3705841,-7.8133459,6.4427618,-5.5604631,-5.7117561,-7.6984885\PG=C01 [X(C16H24N1O4S1)]\@

Nitroxide h.1

1\I\GINC-R3124\FOpt\UM062X\6-31+G(d,p)\C9H17N4O1(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=402653184\NitroxideH.1.freq\0,2\C,0.6920780391,2.8649293597,-0.7543561972\C,-0.7546914253,2.4042171311,-0.8936129272\C,1.5988894788,1.6471173524,-0.7281451987\C,1.2900352276,0.6943252492,0.4320195799\C,-1.2109966983,1.5001800598,0.258456892\N,-0.1801296017,0.4534105011,0.5146928461\H,-0.8416889881,1.860792646,-1.8430722467\H,-1.4366120831,3.2625993009,-0.9425545733\H,2.646773147,1.9578083431,-0.6595751399\H,1.4769623833,1.1186984809,-1.6821189614\C,1.7928106251,1.2475132126,1.7752551501\C,1.9555507252,-0.6570513952,0.1644767267\C,-2.4987312777,0.7797765773,-0.1459581664\C,-1.461946319,2.2990589722,1.5473616392\O,-0.5417126228,-0.5004780092,1.2783098363\H,1.4594739078,2.2716017359,1.9609466384\H,2.8870188425,1.2420370682,1.7858539838\H,1.4304793889,0.6102194834,2.5862235017\H,1.5312739529,-1.1199865914,-0.7308467093\H,1.8064564536,-1.3328337849,1.0075539894\H,3.0278902627,-0.5054234014,0.0089765472\H,-2.3150726679,0.1215023743,-0.9996754007\H,-3.2533789762,1.5206800923,-0.4267116223\H,-2.8771779018,0.177044668,0.6806189619\H,-0.6182514275,2.9384807837,1.8183744127\H,-1.6505696022,1.6044387621,2.3701354596\H,-2.3416689833,2.9368954458,1.4174725037\N,1.1131288556,3.6898114751,-1.9141368572\H,0.8216449094,3.458531988,0.1616263123\N,0.5251528965,4.7709268492,-1.9928134274\N,0.0387994787,5.7810952697,-2.1440675532\Version=ES64L-G09RevD.01\State=2-A\HF=-647.0540016\S2=0.754856\S2-1=0.\S2A=0.750014\RMSD=8.227e-09\RMSF=7.541e-06\Dipole=0.1686548,0.2953109,0.1565607\Quadrupole=6.2214473,-6.5683527,0.3469054,-2.7306833,2.3971937,6.8084976\PG=C01 [X(C9H17N4O1)]\@

Nitroxide h.2

1\I\GINC-R135\FOpt\UM062X\6-31+G(d,p)\C9H17N4O1(2)\ROOT\30-Mar-2017\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=134217728\NitroxideH.1ii.freq\0,2\C,1.2017547893,-0.4901050517,0.0087966985\C,0.8430116657,0.8973159402,-0.5109499133\C,0.1557282103,-1.4900875836,-0.470425696\C,-1.2629243547,-1.1509704441,0.0044829835\C,-0.534526445,1.3792314215,-0.0384345486\N,-1.5421010622,0.2957617428,-0.2282848673\H,0.8511488079,0.870730393,-1.6099592273\H,1.5964803897,1.6266473145,-0.1942259202\H,0.4090928085,-2.4979978223,-0.1242034071\H,0.1668877211,-1.5063531624,-1.5696114386\C,-1.4555636904,-1.4776557472,1.4939626273\C,-2.2763460921,-1.9462972839,-0.8207311444\C,-0.9775505731,2.5652877609,-0.8972432512\C,-0.5105932235,1.8047903737,1.4382872942\O,-2.7603078308,0.6485528319,-0.1047686803\H,-0.671631751,-1.0510064893,2.1244398688\H,-1.4472618931,-2.5628847133,1.6340218696\H,-2.4215356729,-1.0882212651,1.826039768\H,-2.2314957867,-1.6466709921,-1.8715556612\H,-3.2895143112,-1.7739982067,-0.4553018336\H,-2.0429781955,-3.0126933789,-0.7467807102\H,-1.1083272768,2.2549268847,-1.9377201827\H,-0.2123714751,3.3461946097,-0.8546339494\H,-1.9239609134,2.9694527629,-0.5357282647\H,-0.0677523195,1.046681238,2.0888583159\H,-1.5327549287,1.9990498686,1.7736745485\H,0.0745839688,2.7233338551,1.5443653326\N,2.5727825022,-0.8916968992,-0.3921152878\H,1.2539275454,-0.4865860972,1.1001400914\N,2.7430654146,-0.9608956174,-1.6122947162\N,3.0023439725,-1.053726243,-2.7100306983\Version=ES64L-G09RevD.01\State=2-A\HF=-647.0538113\S2=0.754847\S2-1=0.\S2A=0.750014\RMSD=6.220e-09\RMSF=3.071e-06\Dipole=0.1823668,-0.0440137,0.4998641\Quadrupole=-8.8043224,6.7863524,2.01797,4.9327781,1.9379777,-0.6618196\PG=C01 [X(C9H17N4O1)]\@

Nitroxide h.3

1\I\GINC-R3127\FOpt\UM062X\6-31+G(d,p)\C9H17N4O1(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=402653184\NitroxideH.2.freq\0,2\C,0.8621959795,2.8367247456,-0.8060906464\C,-0.6196759176,2.4701542397,-0.8630953946\C,1.7043722633,1.5748931277,-0.6786042873\C,1.3134202221,0.61590979,0.4567835571\C,-1.1293254597,1.5758227365,0.2761127286\N,-0.1691697487,0.4607876047,0.5042734722\H,-0.7737218078,1.9434365784,-1.8133043356\H,-1.2449222367,3.3712126498,-0.9038342154\H,2.7592182537,1.8440721347,-0.5593400792\H,1.6104578427,1.0375720

457,-1.6303545571\C,1.8312996515,1.0773228357,1.8288122564\C,1.8967456981,-0.7660487479,0.1471448546\C,-2.4583323962,0.950264238,-0.1570090306\C,-1.3485932439,2.3451839111,1.5893189975\O,-0.6016415386,-0.5023533408,1.2184418065\H,1.5658375574,2.1113206444,2.0476903382\H,2.9233079256,1.0013771446,1.8450319022\H,1.4233290454,0.4198956615,2.6014715534\H,1.4490584753,-1.1774129921,-0.7622994301\H,1.7049761889,-1.4566906513,0.9691926423\H,2.9772945193,-0.6746547712,-0.0002210066\H,-2.3130816121,0.3071824051,-1.0298548991\H,-3.1631258799,1.7461358802,-0.417045563\H,-2.8798181494,0.3480394065,0.648423099\H,-0.4428855475,2.8421862196,1.9392587501\H,-1.6813650738,1.6435617445,2.3588527782\H,-2.1263619568,3.1025496258,1.445734864\N,1.2170512807,3.7664474567,0.3005777798\H,1.1321471213,3.3326602021,-1.7488634448\N,0.5308629637,4.7885149485,0.3341111007\N,-0.0609544199,5.7464425263,0.4478744091\Version=ES64L-G09RevD.01\State=2-A\HF=-647.0524\S2=0.754883\S2-1=0.\S2A=0.750014\RMSD=4.927e-09\RMSF=7.994e-06\Dipole=0.3126867,0.3473852,-0.9605378\Quadrupole=4.0060703,-8.2170352,4.2109649,-2.8292479,0.2565108,0.9367557\PG=C01 [X(C9H17N4O1)]\@

Nitroxide h.4

1\1\GINC-R56\FOpt\UM062X\6-31+G(d,p)\C9H17N4O1(2)\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\RadH1.freq\0,2\C,0.2349049772,-1.2869062862,-0.6731690773\C,1.313207375,-0.479433274,0.0708820517\C,0.743730414,0.7500841567,0.7862238\C,-0.4991773194,1.353048687,0.1255830719\N,-1.5200508981,0.2852086965,-0.0250351816\C,-1.1824080471,-1.1598694202,-0.1026589029\C,-0.1923021884,1.9566433485,-1.2533443047\C,-1.0741376018,2.4360087191,1.0402484261\C,-2.1693783191,-1.8279015307,-1.0611476555\C,-1.3109015584,-1.7927817104,1.2909499842\O,-2.7430276699,0.6289190055,-0.1057879104\H,0.5094353314,-2.3488872437,-0.6944385751\H,0.2088445961,-0.9594482726,-1.7184340746\H,1.5141870425,1.5240143225,0.8636472135\H,0.4895858929,0.4606362005,1.8106282514\H,0.2838607287,1.2362056069,-1.9244075782\H,0.4766647826,2.8163266625,-1.1442575337\H,-1.1239009455,2.2944013086,-1.7153250977\H,-1.3766010393,2.0051717218,1.9989406998\H,-1.9485169701,2.900246315,0.5829008425\H,-0.3119367052,3.2001931314,1.2195505158\H,-2.1581910575,-1.3297356654,-2.0348507513\H,-3.1842384568,-1.7773242872,-0.6653390641\H,-1.8871590329,-2.8766408225,-1.1942519586\H,-0.5639581318,-1.4118656519,1.990737166\H,-1.1790299949,-2.8773714004,1.217848413\H,-2.3093549512,-1.5881029772,1.687277148\N,1.9966665724,-1.2747073503,1.1284608106\H,2.0718431881,-0.1662541566,-0.6588920475\N,2.6442978452,-2.227930677,0.6908277467\N,3.2556921413,-3.1262171563,0.3752735718\Version=ES64L-G09RevD.01\State=2-A\HF=-647.0487763\S2=0.755233\S2-1=0.\S2A=0.750018\RMSD=5.130e-09\RMSF=9.769e-06\Dipole=0.6408357,0.2210586,-0.3746125\Quadrupole=-6.9299864,3.3320136,3.5979729,7.2018833,-2.3202583,0.6658932\PG=C01 [X(C9H17N4O1)]\@

Nitroxide i

1\1\GINC-R63\FOpt\UM062X\Gen\C9H17Br1N1O1(2)\ROOT\05-Dec-2016\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2684354560\NitroxideJ.New.1.freq\0,2\C,0.6699683432,2.8355364942,-0.678005464\C,-0.771648504,2.391571697,-0.8435412278\C,1.5872058754,1.6267026452,-0.6907333649\C,1.2734394513,0.6485239524,0.4527096468\C,-1.225111347,1.4586901911,0.2908521743\N,-0.1958139226,0.4055486875,0.5237116216\H,-0.8638564412,1.8682026819,-1.8031773476\H,-1.4453399595,3.2536734779,-0.8729320577\H,2.6355075547,1.9304404729,-0.6085725479\H,1.467357922,1.1122960286,-1.6521602\C,1.7731294146,1.1753929458,1.8070248131\C,1.9418682471,-0.6953103633,0.156256417\C,-2.5127485659,0.7491190037,-0.1323160702\C,-1.4764707657,2.2290902959,1.5965139553\O,-0.5589777304,-0.5667392431,1.263055715\H,1.4400033732,2.1958726938,2.0116929734\H,2.8672813634,1.1689537544,1.820648078\H,1.4080596223,0.5229487419,2.6045812854\H,1.5193846203,-1.1397064558,-0.7491728589\H,1.7919790064,-1.3889573311,0.9846683605\H,3.0143466725,-0.5392207571,0.0063714737\H,-2.3275894895,0.107692055,-0.998381923\H,-3.265063896,1.4969061228,-0.4004121402\H,-2.8946571135,0.1307053309,0.6810655371\H,-0.6363512399,2.8691399366,1.8771855982\H,-1.6579251798,1.5171079868,2.4059651312\H,-2.3602965459,2.8640192039,1.4820027528\Br,1.1603408239,4.0558369822,-2.1396265619\H,0.8077795423,3.4400050575,0.2202647152\Version=ES64L-G09RevE.01\State=2-A\HF=-3056.8170384\S2=0.75485\S2-1=0.\S2A=0.750014\RMSD=4.319e-09\RMSF=1.626e-05\Dipole=0.0964967,0.3369658,0.1970647\Quadrupole=5.3522629,-5.2812673,-0.0709955,-4.3426665,2.3938028,5.9867062\PG=CS [SG(C1H1Br1N1O1),X(C8H16)]\@

Nitroxide k.1

1\1\GINC-R124\FOpt\UM062X\6-31+G(d,p)\C12H20N1O2(2)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramanmaxdisk=402653184\NitroxideK.2.freq\0,2\C,0.4089588662,2.6688094047,-0.837025816\C,-1.006059974,2.1114728378,-0.8704415329\C,1.4035194738,1.5194747555,-0.678207448\C,1.1617151079,0.6122055497,0.5351276162\C,-1.3907574876,1.212580537,0.3153936129\N,-0.2832222053,0.2585875408,0.6117453203\H,-1.1036645772,1.5298104039,-1.7955474314\H,-1.7215909474,2.938676572,-0.9253774497\H,2.4366914417,1.883663785,-0.639181177\H,1.3278548262,0.9122829161,-1.5894747951\C,1.6047761925,1.2623785487,1.8563547455\C,1.9368437213,-0.693387448,0.3375323895\C,-2.6

089004637,0.3734583518,-0.0816157415\C,-1.7294679289,2.0178295747,1.5804330733\O,-0.575916911,-0.7035022637,1.3952665895\H,1.1428615989,2.2384403547,2.0113439288\H,2.6934465637,1.3867090575,1.8542217795\H,1.3341351875,0.6026024146,2.6852672664\H,1.5624990847,-1.2329915202,-0.53729794\H,1.8329694376,-1.3385601965,1.2106786404\H,2.9959970386,-0.4636220511,0.1847039987\H,-2.35904796,-0.301682378,-0.9054556784\H,-3.4144208011,1.0408816555,-0.4032528037\H,-2.9555101676,-0.2245429807,0.7621388325\H,-0.9473939665,2.732375246,1.8357979206\H,-1.8860225318,1.3241449947,2.4111239347\H,-2.6552146035,2.5778191737,1.4126803493\O,0.4704651727,3.6443233225,0.1955985404\H,0.6114779798,3.1739909707,-1.7965142615\C,1.6755753794,4.3774276929,0.2225027633\C,1.5438432731,5.484496281,1.1723473965\C,1.4587277774,6.3972146169,1.9549909946\H,1.9035075249,4.7738625643,-0.779279127\H,2.5189469678,3.7439699397,0.5330119255\H,1.3742179101,7.204079776,2.6485195839\Version=ES64L-G09RevD.01\State=2-A\HF=-674.1154541\S2=0.754889\S2-1=0.\S2A=0.750014\RMSD=2.644e-09\RMSF=9.566e-06\Dipole=0.6414308,0.9061012,-0.9036011\Quadrupole=2.6658693,-4.9889689,2.3230996,-1.3644843,0.5367101,4.1864835\PG=C01 [X(C12H20N1O2)]\@@

Nitroxide k.2

1\1\GINC-R65\FOpt\UM062X\6-31+G(d,p)\C12H20N1O2(2)\ROOT\30-Mar-2017\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\NitroxideK.3.freq\0,2\C,-0.7751637144,-0.6988145725,0.5286239098\C,0.1706086688,-1.5080301727,-0.3507045511\C,-0.740173949,0.7531075717,0.0874487261\C,0.6513371691,1.3872855586,0.1801620221\C,1.6216143748,-1.012491205,-0.2904913234\N,1.6644398572,0.4723025536,-0.4193182669\H,-0.2022343332,-1.4488798087,-1.3814672314\H,0.1676177062,-2.5667887326,-0.0690599661\H,-1.4384570771,1.3416375205,0.6920882182\H,-1.0936928501,0.7906690583,-0.9505919602\C,1.0427789118,1.6991046678,1.6338046638\C,0.6728443042,2.6826931005,-0.6336932922\C,2.402078001,-1.591405453,-1.4724358735\C,2.3102356378,-1.429108949,1.0198882117\O,2.817571644,0.9775004532,-0.6185280298\H,0.919489073,0.8384529314,2.2957900845\H,0.4149317513,2.5103896156,2.0149636857\H,2.0878838408,2.0184067996,1.6660185541\H,0.5032379501,2.4693259941,-1.6927732596\H,1.6352691678,3.1859010196,-0.5314035718\H,-0.1209477812,3.3453393874,-0.2758835598\H,1.9935392922,-1.219593622,-2.416255197\H,2.3194462684,-2.6823444298,-1.4579034563\H,3.454160507,-1.3087437239,-1.4147664456\H,1.7284507638,-1.158970389,1.9047277223\H,3.2884130594,-0.9450391865,1.0838068917\H,2.4532683739,-2.5141357698,1.0280474916\O,-2.1295305351,-1.1131288174,0.4090886496\H,-0.4810918782,-0.7870462293,1.5878878805\C,-2.4173024241,-2.397503849,0.9157495926\C,-2.3001457473,-3.4715935392,-0.0868603167\C,-2.2312167443,-4.3634402841,-0.8964854533\H,-3.4507366815,-2.3679170879,1.2734874642\H,-1.7726255532,-2.6285078549,1.7767038003\H,-2.1693065742,-5.1455025554,-1.620275814\Version=ES64L-G09RevD.01\State=2-A\HF=-674.1165814\S2=0.754869\S2-1=0.\S2A=0.750014\RMSD=2.153e-09\RMSF=4.553e-06\Dipole=-0.5911167,-0.6682355,0.6290382\Quadrupole=-7.493778,4.3569638,3.1368142,-3.5537555,0.4681077,2.8231365\PG=C01 [X(C12H20N1O2)]\@@

Nitroxide k.3

1\1\GINC-R66\FOpt\UM062X\6-31+G(d,p)\C12H20N1O2(2)\ROOT\30-Mar-2017\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\NitroxideK.3i.freq\0,2\C,-0.6494301198,-0.8085444249,0.6275332757\C,0.2896714248,-1.587985811,-0.2847793026\C,-0.7306347895,0.6270450042,0.1428567958\C,0.6231441626,1.3442482344,0.1446025823\C,1.7101204894,-1.0086902735,-0.3124046504\N,1.6564348549,0.4715774253,-0.4843331101\H,-0.1354450392,-1.5775755691,-1.2975318455\H,0.3746874365,-2.6344260624,0.0312578595\H,-1.430430919,1.1897745359,0.7698743448\H,-1.1394579895,0.6149739271,-0.8755424375\C,1.0712249633,1.7201494551,1.5662476383\C,0.5263572486,2.6138104833,-0.7035802495\C,2.4666913849,-1.5757448398,-1.5152158181\C,2.480483836,-1.3469134031,0.974980486\O,2.7654850811,1.0360267525,-0.7598478663\H,1.0337236995,0.8733744559,2.2557467288\H,0.4170194296,2.5043623087,1.959475353\H,2.0956759695,2.1006285954,1.5329863979\H,0.3139729516,2.3600317347,-1.7459659067\H,1.4616997139,3.1739914561,-0.6670729393\H,-0.2849375858,3.2403217385,-0.3208554047\H,1.9930489704,-1.2567992255,-2.4480199881\H,2.4517285495,-2.6688472276,-1.4669015737\H,3.5014172776,-1.2303044986,-1.5169296834\H,1.9184135778,-1.0969983503,1.8781278045\H,3.4263328191,-0.7986752674,0.9842979883\H,2.6946073715,-2.4199322295,1.0001231528\O,-1.9811829789,-1.3082087251,0.5974300087\H,-0.2883497876,-0.8460941389,1.6652355197\C,-2.1440204488,-2.6480760988,1.0093505969\C,-1.5513715614,-2.9429536838,2.3261125566\C,-1.0513570299,-3.1925252546,3.3957956685\H,-1.7262659748,-3.3439236971,0.2690250363\H,-3.2229775995,-2.816250092,1.050163358\H,-0.6201093883,-3.4136672339,4.3470476235\Version=ES64L-G09RevD.01\State=2-A\HF=-674.1184909\S2=0.754869\S2-1=0.\S2A=0.750014\RMSD=1.616e-09\RMSF=4.378e-06\Dipole=-0.5359111,-0.7773538,0.551236\Quadrupole=-5.898636,3.0878456,2.8107904,-3.261846,3.9449332,1.2394896\PG=C01 [X(C12H20N1O2)]\@@

Nitroxide k.5

I\1\GINC-R39\FOpt\UM062X\6-31+G(d,p)\C12H20N1O2(2)\ROOT\03-Dec-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\RadK5.freq\0,2\C,-0.0488279775,-1.193484
5117,-1.0955689519\C,1.1343747618,-0.2618015141,-0.7845382484\C,0.749190944,0.8885210507,0.1483844
532\C,-0.7058152668,1.3503017826,0.0354282863\N,-1.5908971412,0.1742452681,0.2258100204\C,-1.15394
91184,-1.2222756194,-0.0315750366\C,-1.0079127852,1.9893644748,-1.3285082665\C,-1.0020680728,2.3562
389384,1.1489990515\C,-2.3534564764,-2.0010860319,-0.5734834845\C,-0.676714948,-1.8629009598,1.2808
649078\O,-2.7866235508,0.3779265862,0.612729442\H,0.3205200189,-2.2169406794,-1.227265513\H,-0.502
413939,-0.9017747313,-2.0499382248\H,1.4082744153,1.7449620923,-0.0269327201\H,0.9369369895,0.5561
724002,1.1743643442\H,-0.7559674391,1.3242279569,-2.1595800013\H,-0.4340703261,2.9145982776,-1.443
5821514\H,-2.0733192251,2.2276679347,-1.38855014\H,-0.8685892152,1.8898875066,2.1293177396\H,-2.02
89254434,2.7167314655,1.0782104091\H,-0.3150128556,3.2034654674,1.0633650603\H,-2.7691640938,-1.50
43769437,-1.4549415075\H,-3.1397143239,-2.0720603691,0.178969889\H,-2.0301197652,-3.0087710015,-0.8
516948754\H,0.2483095405,-1.4152323884,1.6491339353\H,-0.4880720517,-2.9296245781,1.1217643821\H,-
1.4577439708,-1.7548394419,2.0387712653\O,2.1978289423,-0.9455434493,-0.1274236389\H,1.5192757301,
0.142022271,-1.73438417\C,4.0418406377,-2.395545917,-0.2432563314\C,4.8903644556,-2.9982557291,0.36
45983077\H,5.6384170354,-3.5279157282,0.9113509387\C,3.0226607757,-1.6756694132,-1.0094230305\H,3.
5119790201,-0.9936032089,-1.7214491771\H,2.4385247191,-2.4007012569,-1.5951069631\Version=ES64L-
G09RevD.01\State=2-A\HF=-674.1108118\S2=0.755241\S2-1=0.\S2A=0.750018\RMSD=8.339e-09\RMSF=3.
822e-06\Dipole=0.9808451,-0.1439605,-0.8821749\Quadrupole=-6.7890076,4.5699832,2.2190243,0.765502,1.
7741145,-1.063287\PG=C01 [X(C12H20N1O2)]\@

Nitroxide k.6

I\1\GINC-R38\FOpt\UM062X\6-31+G(d,p)\C12H20N1O2(2)\ROOT\09-Dec-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\RadK3.freq\0,2\C,-0.6692793063,0.99572914
35,-0.0432232585\C,-1.0759874879,-0.2311535136,0.7752984839\C,0.0635803872,-1.2520679557,0.9204193
8\C,1.1168188078,-1.2196126154,-0.194406051\N,1.6193393311,0.17262751,-0.3220924803\C,0.813782318,
1.3644181549,0.045229907\C,0.5472179355,-1.6842190179,-1.5435587745\C,2.2940088431,-2.1137965088,0.1
980159938\C,1.1177225503,2.4746224738,-0.9620089689\C,1.2141956582,1.8254765017,1.4548840951\O,2.
8015757608,0.3551929475,-0.7581024522\H,-1.2703447722,1.8583554995,0.2622624204\H,-0.9212370365,0.
7949606751,-1.0896727881\H,-0.3571520101,-2.2635464369,0.9611546528\H,0.574995194,-1.0923103504,1.
8766437233\H,-0.3631006264,-1.1462502951,-1.8151456326\H,0.3022645764,-2.7502665685,-1.4919895805\
H,1.300281711,-1.5358348231,-2.3226660912\H,2.774826149,-1.7403530397,1.1067648997\H,3.0412695688,
-2.1395427069,-0.5959633825\H,1.9279962204,-3.1287891098,0.3806342574\H,0.9148468813,2.1314303003,
-1.9805566668\H,2.1654588711,2.771691315,-0.9033316103\H,0.484007156,3.3402806445,-0.7471161876\H,
0.9598095758,1.0844883688,2.2180646992\H,0.7013141846,2.7606599675,1.7017159238\H,2.2934565676,1.
9980228395,1.4868176933\O,-2.2043639372,-0.7836113922,0.0959359825\H,-1.3980595065,0.082731852,1.7
780769212\C,-3.7503430079,-0.8054659653,1.9382460761\C,-4.3261212025,-0.1747556274,2.7907203701\H,
-4.841747457,0.3842951653,3.5398165178\C,-3.0436377828,-1.5793301537,0.9012029364\H,-2.4839856492,-
2.3933965406,1.3844174153\H,-3.7721484655,-2.0332707382,0.2250315761\Version=ES64L-G09RevD.01\S
tate=2-A\HF=-674.1132409\S2=0.755244\S2-1=0.\S2A=0.750018\RMSD=6.839e-09\RMSF=5.821e-06\Dipole
=-1.0266715,-0.2769777,0.8356957\Quadrupole=-7.16073,5.5059778,1.6547522,-1.3782657,0.4018852,1.9142
461\PG=C01 [X(C12H20N1O2)]\@

Nitroxide l.1

I\1\GINC-R159\FOpt\UM062X\6-31+G(d,p)\C12H20N1O3(2)\ROOT\16-Jul-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\NitroxideL.1iii.freq\0,2\C,-0.4825903787,0.
0005073515,0.9104748891\C,-0.0365695088,-1.2388254193,0.1603870152\C,-0.0413171331,1.2417565009,0.
1521548669\C,1.4818151858,1.3217441288,-0.0048238325\C,1.487182685,-1.3121555319,0.0004477644\N,2.
0120175376,0.004675296,-0.4648124105\H,-0.508855118,-1.2276064256,-0.8300317655\H,-0.3787769645,-2.
141137799,0.678643483\H,-0.3862890357,2.1432546817,0.6680739976\H,-0.511068803,1.2142376037,-0.839
6113981\C,2.1662088836,1.72036845,1.3126316423\C,1.826647313,2.3494984601,-1.0840208604\C,1.83273
86393,-2.3435806582,-1.0752033421\C,2.1800940429,-1.7023038953,1.316041991\O,3.2214643377,0.004577
9375,-0.8662139228\H,1.8413842623,1.1091472733,2.1578889509\H,1.9274596113,2.7623448275,1.5453689
885\H,3.2493465291,1.622416464,1.2009765023\H,1.4387939397,2.0281604501,-2.0548206422\H,2.9073258
553,2.4725180531,-1.1666985988\H,1.3733103938,3.3102465596,-0.8224517222\H,1.4399405954,-2.0279772
943,-2.0458432929\H,1.3846768795,-3.3055257073,-0.808364421\H,2.9135815457,-2.4618965393,-1.161335
4414\H,1.8662109798,-1.0806064807,2.1579053424\H,3.2622972395,-1.6061052863,1.1950657209\H,1.9445
665493,-2.743212788,1.5582931691\O,-1.9190466171,-0.0522649724,0.9786078269\H,-0.1024140368,0.0144
160177,1.9367431493\C,-2.5041061177,0.7085287248,1.922335626\O,-1.8906907032,1.4068643841,2.697368
6821\C,-3.983469906,0.5660651733,1.8797086789\C,-4.7412752592,1.2393704496,2.742792634\H,-4.392805

4098,-0.0989782233,1.1266014299\H,-4.278766006,1.892422435,3.4773603432\H,-5.822252008,1.153325798
7,2.7345189563\\Version=ES64L-G09RevD.01\State=2-A\HF=-749.3962717\S2=0.754864\S2-1=0.\S2A=0.75
0014\RMSD=5.237e-09\RMSF=2.232e-05\Dipole=-1.2188467,-0.3191326,0.1676962\Quadrupole=1.059591,2.
711531,-3.771122,0.0809178,3.3605803,-1.4940033\PG=C01 [X(C12H20N1O3)]\@

Nitroxide I.2

1\1\GINC-R182\FOpt\UM062X\6-31+G(d,p)\C12H20N1O3(2)\ROOT\16-Jul-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\NitroxideL.1iv.freq\0,2\C,-0.4686244401,-0.
0356342724,0.9264617244\C,-0.0133434849,-1.2668374424,0.1685303798\C,-0.050396138,1.2133530634,0.1
678834529\C,1.469957318,1.3138934574,-0.0027228574\C,1.5098517007,-1.3199093237,-0.0051631309\N,2.
013082658,0.0050416527,-0.4715843055\H,-0.4938100606,-1.2587537632,-0.818118551\H,-0.3389919477,-2.
175113397,0.6871773085\H,-0.401747451,2.1090383129,0.6896272724\H,-0.5290318882,1.1831062682,-0.81
9550314\C,2.1609298788,1.7178743057,1.3096915346\C,1.7917760101,2.348850422,-1.0821637893\C,1.859
1715137,-2.3437534215,-1.0868706203\C,2.2198640684,-1.7044017869,1.3028964973\O,3.2187359129,0.021
7071745,-0.884077822\H,1.849087268,1.1027141698,2.1570282886\H,1.9134151325,2.7570847618,1.545715
6996\H,3.2441095806,1.6312403505,1.1892897077\H,1.3994426093,2.0250012796,-2.0503628788\H,2.87005
20407,2.4859152422,-1.1740444867\H,1.3284647382,3.3029584536,-0.8138831197\H,1.4535327889,-2.03071
10451,-2.0530806962\H,1.426533993,-3.3124258482,-0.8187978431\H,2.9406929537,-2.4473401225,-1.1831
243352\H,1.9076775681,-1.0876172461,2.1489898559\H,3.2996474402,-1.5956750015,1.1712588276\H,1.99
8663861,-2.74834572,1.5456786\O,-1.9034706975,-0.1077942151,1.008364976\H,-0.0780263009,-0.0205848
88,1.9486824426\C,-2.4876306198,0.6447034047,1.9588947282\O,-1.8715488226,1.3456853026,2.730346036
8\C,-3.9682138576,0.526381894,1.9706900466\C,-4.6564377839,-0.2304281335,1.1174505323\H,-4.4474937
311,1.1195710458,2.7425026525\H,-4.1516441323,-0.813189516,0.3538992549\H,-5.7390276784,-0.2818954
181,1.1656549308\\Version=ES64L-G09RevD.01\State=2-A\HF=-749.3954415\S2=0.754865\S2-1=0.\S2A=0.
750014\RMSD=6.123e-09\RMSF=3.798e-06\Dipole=-1.194034,-0.5270306,-0.0634169\Quadrupole=1.583244,
2.9318391,-4.5150831,1.7296145,5.4898612,-2.2083402\PG=C01 [X(C12H20N1O3)]\@

Nitroxide I.3

1\1\GINC-R237\FOpt\UM062X\6-31+G(d,p)\C12H20N1O3(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I
NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramanmaxdisk=536870912\NitroxideL.2i.freq\0,2\C,0.6988669
812,2.5702415366,-0.7475007865\C,-0.7750218883,2.1935807225,-0.8148266754\C,1.5601764007,1.3292335
196,-0.5919510447\C,1.1705796985,0.3831577555,0.5547431453\C,-1.2827192959,1.3071137991,0.33049464
47\N,-0.3094944112,0.2088114375,0.5906201993\H,-0.9133448831,1.6538823027,-1.7604297912\H,-1.38994
36137,3.0970527523,-0.8713564195\H,2.6099695303,1.6162694282,-0.4674532295\H,1.4849549336,0.77748
12182,-1.5371990297\C,1.6641194193,0.8788870043,1.9240459805\C,1.7788961341,-0.9950623992,0.279296
2145\C,-2.5970669869,0.6528309354,-0.1044721391\C,-1.5273430491,2.0963865298,1.6274771497\O,-0.734
0452334,-0.7463658245,1.3205514478\H,1.3590438754,1.9053016693,2.1271754045\H,2.7579576996,0.8389
751204,1.9500007194\H,1.2707681002,0.2200458001,2.7029386692\H,1.3522186586,-1.427611262,-0.63035
87949\H,1.583144488,-1.6749468309,1.1093262886\H,2.8603802075,-0.8906330046,0.1475861408\H,-2.4307
08162,-0.0091883312,-0.9592035538\H,-3.3069178509,1.433281644,-0.3951528055\H,-3.0231315252,0.0651
348557,0.709486627\H,-0.6431302964,2.6448356777,1.9537732807\H,-1.8267881721,1.401100218,2.416485
8935\H,-2.3368978372,2.816017887,1.4673012698\O,0.9808084326,3.4536559327,0.3579573934\H,0.971465
6826,3.1025530461,-1.6639532517\C,0.6249939036,4.7430280887,0.2088918533\O,0.114169613,5.18805471
88,-0.7933567233\C,0.9430404553,5.5246560269,1.4332179112\C,0.6511811654,6.8224778628,1.489356753
3\H,1.4099622197,4.9885226933,2.2534309653\H,0.1837486407,7.310978506,0.6391334278\H,0.8700369656,7
.4147589632,2.3709628651\\Version=ES64L-G09RevD.01\State=2-A\HF=-749.3946071\S2=0.754887\S2-1=0.\
S2A=0.750014\RMSD=5.505e-09\RMSF=8.376e-06\Dipole=0.631975,0.7803638,0.0192756\Quadrupole=2.60
60033,-3.9270687,1.3210654,-2.3128759,1.0896476,9.417889\PG=C01 [X(C12H20N1O3)]\@

Nitroxide I.4

1\1\GINC-R224\FOpt\UM062X\6-31+G(d,p)\C12H20N1O3(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I
NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramanmaxdisk=536870912\NitroxideL.2ii.freq\0,2\C,0.5970298
526,2.6003129846,-0.6996510061\C,-0.8492540992,2.1423307449,-0.8329527932\C,1.5189145947,1.4067775
828,-0.5228049059\C,1.1353820684,0.4215650071,0.5925231423\C,-1.3530568891,1.2140708439,0.27998796
05\N,-0.3324608811,0.1655423938,0.565071906\H,-0.9165367071,1.6079866186,-1.7893393583\H,-1.512317
4356,3.0096340596,-0.9065482272\H,2.545089829,1.7491561791,-0.3504212272\H,1.5142101602,0.8666679
103,-1.477696143\C,1.5393546441,0.9217063696,1.9886181325\C,1.8328842277,-0.9150268387,0.324371490
4\C,-2.6111039202,0.4947004521,-0.2146183554\C,-1.69260977,1.9730178339,1.5739075651\O,-0.73216482
91,-0.8220888022,1.265075288\H,1.1322578132,1.9099925995,2.2014773768\H,2.6308124758,0.9790321911,
2.053884432\H,1.1777653366,0.2135553966,2.7390226299\H,1.4745440942,-1.3531080645,-0.6117181181\H,1

.6370142089,-1.620572505,1.1326321321\H,2.9117601656,-0.7482710205,0.246088781\H,-2.3742775425,-0.1489130482,-1.0667804796\H,-3.3494162516,1.2388648805,-0.5284384612\H,-3.0381262987,-0.1231912767,0.5762227276\H,-0.8628010942,2.5847360211,1.9302972974\H,-1.9650787588,1.252145057,2.3497002049\H,-2.5473894582,2.6327564007,1.3922131264\O,0.7877241517,3.4855375976,0.4247495285\H,0.8765720965,3.1569246968,-1.5993390399\C,0.3551490194,4.7504810032,0.2720970888\O,-0.155182275,5.1663777602,-0.7437381949\C,0.5646893494,5.5887773227,1.4803919793\C,1.1504199858,5.1510809656,2.5940005857\H,0.1957530999,6.6038941833,1.3768412346\H,1.5197586347,4.1333404516,2.672398346\H,1.2787104022,5.8037560482,3.4510033542\Version=ES64L-G09RevD.01\State=2-A\HF=-749.3943255\S2=0.754888\S2-1=0.\S2A=0.50014\RMSD=6.185e-09\RMSF=1.299e-05\Dipole=0.7249545,0.5652729,0.1817763\Quadrupole=3.7719582,-7.0602189,3.2882607,-1.460256,1.0732458,9.5819572\PG=C01 [X(C12H20N1O3)]\@

Nitroxide l.5

1\1\GINC-R166\FOpt\UM062X\6-31+G(d,p)\C12H20N1O3(2)\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\RadL1.freq\0,2\C,-0.1106290447,0.6112446313,1.0451305375\C,0.6115067558,-0.4740402528,0.2381560476\C,-0.3023979531,-1.2027336905,-0.7478426815\C,-1.7653177524,-1.2923208639,-0.3016141415\N,-2.2548033771,0.0792178024,-0.0125764576\C,-1.358705883,1.1986825268,0.3770437998\C,-1.9382240476,-2.1650486601,0.9509006345\C,-2.6027729011,-1.86728875,-1.4449752791\C,-2.1028717286,2.0738835049,1.3866227499\C,-1.0139622071,2.0308989157,-0.8675917359\O,-3.5054516718,0.3022942197,-0.096227009\H,0.5922609847,1.4197199877,1.268245621\H,-0.4024954345,0.1896021948,2.0131104803\H,0.073952455,-2.2147082271,-0.9295055962\H,-0.2633291798,-0.6756842457,-1.7064978676\H,-1.3101506533,-1.8279071145,1.7801459842\H,-1.6756319237,-3.2030514798,0.7225280538\H,-2.9824456529,-2.1308804734,1.2731607667\H,-2.5568337722,-1.2119013164,-2.3194765553\H,-3.6468240412,-1.9640313319,-1.1454258156\H,-2.2129951691,-2.8523737093,-1.7185310812\H,-2.4414441062,1.4756974765,2.2374258695\H,-2.9765645802,2.536747797,0.9263884671\H,-1.4288583279,2.8560595885,1.7486110855\H,-0.4004423209,1.4748215111,-1.5800668478\H,-0.4563911638,2.9251804911,-0.5705881876\H,-1.9388201652,2.3423697422,-1.3611528734\O,1.6651911197,0.0950797045,-0.5693097311\H,1.08280061,-1.172716795,0.934580579\C,2.8039483481,0.4177064611,0.0708121214\O,2.9731291348,0.2599799764,1.2588023301\C,3.803707811,0.985259343,-0.8721616817\C,4.9974909872,1.3682932256,-0.4240594116\H,3.5096831348,1.0648656265,-1.9134696728\H,5.2405982753,1.265883571,0.6296945707\H,5.745453441,1.7846186126,-1.089807072\Version=ES64L-G09RevD.01\State=2-A\HF=-749.3911219\S2=0.755238\S2-1=0.\S2A=0.750018\RMSD=4.667e-09\RMSF=6.793e-06\Dipole=1.0490068,-0.1320037,-0.4997303\Quadrupole=-5.4155795,5.0012405,0.4143391,4.7020335,-5.5341644,-0.2057908\PG=C01 [X(C12H20N1O3)]\@

Nitroxide l.6

1\1\GINC-R170\FOpt\UM062X\6-31+G(d,p)\C12H20N1O3(2)\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\RadL4.freq\0,2\C,-0.35234564,-0.8822953034,-0.5519071225\C,0.7005537199,-0.3295525292,0.4070936696\C,1.2463942233,-1.3820776586,1.3807939454\C,0.2623013044,-2.5095954547,1.7111598248\N,-0.2207213419,-3.1129981626,0.443046145\C,-0.2424439934,-2.3821359504,-0.8500858663\C,-0.9426868278,-2.0057876964,2.5204318682\C,0.9932310553,-3.5926878006,2.5064299794\C,-1.4787600608,-2.8300278193,-1.6306832549\C,1.0232152389,-2.7270051425,-1.6490078799\O,-0.6445015623,-4.3133352392,0.4688389833\H,-0.2945211698,-0.3259200616,-1.4931173984\H,-1.3459636794,-0.6913550629,-0.1325073599\H,1.5612951778,-0.8981867296,2.3093720579\H,2.143448079,-1.8259503274,0.9342956215\H,-1.4596393221,-1.1804749773,2.0228529251\H,-0.6117083756,-1.6572055412,3.5037535825\H,-1.6533353148,-2.8252068973,2.6585464102\H,1.8019862095,-4.0245821774,1.9099916566\H,0.3078917157,-4.3943204414,2.7839923798\H,1.4177945018,-3.149932639,3.4122703844\H,-2.384825115,-2.675662782,-1.0375777355\H,-1.4132675602,-3.8891171735,-1.8821075011\H,-1.5530733937,-2.2448125765,-2.5522892095\H,1.9296305767,-2.3562670305,-1.1657128835\H,0.966445045,-2.2773088496,-2.6455854359\H,1.0956953433,-3.81289632,-1.7562228485\O,1.78327552,0.1816914001,-0.402793832\H,0.2895777813,0.5196516568,0.9611929613\C,2.6334926637,1.0281914877,0.2057721899\O,2.5296593434,1.3646193039,1.3636869417\C,3.6940807714,1.4858660519,-0.7305898416\C,4.6335903228,2.3299048004,-0.3093159359\H,3.6563368405,1.1012702438,-1.7444098911\H,4.6244416,2.6839612907,0.7175878444\H,5.4185063232,2.6799321088,-0.9706553747\Version=ES64L-G09RevD.01\State=2-A\HF=-749.3913538\S2=0.755241\S2-1=0.\S2A=0.750018\RMSD=9.447e-09\RMSF=1.000e-05\Dipole=0.4456935,0.9382995,-0.5644039\Quadrupole=4.7981923,-8.1549147,3.3567225,-1.6737626,-2.7514454,-3.6926495\PG=C01 [X(C12H20N1O3)]\@

Nitroxide m.1

1\1\GINC-R125\FOpt\UM062X\6-31+G(d,p)\C10H18N1O3(2)\ROOT\13-Jul-2017\0\#M062X/6-31+G** SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610612736\NitroxideM.li.freq\0,2\C,-2.1233100453,-0.0146012816,0.8491445535\C,-1.5899251663,1.2358475825,0.1428014418\C,-1.5441535798,-1.2467054488,0.146594488\C,-1.9489426562,-1.331247231,-1.3300577001\C,-1.9974739913,1.3009027815,-1.3340785722\N,

-1.7334113618,-0.0117568096,-1.9902971514\H,-0.4959160981,1.2351403985,0.2171680376\H,-1.951666062,2.1462928597,0.6347312679\H,-1.8721331073,-2.1683502158,0.6413284082\H,-0.4509165252,-1.2054422333,0.2208973815\C,-3.4169061262,-1.7534136563,-1.4966666256\C,-1.0489557747,-2.3449172978,-2.0398671552\C,-1.1354261333,2.3448861272,-2.0470342249\C,-3.4799921949,1.6681572989,-1.5018995908\O,-1.7989382395,-0.0149111154,-3.2631037155\H,-4.1000325917,-1.148157173,-0.8958780301\H,-3.5341091717,-2.7977182417,-1.1910921258\H,-3.701299714,-1.661317482,-2.5481851971\H,-0.0092437853,-2.0059159135,-2.0273328094\H,-1.3582337421,-2.4736682618,-3.0778823813\H,-1.1131972069,-3.3072867157,-1.5230431603\H,-0.08392482,2.0444824121,-2.0335210174\H,-1.2351286457,3.3058076726,-1.5331489537\H,-1.4491796753,2.4589776861,-3.0854209691\H,-4.1403815397,1.0399612657,-0.8992390544\H,-3.760731418,1.5624394017,-2.5531189229\H,-3.635631548,2.7083575514,-1.1995015977\H,-3.2167196164,-0.0348155745,0.8290308889\C,-1.7595378354,-0.0057785101,2.3149346861\O,-2.5437028072,-0.0192445381,3.2319827645\O,-0.4236764401,0.020083893,2.5108942575\H,-0.2715843801,0.0243507691,3.4685297797\Version=ES64L-G09RevE.01\State=2-A\HF=-672.0400847\S2=0.754859\S2-1=0.\S2A=0.750014\RMSD=6.732e-09\RMSF=1.612e-05\Dipole=0.3358191,0.0073149,0.5696553\Quadrupole=2.3486268,6.3936681,-8.7422949,-0.0651166,6.8802451,0.1071123\PG=C01 [X(C10H18N1O3)]\@

Nitroxide m.2

1\1\GINC-R53\FOpt\UM062X\Gen\C10H18N1O3(2)\ROOT\14-Dec-2016\0\#M062X/gen 6D SCF=Tight INT (grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610612736\NitroxideM.1ii.freq\0,2\C,1.2691133857,0.0753384466,0.2868221521\C,0.5530420014,1.2878725707,-0.2919017839\C,0.6100675497,-1.2000779622,-0.253116339\C,-0.8756206324,-1.2998959862,0.1126017993\C,-0.9350221573,1.3320493453,0.0711020064\N,-1.5572739234,-0.0032996653,-0.1646857527\H,0.6634756891,1.2639630197,-1.3827638587\H,1.0229367269,2.2162661514,0.0492086642\H,1.1198462259,-2.0909921696,0.1272719434\H,0.7096025514,-1.2026556197,-1.3468590643\C,-1.0710953879,-1.6754751192,1.5897051558\C,-1.5395325551,-2.3593469425,-0.7693742914\C,-1.6480954256,2.3303769181,-0.8429836445\C,-1.1526774535,1.7435727193,1.5358866671\O,-2.8310168224,-0.0335457709,-0.1304669663\H,-0.4980527194,-1.036146407,2.2658638731\H,-0.7506267175,-2.7094133736,1.7502891068\H,-2.1306433933,-1.5917292171,1.8454860716\H,-1.5067834718,-2.0557824958,-1.8195483011\H,-2.5825306354,-2.4998221848,-0.4828981344\H,-1.0044651262,-3.3073941762,-0.6583024432\H,-1.5991971189,1.9961377582,-1.8831060489\H,-1.1569013211,3.3047924885,-0.7627744639\H,-2.6968223089,2.4316867096,-0.5607118976\H,-0.55339654,1.1519532856,2.2326365884\H,-2.2081346201,1.6213933014,1.7932857038\H,-0.8788191738,2.7952882049,1.6642029725\H,1.2222540583,0.0701214509,1.3836065471\C,2.7371412882,0.0914393975,-0.0725181619\O,3.2759990235,0.8774966519,-0.8123105891\O,3.4111458281,-0.9101792616,0.5308362555\H,4.3365131759,-0.8489920682,0.2476362335\Version=ES64L-G09RevE.01\State=2-A\HF=-672.0413103\S2=0.754856\S2-1=0.\S2A=0.750014\RMSD=1.338e-09\RMSF=9.054e-06\Dipole=0.8318481,-0.4211629,0.5534267\Quadrupole=-4.9352156,3.867389,1.0678267,-4.1682758,1.4554874,1.9454649\PG=C01 [X(C10H18N1O3)]\@

Nitroxide m.3

1\1\GINC-R243\FOpt\UM062X\6-31+G(d,p)\C10H18N1O3(2)\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\RadM2.freq\0,2\C,0.1827076103,-1.4366451248,0.5916480628\C,0.417718924,0.0413274964,0.2102107941\C,0.0958397973,1.0088408009,1.3683313032\C,-1.1454164367,0.5971662053,2.1654264564\N,-0.9460388188,-0.7804041103,2.6787361421\C,0.0228368202,-1.7402886272,2.0913780589\C,-2.4147279102,0.6181637387,1.3028012671\C,-1.3103482477,1.5385575336,3.3595765011\C,-0.5581788727,-3.1483631806,2.2399876864\C,1.3469412109,-1.6612929598,2.8664353068\O,-1.6357000307,-1.1481394339,3.6839227273\H,0.9948239463,-2.0635798543,0.211227936\H,-0.7324612319,-1.7731861938,0.0926550243\H,-0.0595154194,2.0147675719,0.9653334317\H,0.9457000139,1.0708879428,2.0569743852\H,-2.3268239766,-0.0407230399,0.433832713\H,-2.6163013101,1.6343162627,0.9488946954\H,-3.2625184749,0.2790166611,1.9037763586\H,-0.4347750118,1.4835226955,4.0133481912\H,-2.1903056944,1.2656293674,3.9428912669\H,-1.4198537721,2.5659655221,2.9996336587\H,-1.5557346482,-3.2022645429,1.7951076939\H,-0.6396984109,-3.4244380914,3.2917070639\H,0.0978213524,-3.8610332316,1.7308354793\H,1.8466108292,-0.6987016592,2.7477958557\H,2.0326962416,-2.4347845374,2.5064543932\H,1.1468338425,-1.830712004,3.9281796116\C,1.8126181391,0.366015077,-0.2727835243\H,-0.2280960391,0.300670581,-0.6330550057\O,2.0725438445,1.2139397971,-1.0916061635\O,2.7740097408,-0.3506260989,0.347613658\H,3.6273819932,-0.0408045635,0.0063489707\Version=ES64L-G09RevD.01\State=2-A\HF=-672.0341317\S2=0.755232\S2-1=0.\S2A=0.750018\RMSD=8.287e-09\RMSF=6.503e-06\Dipole=0.5408241,-0.0877012,-0.4240907\Quadrupole=4.7235732,1.9161892,-6.6397624,-4.3926015,5.616092,6.312108\PG=C01 [X(C10H18N1O3)]\@

Nitroxide m.4

1\1\GINC-R245\FOpt\UM062X\6-31+G(d,p)\C10H18N1O3(2)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=normanmaxdisk=402653184\NitroxideM.2i.freq\0,2\C,-2.071495 0349,-0.1905044181,0.7977177291\C,-1.580579133,1.0919840055,0.1198421915\C,-1.5370385691,-1.418290 8007,0.0592870488\C,-1.7287877973,-1.4391159588,-1.4683730427\C,-1.8973134907,1.1811183007,-1.37695 24324\N,-1.4833457452,-0.0842933461,-2.0441605724\H,-0.4904261649,1.123707302,0.2366154125\H,-1.98 89269312,1.9753649273,0.6190940759\H,-1.981472249,-2.3299181822,0.4704858967\H,-0.4599031264,-1.45 93552831,0.2606964094\C,-3.120827835,-1.9323162592,-1.8950151495\C,-0.6760041868,-2.3754997714,-2.0 706750953\C,-1.0675096797,2.3123641434,-1.9876416751\C,-3.3855137389,1.4472524563,-1.6520374938\O, -1.3818230459,-0.0361396947,-3.3140389583\H,-3.9336930836,-1.3826901851,-1.4225124479\H,-3.23258760 72,-2.9833114029,-1.6115527358\H,-3.2071567473,-1.8458272328,-2.9814441234\H,0.330517862,-1.9853453 24,-1.8932647764\H,-0.8229245972,-2.4779502033,-3.1465086178\H,-0.7611237998,-3.36026979,-1.6009086 313\H,0.0004084063,2.093074164,-1.8997426535\H,-1.2829214643,3.2433967501,-1.4544950779\H,-1.30575 71707,2.4399084688,-3.0440325458\H,-4.0448368517,0.7084993789,-1.1919487794\H,-3.5562800582,1.4290 068833,-2.7319351519\H,-3.6607603958,2.4322384112,-1.2626756787\C,-3.5602499152,-0.2398954537,1.075 7472448\H,-1.6424643475,-0.1988190062,1.8104885185\O,-4.2664318577,-1.2149509741,0.9843266878\O,-4.0 281770575,0.9387375358,1.5384356136\H,-4.9643745868,0.8100805593,1.7560288106\Version=ES64L-G09 RevD.01\State=2-A\HF=-672.0381221\S2=0.754889\S2-1=0.\S2A=0.750014\RMSD=5.145e-09\RMSF=1.955e -05\Dipole=-0.0237534,0.4701528,1.2301581\Quadrupole=2.0234508,1.7662855,-3.7897363,-3.8694692,2.540 6662,2.0025022\PG=C01 [X(C10H18N1O3)]\@

Nitroxide n

1\1\GINC-R260\FOpt\UM062X\6-31+G(d,p)\C9H15N2O2(2)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) IN T(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=402653184\NitroxideN.2.freq\0,2\C,-0.56745890 57,-1.0281122614,-0.5851140329\C,0.1981257767,0.1349518415,-1.1812207395\N,0.7266598365,0.74663466 97,0.0624595765\C,0.1902444238,0.1687528346,1.3128627174\C,-0.5820619138,-0.9946692052,0.751448211 3\O,1.3843882667,1.8273552119,0.0565764172\C,-0.7040865852,1.1406504002,-1.9047338978\C,1.36059918 51,-0.2982783181,-2.0746605034\C,-0.7080229801,1.1891279695,2.0207554225\C,1.3470790855,-0.2615054 985,2.2180511889\H,-1.1050945934,-1.6894050439,1.4032776173\H,-1.5466164884,1.4294692058,-1.269506 9678\H,-1.0895158605,0.6961404321,-2.8236598208\H,-0.1163685377,2.0332403815,-2.1361110401\H,1.995 0209296,-1.0248025735,-1.5581552103\H,1.9642750516,0.5788483638,-2.322730674\H,0.9732145249,-0.744 333004,-2.9937546383\H,-1.5385531729,1.487008141,1.3754344714\H,-0.1168624162,2.0755738066,2.26543 42275\H,-1.1121714003,0.763264616,2.9439431828\H,1.9762400007,-1.0000576552,1.7139213691\H,0.9643 619536,-0.6924798893,3.1481072592\H,1.9570871834,0.6135802159,2.4581302417\C,-1.2363664374,-2.0296 038339,-1.4669023933\N,-1.5814110317,-3.2132747203,-0.8790369131\O,-1.4797515202,-1.7893808037,-2.6 388915117\H,-1.1562394118,-3.5077471305,-0.0151507871\H,-1.9677449629,-3.9222081526,-1.4848227728\ Version=ES64L-G09RevD.01\State=2-A\HF=-611.6557982\S2=0.7552\S2-1=0.\S2A=0.750017\RMSD=6.255e -09\RMSF=9.247e-06\Dipole=-0.4008275,-1.5192293,1.2925416\Quadrupole=-3.2172498,3.9607936,-0.74354 37,-2.1298308,-3.6326822,-3.3417341\PG=C01 [X(C9H15N2O2)]\@

Nitroxide o.1

1\1\GINC-R537\FOpt\UM062X\6-31+G(d,p)\C9H14N1O3(2)\ROOT\28-Apr-2016\0\#M062X/6-31+G(d,p) IN T(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=402653184\NitroxideO.2.freq\0,2\C,-0.53384602 76,-1.0347489105,-0.6032007895\C,0.1874935423,0.1527875185,-1.2011268251\N,0.6096325636,0.82906683 97,0.0477405375\C,0.2055767991,0.1537386689,1.2987024531\C,-0.5236481321,-1.033366295,0.7337177402 \O,1.2690176791,1.9084854769,0.0471009742\C,-0.7311167867,1.0780045073,-2.0032693142\C,1.421516093 3,-0.2372574854,-2.0186431452\C,-0.7054643231,1.0746401051,2.1167081063\C,1.4488300384,-0.24165357 27,2.1019209153\H,-0.9823668393,-1.7913518389,1.3604923657\H,-1.6185640175,1.3404914231,-1.4199370 703\H,-1.0414409468,0.5840885225,-2.9267783074\H,-0.1859714657,1.9946914738,-2.2437194766\H,2.0660 410937,-0.9108309058,-1.4462577487\H,1.9859480928,0.6676504617,-2.2592098429\H,1.1140262291,-0.732 8763619,-2.9421878222\H,-1.5983096569,1.3418780689,1.5452049851\H,-0.1582031364,1.9887257334,2.362 0497892\H,-1.0110041333,0.581733966,3.0441749645\H,2.088284772,-0.9106301726,1.5198787396\H,1.158 9209232,-0.7441433152,3.0292627117\H,2.0149218837,0.6609166137,2.3471676662\C,-1.1667311929,-2.060 782268,-1.4557574894\O,-1.7610700756,-3.0419334291,-0.7481555678\O,-1.1640489712,-2.0421943798,-2.6 657214988\H,-2.144434005,-3.6619204446,-1.3869270505\Version=ES64L-G09RevD.01\State=2-A\HF=-631.5 233926\S2=0.75524\S2-1=0.\S2A=0.750018\RMSD=6.982e-09\RMSF=3.172e-05\Dipole=-0.6177021,-1.0198 563,0.7843539\Quadrupole=0.360181,-1.0757772,0.7155962,-1.4210675,-0.79526,-1.2943109\PG=C01 [X(C9 H14N1O3)]\@

Nitroxide o.2

1\1\GINC-R1356\FOpt\UM062X\6-31+G(d,p)\C9H14N1O3(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noramanmaxdisk=402653184\NitroxideO.1.freq\0,2\C,-0.5567791 926,-1.0192204081,-0.6187665938\C,0.1689440807,0.1699153949,-1.2151255181\N,0.6065677562,0.8329364 722,0.0374000568\C,0.2076640445,0.1512280341,1.2867424044\C,-0.5331087038,-1.0242958826,0.71773425 96\O,1.2726267123,1.9079362268,0.0373015901\C,-0.7431125209,1.1200652187,-1.9964709267\C,1.4010480 705,-0.2107916416,-2.0409934501\C,-0.6902199397,1.0728830944,2.118403965\C,1.4547715462,-0.2583821 04,2.0767761988\H,-0.9956549057,-1.7897710616,1.3332746623\H,-1.631158483,1.3716802501,-1.40948575 25\H,-1.0539756385,0.6579576938,-2.9358732216\H,-0.1913817102,2.0397441962,-2.2090739211\H,2.03771 48231,-0.9055964133,-1.4856657253\H,1.9739986592,0.6957340018,-2.2539719305\H,1.0967444548,-0.6768 775845,-2.9805822695\H,-1.5855083887,1.3506022723,1.5558401804\H,-0.1343203332,1.9809821365,2.3664 972629\H,-0.9925407797,0.5748432502,3.0440320665\H,2.0847489942,-0.927465306,1.4846590128\H,1.168 5932086,-0.7662832348,3.0021775463\H,2.0288242292,0.6384869779,2.3243907162\C,-1.2355822158,-2.088 4383311,-1.386266952\O,-1.1504545363,-1.9066586058,-2.7207859413\O,-1.8103376476,-3.0316949858,-0.8 968594929\H,-1.6176415837,-2.6461496607,-3.1397482268\Version=ES64L-G09RevD.01\State=2-A\HF=-63 1.5222243\S2=0.755236\S2-1=0.\S2A=0.750018\RMSD=5.019e-09\RMSF=1.111e-05\Dipole=-0.2956331,-0.4 717774,-0.0972997\Quadrupole=-1.7895781,-7.4129073,9.2024854,-5.5659366,1.5177818,2.2013135\PG=C01 [X(C9H14N1O3)]\@

Nitroxide p

1\1\GINC-R1063\FOpt\UM062X\6-31+G(d,p)\C8H14N1O3(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\NitroxideP.freq\0,2\O,-1.84598374 26,-0.1940138146,0.6782087125\C,-2.3264926227,0.9101074797,0.0747552615\C,-1.1183782547,-1.1592515 202,-0.0805205043\C,-1.7312171705,-1.4036659623,-1.4526895093\C,-2.0684080214,1.1429951961,-1.42269 4484\N,-1.6891943498,-0.098360332,-2.1340415639\H,-1.1412545482,-2.072610271,0.5174456291\H,-0.0783 286217,-0.8279292288,-0.1879285444\C,-3.181628903,-1.8931445755,-1.3536650645\C,-0.8665651058,-2.39 35307432,-2.2242830714\C,-0.9005931875,2.1375738166,-1.5360363438\C,-3.3357429656,1.7258779408,-2.0 5670927\O,-1.6496232791,-0.0519772513,-3.4038630138\H,-3.8003777634,-1.2176404313,-0.7556824568\H,- 3.2139446625,-2.8825744226,-0.8875520291\H,-3.6068963714,-1.9619572745,-2.3583969908\H,0.151932945 5,-2.0130702432,-2.3399992021\H,-1.2813187672,-2.5575395344,-3.2193834768\H,-0.8362444418,-3.346098 6727,-1.687524079\H,-0.0016512778,1.7508225529,-1.0464364331\H,-1.1792862071,3.0854021222,-1.07081 41599\H,-0.684255768,2.2947456839,-2.5952008086\H,-4.1644032256,1.0149711705,-1.9915230616\H,-3.13 68232166,1.9380924513,-3.1079702198\H,-3.615997387,2.6393579125,-1.5316356919\O,-2.9204330844,1.72 58979511,0.7278603758\Version=ES64L-G09RevD.01\State=2-A\HF=-593.4240342\S2=0.755134\S2-1=0.\S 2A=0.750016\RMSD=4.798e-09\RMSF=1.349e-05\Dipole=0.5570485,-1.0070331,-0.2084769\Quadrupole=3.5 258555,5.8612741,-9.3871296,1.27438,4.0195677,-4.5048701\PG=C01 [X(C8H14N1O3)]\@

Nitroxide r

1\1\GINC-R819\FOpt\UM062X\6-31+G(d,p)\C8H16N1O2(2)\ROOT\28-Apr-2016\0\#M062X\6-31+G(d,p) I NT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\NitroxideR.freq\0,2\C,-0.726042442, -1.2498042694,-1.1551232657\C,0.064020711,0.0534866329,-1.30106381\N,0.0141619112,0.7716858484,0.\ C,0.064020711,0.0534866329,1.30106381\C,-0.726042442,-1.2498042694,1.1551232657\O,-0.3545042927,-1. 9699132171,0.\O,0.425927703,1.9770980791,0.\C,-0.6005184904,0.9392951061,-2.3522305399\C,1.52174760 77,-0.2316271583,-1.6852887974\C,-0.6005184904,0.9392951061,2.3522305399\C,1.5217476077,-0.2316271 583,1.6852887974\H,-1.8053798497,-1.0284666033,1.1220364446\H,-0.526740722,-1.8937469947,2.0163215 57\H,-1.6052890595,1.2303986455,-2.0331045282\H,-0.6725722338,0.3918257456,-3.2974493062\H,-0.0137 986416,1.8452784752,-2.5107366973\H,1.946621344,-1.0300994771,-1.0733478135\H,2.118025109,0.676556 6789,-1.5629822927\H,1.5691590068,-0.5430971361,-2.7335909652\H,-1.6052890595,1.2303986455,2.03310 45282\H,-0.0137986416,1.8452784752,2.5107366973\H,-0.6725722338,0.3918257456,3.2974493062\H,1.946 621344,-1.0300994771,1.0733478135\H,1.5691590068,-0.5430971361,2.7335909652\H,2.118025109,0.67655 66789,1.5629822927\H,-0.526740722,-1.8937469947,-2.016321557\H,-1.8053798497,-1.0284666033,-1.12203 64446\Version=ES64L-G09RevD.01\State=2-A\HF=-519.4119985\S2=0.75487\S2-1=0.\S2A=0.750014\RMS D=5.051e-09\RMSF=3.336e-05\Dipole=-0.3126997,-0.6346928,0.\Quadrupole=1.5857267,-7.4036194,5.81789 27,-0.5280929,0,0.\PG=CS [SG(N1O2),X(C8H16)]\@

Model a.1

1\1\GINC-R37\SP\RM062X\6-31+G(d,p)\C10H18O1\ROOT\15-Jun-2017\0\#M062X\6-31+G(d,p) INT(grid= ultrafine) Nosymm maxdisk=12GB\CycloA.ext.retry.1.freq\0,1\C\C,1,2.862859\C,2,1.544538,1,61.151\C,1,1. 514308,2,61.42,3,29.012,0\C,1,1.514331,4,114.347,3,-59.503,0\C,2,1.544372,3,118.233,4,-49.544,0\C,6,1.5339 06,2,108.088,3,167.493,0\O,1,1.213755,4,122.796,3,117.551,0\C,3,1.533544,2,108.123,6,-168.049,0\C,3,1.537 239,2,113.103,6,72.347,0\C,6,1.537444,2,113.021,3,-73.076,0\H,2,1.099084,3,108.981,4,-174.651,0\H,2,1.1004

5,3,106.852,4,71.053,0\H,4,1.098967,1,108.373,5,59.615,0\H,4,1.094156,1,109.311,5,177.992,0\H,5,1.094149,1,109.281,4,-178.434,0\H,5,1.099068,1,108.208,4,-60.246,0\H,10,1.095305,3,109.647,2,166.93,0\H,10,1.091825,3,112.861,2,-74.071,0\H,10,1.095408,3,110.901,2,47.727,0\H,9,1.095228,3,110.725,2,177.447,0\H,9,1.096,3,110.524,2,-63.131,0\H,9,1.09521,3,111.292,2,56.985,0\H,11,1.09524,6,109.696,2,-166.007,0\H,11,1.095466,6,110.798,2,-46.994,0\H,11,1.091693,6,112.901,2,74.678,0\H,7,1.09527,6,110.7,2,-177.028,0\H,7,1.095186,6,111.268,2,-56.666,0\H,7,1.096,6,110.574,2,63.475,0\Version=ES64L-G09RevD.01\HF=-466.9520441\RMSD=4.516e-09\Dipole=-0.0998569,-0.4632349,1.1774599\Quadrupole=1.2510036,-0.1113309,-1.1396726,-0.300244,0.3366395,1.5915375\PG=C01 [X(C10H18O1)]\@

Model a.2

1\1\GINC-R40\FOpt\RM062X\6-31+G(d,p)\C10H18O1\ROOT\10-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\CatA.parameter.freq\0,1\C,1.1388236474,1.0564523784,-0.6101049869\C,0.0004517991,1.8531950589,0.002816019\C,-1.1397111246,1.0546142413,0.6100483616\C,-1.3294415685,-0.3297675095,-0.0290246319\C,-0.0029805063,-1.139661138,-0.0080727251\C,1.3253164749,-0.3329450012,0.0189279024\O,0.0018262543,3.065977537,0.007211298\C,-1.8284362896,-0.1519955073,-1.4729535429\C,-2.4012925948,-1.0984222825,0.7517487876\C,2.3955403335,-1.0983347375,-0.7672791227\C,1.8246051862,-0.1667478491,1.4641348313\H,-2.0509103174,1.6576570911,0.5343317072\H,-0.9249483733,0.9483746879,1.6822891722\H,-1.1053048729,0.3713082483,-2.1056629173\H,-2.760574939,0.4230521302,-1.4892500161\H,-2.0239737183,-1.1274166048,-1.9309781644\H,-2.1153520871,-1.2101409756,1.8031999967\H,-2.5407495548,-2.1003822121,0.3304607099\H,-3.364695489,-0.578192008,0.71263273\H,2.1094930666,-1.201760059,-1.8195484355\H,2.5326422144,-2.1036406793,-0.3532546755\H,3.3601287047,-0.5806120376,-0.7242650241\H,1.1026058956,0.3535324843,2.1006168367\H,2.7580061277,0.4061174263,1.4846259044\H,2.0179814301,-1.1458977271,1.9150606861\H,-0.0033758594,-1.8055650205,0.8647340304\H,-0.0041322879,-1.7989856954,-0.885856643\Version=ES64L-G09RevD.01\State=1-A\HF=-466.9476707\RMSD=5.211e-09\RMSF=4.856e-06\Dipole=-0.0014814,-1.3262577,-0.004803\Quadrupole=4.1878835,-7.4912313,3.3033478,-0.01277,-0.0809417,-0.0389191\PG=C01 [X(C10H18O1)]\@

Model b.1

1\1\GINC-R96\SP\RM062X\6-31+G(d,p)\C10H20O1\ROOT\26-Sep-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloC.ext1.retry.freq\0,1\C\C,1,2.928143\C,2,1.544035,1,61.068\C,1,1.527069,2,59.059,3,-28.167,0\C,1,1.526901,4,110.554,3,57.017,0\C,2,1.544002,3,118.06,4,48.053,0\C,6,1.537779,2,112.997,3,75.275,0\O,1,1.421104,5,111.263,6,178.841,0\C,6,1.534863,2,107.934,3,-166.289,0\C,3,1.537794,2,112.998,6,-75.287,0\C,3,1.534844,2,107.929,6,166.282,0\H,1,1.095754,5,109.795,6,64.261,0\H,8,0.965225,1,108.382,5,61.848,0\H,4,1.102593,1,107.656,5,-63.358,0\H,4,1.097207,1,109.384,5,-179.247,0\H,5,1.102587,1,107.668,4,63.357,0\H,5,1.097198,1,109.406,4,179.265,0\H,2,1.099625,6,109.309,5,-173.781,0\H,2,1.100515,6,106.68,5,71.889,0\H,9,1.095614,6,110.739,2,177.871,0\H,9,1.09611,6,110.773,2,-62.41,0\H,9,1.095316,6,111.164,2,57.714,0\H,7,1.095599,6,109.759,2,169.189,0\H,7,1.090953,6,113.414,2,-70.94,0\H,7,1.095793,6,110.612,2,50.296,0\H,10,1.0956,3,109.759,2,-169.199,0\H,10,1.095788,3,110.612,2,-50.305,0\H,10,1.090953,3,113.413,2,70.932,0\H,11,1.095611,3,110.737,2,-177.868,0\H,11,1.095319,3,111.164,2,-57.712,0\H,11,1.096104,3,110.771,2,62.412,0\Version=ES64L-G09RevD.01\HF=-468.1538404\RMSD=2.763e-09\Dipole=-0.0487338,0.2367704,0.6916857\Quadrupole=0.0336595,2.2464241,-2.2800837,-0.4731391,0.1804398,-0.8794821\PG=C01 [X(C10H20O1)]\@

Model b.2

1\1\GINC-R51\SP\RM062X\6-31+G(d,p)\C10H20O1\ROOT\15-Jun-2017\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloC.ext.retry.freq\0,1\C\C,1,2.92411\C,2,1.544275,1,60.89\C,1,1.521869,2,59.23,3,28.291,0\C,1,1.527069,4,110.521,3,-57.454,0\C,2,1.544145,3,118.037,4,-47.981,0\C,6,1.53774,2,112.985,3,-75.578,0\O,1,1.422797,4,106.562,3,-178.431,0\C,3,1.53489,2,107.848,6,-165.989,0\C,3,1.537836,2,112.942,6,75.744,0\C,6,1.534775,2,107.95,3,165.996,0\H,1,1.100896,4,109.575,3,63.743,0\H,8,0.963945,1,108.934,4,178.342,0\H,5,1.099425,1,107.132,4,-63.393,0\H,5,1.100474,1,110.083,4,-179.399,0\H,4,1.099365,1,107.092,5,63.496,0\H,4,1.097078,1,109.325,5,179.056,0\H,2,1.099685,3,109.355,4,-173.671,0\H,2,1.100174,3,106.679,4,71.915,0\H,9,1.095595,3,110.708,2,178.001,0\H,9,1.096179,3,110.786,2,-62.267,0\H,9,1.095123,3,111.134,2,57.931,0\H,10,1.095655,3,109.734,2,169.517,0\H,10,1.091029,3,113.434,2,-70.633,0\H,10,1.095917,3,110.64,2,50.638,0\H,7,1.095942,6,109.783,2,-169.733,0\H,7,1.095784,6,110.594,2,-50.925,0\H,7,1.090944,6,113.424,2,70.242,0\H,11,1.095804,6,110.778,2,-178.045,0\H,11,1.095091,6,111.144,2,-57.87,0\H,11,1.096131,6,110.745,2,62.268,0\Version=ES64L-G09RevD.01\HF=-468.1539929\RMSD=4.920e-09\Dipole=-0.3903933,0.4738556,0.2766959\Quadrupole=0.8331279,-1.3303716,0.4972437,0.0866325,1.8976163,-1.3361585\PG=C01 [X(C10H20O1)]\@

Model b.3

Model c.1

I1\GINC-R37\SP\RM062X\6-31+G(d,p)\C10H19N1O1\ROOT\15-Jun-2017\0\#M062X\6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloB.EXT.retry.freq\0,1\C\C,1,2.902315\C,2,1.530844,1,59.376\C,1,1.505475,2,60.508,3,-29.618,0\C,1,1.506361,4,116.434,3,52.183,0\C,2,1.530721,3,111.076,4,56.889,0\C,6,1.45,2,110.576,3,-178.965,0\N,1,1.275876,4,117.073,3,-126.25,0\O,8,1.397701,1,112.608,4,179.716,0\C,3,1.45,2,110.62,6,178.999,0\C,3,1.45,2,109.309,6,-63.345,0\C,6,1.450001,2,109.245,3,63.581,0\H,9,0.963243,8,102.888,1,-179.445,0\H,4,1.092789,1,109.349,5,175.655,0\H,4,1.099444,1,108.395,5,-66.96,0\H,5,1.089912,1,110.66,4,-175.227,0\H,5,1.099215,1,107.76,4,67.061,0\H,2,1.099304,3,109.23,4,-63.692,0\H,2,1.095159,3,110.231,4,179.213,0\H,7,1.089,6,109.47122063,2,180.,0\H,7,1.089,6,109.47122063,2,-60.,0\H,7,1.089,6,109.47122063,2,60.,0\H,12,1.089001,6,109.47122063,2,180.,0\H,12,1.089,6,109.47122063,2,-60.,0\H,12,1.089,6,109.47122063,2,60.,0\H,10,1.089,3,109.47122063,2,180.,0\H,10,1.089,3,109.47122063,2,-60.,0\H,10,1.089,3,109.47122063,2,60.,0\H,11,1.089,3,109.47122063,2,180.,0\H,11,1.089,3,109.47122063,2,-60.,0\H,11,1.089,3,109.47122063,2,60.,0\Version=ES64L-G09RevD.01\HF=-522.1317443\RMSD=4.921e-09\Dipole=-0.0194803,0.04447,0.3019812\Quadrupole=-2.2317209,-0.5180819,2.7498027,-0.1689202,0.2440525,1.3145924\PG=C01 [X(C10H19N1O1)]\@\

Model c.2

I1\GINC-R41\FOpt\RM062X\6-31+G(d,p)\C10H19N1O1\ROOT\10-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\CatC2.parameter.freq\0,1\C,0.3646132552,-1.2806389973,-0.8362077234\C,1.4366848544,-0.3867456577,-0.2727748409\C,1.0314504061,0.9324391739,0.3345788103\C,-0.3884902941,1.3757895087,-0.0557701499\C,-1.4240367682,0.2322271645,0.1391296124\C,-0.8992406609,-1.226410118,0.0396050644\N,2.6325483782,-0.8324312225,-0.2751528236\C,-0.3811153437,1.8533283085,-1.5184044504\C,-0.790296777,2.5668921103,0.822082023\C,-1.9807756286,-2.1153083646,-0.5812130112\C,-0.565973453,-1.7682189334,1.438502355\H,0.7508494492,-2.3032668452,-0.8984295743\H,0.111525146,-0.9698375365,-1.8577428174\H,1.7598445932,1.6997565249,0.0479972884\H,1.1209298101,0.8405863989,1.4266319061\H,-0.0890163903,1.064903533,-2.2172624843\H,0.3224236855,2.6836205695,-1.6441120821\H,-1.3762927977,2.2061965372,-1.8098081173\H,-0.7792082933,2.2931683116,1.8825360446\H,-1.8009620495,2.9079775067,0.570751633\H,-0.1037580941,3.4088998888,0.6793044344\H,-2.2035016257,-1.8026802473,-1.6073105324\H,-2.9084623331,-2.0564217749,-0.0008318043\H,-1.6620728311,-3.1633894149,-0.6041087421\H,0.1640512254,-1.1420252147,1.9606123182\H,-0.1488627088,-2.7790959844,1.3719871854\H,-1.4706226433,-1.8116781366,2.0545578417\O,3.5169377571,0.0757576827,0.313735286\H,4.3682087152,-0.3690402087,0.2385888141\H,-2.2205609519,0.3784232847,-0.6024260713\H,-1.9049576313,0.3464721528,1.1195946078\Version=ES64L-G09RevD.01\State=1-A\HF=-522.2320122\RMSD=7.232e-09\RMSF=6.346e-06\Dipole=-0.3602772,0.1049043,0.0296509\Quadrupole=1.8933015,-0.8988364,-0.9944651,0.011232,0.6032669,-0.4151701\PG=C01 [X(C10H19N1O1)]\@\

Model d.1

I1\GINC-R87\SP\RM062X\6-31+G(d,p)\C11H20O1\ROOT\14-Jul-2017\0\#M062X\6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloD.1.ext.retry.freq\0,1\C\C,1,2.882631\C,2,1.545199,1,61.361\C,1,1.511576,2,60.583,3,-27.803,0\C,1,1.511557,4,113.866,3,56.346,0\C,2,1.545204,3,118.302,4,48.832,0\C,6,1.534295,2,107.947,3,-167.127,0\O,1,1.423529,5,115.207,6,167.336,0\C,8,1.42268,1,62.34,5,-112.139,0\C,3,1.53423,2,107.95,6,167.127,0\C,3,1.537246,2,112.977,6,-74.086,0\C,6,1.537145,2,112.99,3,74.09,0\H,9,1.089218,1,119.536,5,-0.455,0\H,9,1.089211,1,119.54,5,-154.299,0\H,4,1.099875,1,107.485,5,-63.838,0\H,4,1.09688,1,109.854,5,179.94,0\H,5,1.099878,1,107.489,4,63.821,0\H,5,1.096878,1,109.853,4,-179.954,0\H,2,1.099563,3,109.147,4,174.379,0\H,2,1.1004,3,106.719,4,-71.35,0\H,12,1.095934,6,109.731,2,168.709,0\H,12,1.090984,6,112.974,2,-71.609,0\H,12,1.095754,6,110.786,2,49.729,0\H,7,1.095668,6,110.733,2,177.577,0\H,7,1.095996,6,110.75,2,-62.74,0\H,7,1.095194,6,111.191,2,57.433,0\H,10,1.095674,3,110.735,2,-177.586,0\H,10,1.095201,3,111.192,2,-57.443,0\H,10,1.096003,3,110.751,2,62.731,0\H,11,1.095919,3,109.736,2,-168.644,0\H,11,1.095738,3,110.791,2,-49.649,0\H,11,1.090958,3,112.947,2,71.679,0\Version=ES64L-G09RevD.01\HF=-506.2152843\RMSD=8.170e-09\Dipole=0.1018649,-0.4799433,0.7106193\Quadrupole=1.0149309,0.5825191,-1.5974501,0.0963586,-0.4311543,2.0330938\PG=C01 [X(C11H20O1)]\@\

Model d.2

I1\GINC-R107\SP\RM062X\6-31+G(d,p)\C11H20O1\ROOT\14-Jul-2017\0\#M062X\6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloD.2.ext.retry.freq\0,1\C\C,1,2.884339\C,2,1.544176,1,61.546\C,1,1.513031,2,60.467,3,27.51,0\C,1,1.513023,4,114.46,3,-54.515,0\C,2,1.544169,3,118.171,4,-49.846,0\C,6,1.534175,2,107.931,3,168.044,0\C,1,1.469812,5,120.122,6,-151.141,0\O,8,1.423279,1,59.298,5,103.555,0\C,6,1.537576,2,113.016,3,-72.852,0\C,3,1.537602,2,113.017,6,72.858,0\C,3,1.534177,2,107.926,6,-168.037,0\H,4,1.099728,1,107.775,5,65.916,0\H,4,1.097013,1,109.5,5,-177.438,0\H,5,1.09973,1,107.777,4,-65.91,0\H,5,1.097009,1,109.5,4,177.442,0\H,8,1.088671,1,119.461,5,0.322,0\H,8,1.088671,1,119.46,5,-153.211,0\H,2,1.099564,6,109.067,5,1

75.102,0\H,2,1.100999,6,106.871,5,-70.575,0\H,10,1.095923,6,109.58,2,-167.039,0\H,10,1.095974,6,110.648,2,-48.233,0\H,10,1.089869,6,112.793,2,73.802,0\H,7,1.095809,6,110.715,2,-176.959,0\H,7,1.095601,6,111.332,2,-56.66,0\H,7,1.096012,6,110.658,2,63.522,0\H,12,1.095804,3,110.716,2,176.984,0\H,12,1.096015,3,110.657,2,-63.496,0\H,12,1.095601,3,111.332,2,56.684,0\H,11,1.095922,3,109.58,2,166.956,0\H,11,1.089871,3,112.791,2,-73.887,0\H,11,1.095975,3,110.652,2,48.149,0\Version=ES64L-G09RevD.01\HF=-506.2154815\RMSD=4.461e-09\Dipole=-0.1541543,-0.6887477,0.0341853\Quadrupole=0.7486298,-2.3407207,1.5920909,-0.7281304,0.3097595,1.3822216\PG=C01 [X(C11H20O1)]\@

Model e.1

1\1\GINC-R38\SP\RM062X\6-31+G(d,p)\C11H22O2\ROOT\14-Jul-2017\0\#M062X\6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\Cyclo.E.ii.ext.retry.freq\0,1\C\C,1,2.957368\C,2,1.542037,1,61.501\C,3,1.539809,2,109.021,1,-24.049,0\C,1,1.529205,4,110.895,3,-51.752,0\C,5,1.540581,1,115.725,4,51.35,0\C,6,1.537755,5,111.341,1,76.479,0\C,3,1.537334,4,111.772,1,-75.857,0\C,3,1.536303,4,108.082,1,166.595,0\C,1,1.531225,4,109.836,3,-172.179,0\C,10,1.422702,1,106.963,4,-64.89,0\C,1,1.425073,4,111.629,3,69.078,0\C,6,1.536111,5,108.167,1,-166.045,0\H,4,1.100247,3,108.064,2,-70.322,0\H,4,1.097677,3,110.168,2,173.719,0\H,5,1.100276,1,107.175,4,-69.358,0\H,5,1.098033,1,108.598,4,175.105,0\H,8,1.087944,3,112.854,4,54.439,0\H,8,1.096599,3,109.575,4,-65.356,0\H,8,1.096334,3,110.143,4,176.328,0\H,9,1.095628,3,111.366,4,-60.239,0\H,9,1.09615,3,110.635,4,179.587,0\H,9,1.095877,3,110.714,4,60.04,0\H,13,1.095717,6,111.4,5,60.88,0\H,13,1.095923,6,110.756,5,-59.524,0\H,13,1.096044,6,110.569,5,-178.996,0\H,7,1.087893,6,112.861,5,-52.154,0\H,7,1.096241,6,110.162,5,-174.345,0\H,7,1.096245,6,109.553,5,67.245,0\H,10,1.097937,1,110.434,4,55.795,0\H,10,1.098192,1,108.514,4,175.674,0\H,12,0.968117,1,106.516,4,72.095,0\H,11,0.961723,10,109.987,1,-165.699,0\H,2,1.101155,3,106.788,4,70.763,0\H,2,1.099696,3,109.347,4,-174.825,0\Version=ES64L-G09RevD.01\HF=-582.649686\RMSD=5.442e-09\Dipole=-0.2210349,-0.7108428,-0.6467061\Quadrupole=-1.7582449,-2.1243155,3.8825604,1.2347345,0.1614758,1.4742818\PG=C01 [X(C11H22O2)]\@

Model e.2

1\1\GINC-R42\SP\RM062X\6-31+G(d,p)\C11H22O2\ROOT\14-Jul-2017\0\#M062X\6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\Cyclo.E.iii.ext.retry.freq\0,1\C\C,1,2.960325\C,2,1.542004,1,61.587\C,3,1.540809,2,108.923,1,-23.919,0\C,3,1.537255,4,111.571,1,-75.823,0\C,3,1.536094,4,108.19,1,166.546,0\C,2,1.542181,3,117.873,4,-49.409,0\C,7,1.540313,2,109.123,3,49.264,0\C,1,1.535044,4,110.209,3,-171.959,0\C,9,1.421489,1,111.157,4,-68.071,0\C,1,1.424378,4,111.33,3,69.415,0\C,7,1.536019,8,108.226,1,-166.344,0\C,7,1.537658,8,111.336,1,76.082,0\H,4,1.101113,3,107.972,2,-70.876,0\H,4,1.100146,3,108.896,2,173.191,0\H,8,1.10061,1,107.198,4,-69.383,0\H,8,1.097807,1,108.426,4,175.205,0\H,5,1.087852,3,112.816,4,53.373,0\H,5,1.096683,3,109.598,4,-66.366,0\H,5,1.09612,3,110.116,4,175.346,0\H,6,1.095655,3,111.412,4,-60.455,0\H,6,1.09596,3,110.594,179.412,0\H,6,1.096077,3,110.766,4,59.968,0\H,12,1.095714,7,111.414,8,60.781,0\H,12,1.095792,7,110.731,8,-59.599,0\H,12,1.096026,7,110.584,8,-179.065,0\H,13,1.08794,7,112.909,8,-51.903,0\H,13,1.096227,7,110.179,8,-174.136,0\H,13,1.096093,7,109.531,8,67.454,0\H,9,1.097525,1,110.839,4,56.249,0\H,9,1.094153,1,108.755,4,175.775,0\H,11,0.968651,1,106.686,4,79.199,0\H,10,0.96343,9,109.408,1,80.534,0\H,2,1.101152,3,106.837,4,70.808,0\H,2,1.099538,3,109.225,4,-174.81,0\Version=ES64L-G09RevD.01\HF=-582.6494662\RMSD=4.890e-09\Dipole=0.2278024,-0.8391834,0.1934914\Quadrupole=2.5122085,0.0805937,-2.5928023,-0.706808,-0.5730813,0.520353\PG=C01 [X(C11H22O2)]\@

Model e.3

1\1\GINC-R38\FOpt\RM062X\6-31+G(d,p)\C11H22O2\ROOT\10-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\ModelE.3.freq\0,1\C,0.5777841411,1.3870138086,-0.0359557918\C,-0.8612778594,1.0440819296,-0.4645492875\C,-1.3594933698,-0.3532408499,-0.0866473341\C,-0.3566702748,-1.4283038247,-0.5106121924\C,1.1031486167,-1.2032624912,-0.073104188\C,1.5202450739,0.2345447126,-0.4421296859\C,0.6539714305,1.7349856487,1.4604085886\C,1.0181073223,2.6393153161,-0.8101232122\H,-0.9208222486,1.1113471057,-1.5600509091\H,-1.5618746311,1.7883228877,-0.068447609\H,-0.3834936506,-1.4757795094,-1.6091309723\H,-0.7020103382,-2.411970491,-0.1549171095\C,1.9926641296,-2.17475194,-0.8631074215\C,1.3078250152,-1.5166593426,1.417695813\H,0.1835755831,0.9867191846,2.0949133705\H,0.1347523749,2.6831313783,1.6413836751\H,1.6982440497,1.8616223015,1.7690635922\H,1.010045434,2.464197658,-1.8915156012\H,2.0334069814,2.9345134843,-0.5212445876\H,0.3496396204,3.4808042333,-0.5971821105\H,1.9038382796,-2.0082826051,-1.9420806066\H,1.7154455078,-3.2146139708,-0.6550989719\H,3.0450151461,-2.0459708869,-0.5861015375\H,0.6768739338,-0.9160371157,2.070313644\H,2.3526184584,-1.3415264513,1.6980300154\H,1.0868570778,-2.573957456,1.6099344654\C,-2.7203884862,-0.6295617615,-0.7422341238\O,-1.5856738065,-0.3606538088,1.333549463\O,-3.7051976088,0.2727923908,-0.2970496546\H,-2.6534068062,-0.5259643541,-1.8295963485\H,-3.0122803118,-1.6703244424,-0.5172867087\H,-1.6952011231,-1.2761104777,1.6229710216\H,-3.5944416138,0.3531657776,0.6609243426\H,1.6101742196,0.2668021203,-1.5387949058\H,2.5274997331,0.4315018414,-0.0475871214\Version=ES64L-G

09RevD.01\State=1-A\HF=-582.6489986\RMSD=4.465e-09\RMSF=1.025e-05\Dipole=0.6282576,-0.7302977,0.0749307\Quadrupole=-5.3280951,3.1727004,2.1553947,3.0075732,-2.5997978,-0.8126851\PG=C01 [X(C11H22O2)]\@

Model f

1\1\GINC-R37\SP\RM062X\6-31+G(d,p)\C12H20O3\ROOT\15-Jun-2017\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloF.ext.retry.freq\0,1\C\C,1,2.943026\C,2,1.542923,1,61.678\C,1,1.530042,2,58.324,3,-26.983,0\C,1,1.522488,4,111.94,3,51.375,0\C,2,1.543051,3,118.045,4,49.596,0\C,6,1.537816,2,113.037,3,75.232,0\C,1,1.538043,5,112.401,6,-176.812,0\O,8,1.425518,1,103.689,5,-140.993,0\C,9,1.353321,8,109.224,1,20.119,0\O,10,1.351001,9,110.125,8,-7.38,0\C,3,1.536129,2,107.818,6,166.414,0\C,3,1.537501,2,113.26,6,-75.195,0\C,6,1.53569,2,107.879,3,-166.327,0\O,10,1.191767,9,124.859,8,172.572,0\H,8,1.091136,1,113.196,5,101.469,0\H,8,1.095791,1,111.973,5,-23.726,0\H,4,1.098966,1,109.159,5,176.427,0\H,4,1.099775,1,106.336,5,-68.676,0\H,5,1.097601,1,108.879,4,-174.844,0\H,5,1.100662,1,106.288,4,70.211,0\H,2,1.098956,3,109.186,4,174.817,0\H,2,1.10092,3,106.866,4,-70.826,0\H,12,1.09558,3,110.475,2,62.902,0\H,12,1.095526,3,111.434,2,-57.183,0\H,12,1.095599,3,110.797,2,-177.678,0\H,13,1.095707,3,109.976,2,-53.031,0\H,13,1.095905,3,109.646,2,-171.334,0\H,13,1.088058,3,113.501,2,68.826,0\H,7,1.095625,6,110.073,2,51.4,0\H,7,1.088406,6,113.359,2,-70.427,0\H,7,1.095907,6,109.647,2,169.806,0\H,14,1.095538,6,110.505,2,-63.025,0\H,14,1.095693,6,110.797,2,177.549,0\H,14,1.095518,6,111.417,2,57.062,0\Version=ES64L-G09RevD.01\HF=-694.7656096\RMSD=6.431e-09\Dipole=-0.8514447,1.5569109,1.2936066\Quadrupole=3.4140437,-1.8241144,-1.5899293,3.4021998,4.4915297,-6.0072622\PG=C01 [X(C12H20O3)]\@

Model g.1

1\1\GINC-R96\SP\RM062X\6-31+G(d,p)\C17H26O3S1\ROOT\26-Sep-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloG.1.ext.retry.freq\0,1\C\C,1,2.897051\C,2,1.544693,1,60.984\C,1,1.521432,2,60.053,3,28.797,0\C,2,1.545207,3,118.16,4,-48.151,0\C,1,1.519717,4,111.808,3,-59.253,0\O,1,1.45486,6,107.491,5,177.567,0\S,7,1.610515,1,117.695,6,127.105,0\C,8,1.774411,7,102.014,1,67.274,0\C,9,1.390495,8,119.569,7,-97.643,0\C,10,1.393398,9,118.783,8,175.147,0\C,11,1.397872,10,121.015,9,0.207,0\C,12,1.401877,11,118.765,10,0.208,0\C,13,1.389358,12,121.075,11,-0.302,0\C,3,1.537977,4,110.363,1,-73.353,0\C,3,1.534496,4,108.721,1,169.171,0\C,5,1.534721,6,108.654,1,-168.334,0\C,5,1.538121,6,110.506,1,74.175,0\C,12,1.506626,11,120.872,10,178.735,0\O,8,1.445007,7,104.604,1,-178.531,0\O,8,1.45226,7,108.81,1,-46.867,0\H,6,1.098776,1,107.705,4,-62.054,0\H,6,1.096476,1,109.373,4,-178.494,0\H,4,1.097938,1,110.186,6,177.993,0\H,4,1.098876,1,107.567,6,61.329,0\H,15,1.091639,3,113.471,4,52.924,0\H,15,1.096071,3,109.669,4,-66.867,0\H,15,1.095657,3,110.629,4,174.058,0\H,16,1.095044,3,111.148,4,-60.429,0\H,16,1.095938,3,110.708,4,179.452,0\H,16,1.095686,3,110.721,4,59.741,0\H,17,1.095083,5,111.18,6,60.741,0\H,17,1.09537,5,110.724,6,-59.437,0\H,17,1.095948,5,110.677,6,-179.11,0\H,18,1.091343,5,113.574,6,-51.776,0\H,18,1.095692,5,110.548,6,-173.043,0\H,18,1.095228,5,109.781,6,68.,0\H,1,1.095494,6,109.729,5,-65.162,0\H,10,1.085755,9,119.801,8,-5.344,0\H,11,1.08651,10,119.459,9,-179.884,0\H,13,1.086658,12,119.39,11,179.659,0\H,14,1.085632,9,119.764,8,4.647,0\H,19,1.092213,12,111.291,11,20.937,0\H,19,1.094977,12,110.433,11,-98.784,0\H,19,1.092976,12,111.141,11,141.894,0\H,2,1.099414,3,109.286,4,-173.787,0\H,2,1.100055,3,106.608,4,71.879,0\Version=ES64L-G09RevD.01\HF=-1286.9143395\RMSD=2.656e-09\Dipole=1.959491,0.2204384,1.650377\Quadrupole=14.4399555,-1.5016324,-12.9383231,1.4344278,-9.2177327,0.7979186\PG=C01 [X(C17H26O3S1)]\@

Model g.2

1\1\GINC-R38\FOpt\RM062X\6-31+G(d,p)\C17H26O3S1\ROOT\10-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\ModelG.2.freq\0,1\C,-1.0507653855,0.1071818369,0.2212766082\C,-1.6672643423,1.3698827861,-0.3560463107\C,-1.5882835102,-1.1484691252,-0.4464233082\C,-3.1184397375,-1.2656922632,-0.3220554153\C,-3.202516266,1.3805694303,-0.2334361602\C,-3.7661923088,0.0552430911,-0.7916041559\H,-1.3836619315,1.4219841513,-1.416641928\H,-1.2381655714,2.2477253569,0.1418983012\H,-1.0985690823,-2.0298518353,-0.0162008065\H,-1.3102571356,-1.0993657918,-1.508767785\C,-3.5154035206,-1.6565770204,1.1114308053\C,-3.6021958786,-2.3862500429,-1.2523984558\C,-3.7544778786,2.5277539876,-1.0905450251\C,-3.6266703542,1.6495680904,1.2201667027\H,-3.0738351812,-1.015924978,1.8762459018\H,-3.1857884778,-2.6798141153,1.3207807784\H,-4.6038076294,-1.6204591987,1.2326542859\H,-3.3534244814,-2.168586083,-2.2965489414\H,-4.6890564568,-2.5074038717,-1.1798801003\H,-3.1373571868,-3.3409591563,-0.9832817775\H,-3.4905348296,2.3961417425,-2.1452473221\H,-3.352389496,3.4904905127,-0.7562883723\H,-4.8469182474,2.5744579901,-1.0166910293\H,-3.1474077934,0.9887751837,1.9440675907\H,-4.7107056041,1.5357521556,1.3312807537\H,-3.365695639,2.6763843231,1.498628306\H,-1.2000546556,0.0728103973,1.3070696177\O,0.3853805862,0.1892790637,-0.034436986\S,1.3247522086,-0.2153796706,1.210925605\O,1.1909076313,0.8020888624,2.2397019533\O,1.0763059284,-1.6079808075,1.546345091\C,2.8939856861,-0.0579643954,0.4145164667\C,3.4423009931,-1.1665077387,-0.2221639768\C,4.6722848087,-1.0285291528,-0.8569991135\C,5.3508936972,0.1953463251,-0.8567695854\C,4.77045007,

1.289601129,-0.2046966834\C,3.5418985751,1.1730583769,0.4363919037\C,6.6994537674,0.3248905943,-1.5159711732\H,2.9135764095,-2.1140726771,-0.2071620267\H,5.1149948421,-1.8849025173,-1.3579101622\H,5.2899278999,2.2437763078,-0.196564465\H,3.0892160692,2.0121719804,0.9546509268\H,6.808409859,-0.3870394987,-2.3373827657\H,7.498216663,0.1257156403,-0.7937907099\H,6.8517489071,1.332620199,-1.9097910451\H,-4.8487726258,0.0156063338,-0.6039348698\H,-3.6459433945,0.0953940916,-1.884561142\Version=ES64L-G09RevD.01\State=1-A\HF=-1286.9123881\RMSD=7.722e-09\RMSF=1.156e-06\Dipole=0.5685917,0.3228349,-1.436182\Quadrupole=15.8622361,-3.8912873,-11.9709488,1.2497558,-6.3645794,2.0220042\PG=C01 [X(C17H26O3S1)]\@

Model h.1

1\1\GINC-R122\SP\RM062X\6-31+G(d,p)\C10H19N3\ROOT\14-Jul-2017\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\Cyclo.H.ext.retry.freq\0,1\C,C,1,2.917191\C,2,1.54411,1,60.895\C,1,1.523214,2,59.479,3,28.419,0\C,1,1.528944,4,110.817,3,-57.923,0\C,2,1.543844,3,118.028,4,-48.181,0\C,6,1.537585,2,113.111,3,-75.417,0\N,1,1.488143,4,106.693,3,-178.988,0\N,8,1.231548,1,113.82,4,-172.734,0\N,9,1.132273,8,175.166,1,178.683,0\C,3,1.537736,2,112.993,6,75.506,0\C,3,1.534916,2,107.903,6,-166.075,0\C,6,1.534933,2,107.967,3,166.036,0\H,1,1.099365,8,108.035,9,-54.534,0\H,5,1.099124,1,107.39,8,55.843,0\H,5,1.099131,1,10.349,8,-60.571,0\H,4,1.096823,1,109.615,8,57.715,0\H,4,1.099079,1,107.414,8,-58.144,0\H,2,1.100129,3,106.709,4,71.781,0\H,2,1.099447,3,109.305,4,-173.822,0\H,11,1.095672,3,110.604,2,50.409,0\H,11,1.091209,3,113.491,2,-70.745,0\H,11,1.095567,3,109.78,2,169.292,0\H,12,1.095941,3,110.706,2,-62.369,0\H,12,1.095537,3,110.761,2,177.935,0\H,12,1.095085,3,111.163,2,57.771,0\H,13,1.095942,6,110.673,2,62.383,0\H,13,1.095067,6,111.174,2,-57.715,0\H,13,1.095591,6,110.8,2,-177.949,0\H,7,1.095615,6,110.532,2,-50.888,0\H,7,1.095656,6,109.798,2,-169.701,0\H,7,1.09111,6,113.554,2,70.22,0\Version=ES64L-G09RevD.01\HF=-556.4889598\RMSD=4.489e-09\Dipole=0.1760472,0.3001225,1.0031734\Quadrupole=0.8184449,0.8235374,-1.6419823,0.5676606,-1.958776,-0.1355122\PG=C01 [X(C10H19N3)]\@

Model h.2

1\1\GINC-R38\SP\RM062X\6-31+G(d,p)\C10H19N3\ROOT\14-Jul-2017\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\Cyclo.H.2.ext.retry.freq\0,1\C,C,1,2.919764\C,2,1.543781,1,61.079\C,1,1.52899,2,59.359,3,28.376,0\C,1,1.529003,4,110.939,3,-57.515,0\C,2,1.543779,3,118.045,4,-48.474,0\C,6,1.534895,2,107.942,3,166.442,0\N,1,1.487914,5,111.395,6,-177.767,0\N,8,1.232123,1,114.184,5,-62.262,0\N,9,1.13267,8,174.646,1,-179.986,0\C,6,1.537503,2,113.077,3,-75.007,0\C,3,1.534896,2,107.942,6,-166.442,0\C,3,1.537503,2,113.078,6,75.007,0\H,5,1.101114,1,108.155,4,-62.784,0\H,5,1.097094,1,109.667,4,-179.261,0\H,4,1.097097,1,109.668,5,179.261,0\H,4,1.101112,1,108.158,5,62.781,0\H,1,1.092736,5,110.04,6,-64.498,0\H,2,1.099379,6,109.26,5,174.067,0\H,2,1.100257,6,106.725,5,-71.563,0\H,12,1.095914,3,110.678,2,-62.54,0\H,12,1.09554,3,110.776,2,177.793,0\H,12,1.095122,3,111.202,2,57.563,0\H,13,1.095589,3,110.57,2,50.227,0\H,13,1.091033,3,113.507,2,-70.928,0\H,13,1.095532,3,109.781,2,169.093,0\H,11,1.095589,6,110.57,2,-50.227,0\H,11,1.09553,6,109.781,2,-169.093,0\H,11,1.091033,6,113.506,2,70.928,0\H,7,1.095913,6,110.678,2,62.54,0\H,7,1.095122,6,111.202,2,-57.563,0\H,7,1.095541,6,110.776,2,-177.793,0\Version=ES64L-G09RevD.01\HF=-556.4890417\RMSD=5.875e-09\Dipole=0.1178409,0.5732534,0.9589397\Quadrupole=2.2854709,-2.4999484,0.2144774,-1.0250893,-0.2866827,-1.3964309\PG=C01 [X(C10H19N3)]\@

Model h.3

1\1\GINC-R37\FOpt\RM062X\6-31+G(d,p)\C10H19N3\ROOT\11-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\Modell.H.3.freq\0,1\C,0.9942218691,-0.7887605924,-1.0541352665\C,0.8089112532,0.728571306,-1.1618384302\C,-0.3485603955,-1.515672529,-1.0000722909\C,-1.3591020548,-0.9824655821,0.0346510073\C,-0.1314200973,1.3586955079,-0.1178254233\C,-1.4475960985,0.554815081,-0.0807426327\H,0.3915716096,0.9147959857,-2.1613618656\H,1.7840013326,1.2356015727,-1.1413915512\H,-0.1730619745,-2.5857584403,-0.835727818\H,-0.79430009,-1.4140991675,-1.9992648743\C,-1.0194391534,-1.462587147,1.4557963482\C,-2.7418878738,-1.5543199779,-0.3132535646\C,-0.4609614518,2.7866518656,-0.5776069096\C,0.5407671394,1.4747453949,1.2600195417\H,0.0111671926,-1.2620119349,1.7422453425\H,-1.1648331818,-2.5468870655,1.5213385492\H,-1.68781146,-0.9899458094,2.1847708498\H,-3.0649823329,-1.2392661329,-1.3115082143\H,-3.4924319154,-1.2142210946,0.4093130355\H,-2.7258612964,-2.6497048702,-0.2901800359\H,-0.9421606132,2.7870311409,-1.5616447485\H,0.4485937416,3.3944364048,-0.6427557061\H,-1.1398825593,3.2729671755,0.1318058741\H,0.8576478684,0.5163627041,1.669099564\H,-0.1492899711,1.9353021402,1.9759794145\H,1.4263556424,2.1174493187,1.1900525035\N,1.8084957613,-1.2114964463,0.1226308477\H,1.5296092004,-1.1337367925,-1.9502896196\N,2.8887753817,-0.6325216046,0.2222678972\N,3.8931739931,-0.1391625735,0.3978867511\H,-1.9785615561,0.7745741691,-1.019668609\H,-2.0853779098,0.9410579934,0.7273800341\Version=ES64L-G09RevD.01\State=1-A\HF=-556.4869411\RMSD=4.340e-09\RMSF=2.203e-06\Dipole=-0.6649515,0.1590632,-0.5582702\Quadrupole=-4.077223,1.1796557,2.8975672,0.0760545,-1.8155874,0.8668851\PG=C01 [X(C10H19N3)]\@

Model h.4

1\1\GINC-R37\FOpt\RM062X\6-31+G(d,p)\C10H19N3\ROOT\11-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\Modell.4.freq\0,1\C,-0.7155817833,0.6430299861,
-0.8462599519\C,-1.119844026,-0.7551034028,-0.3371178406\C,-0.0058966548,-1.4630545576,0.444442425
7\C,1.4044540193,-1.0934018137,-0.0310213022\C,1.6239836535,0.4392747474,0.0937195436\C,0.36043761
96,1.339272178,-0.0022515961\C,1.6165066668,-1.565697933,-1.4794265758\C,2.4273959639,-1.818254657
5,0.8512998351\C,0.7409518413,2.6606815462,-0.6807984236\C,-0.1922231574,1.6697158816,1.3942822076
\H,-1.6058269135,1.2839903929,-0.9088791229\H,-0.3475197592,0.5482127801,-1.8744678742\H,-0.151848
6097,-2.5479787707,0.3805256139\H,-0.1090359234,-1.2026431881,1.5030773954\H,0.9573664275,-1.06140
32952,-2.1915254519\H,1.4352633822,-2.6435863302,-1.560936932\H,2.647973542,-1.373466312,-1.794313
4596\H,2.2809586877,-1.5670229698,1.9072453215\H,3.4477894903,-1.5311398045,0.573153889\H,2.34071
51799,-2.9052740824,0.743253891\H,1.0936522717,2.4907316603,-1.7040495319\H,1.5429752928,3.160593
1359,-0.1259719834\H,-0.1156836652,3.3427769,-0.7226286606\H,-0.4784140002,0.7802344053,1.95958281
34\H,-1.083180883,2.3026504722,1.3107185501\H,0.5579208247,2.2172238168,1.9757033761\N,-2.2925810
45,-0.7084210807,0.5843803449\H,-1.4037702146,-1.3686963575,-1.2034275994\N,-3.3249014083,-0.294851
2841,0.0567624634\N,-4.3136294015,0.0799428803,-0.3487529441\H,2.1141246927,0.6531101365,1.052738
5614\H,2.3399378894,0.7406649203,-0.6827069818\Version=ES64L-G09RevD.01\State=1-A\HF=-556.4811
201\RMSD=3.542e-09\RMSF=1.345e-05\Dipole=0.9155725,-0.0418301,-0.3369212\Quadrupole=-4.8607608,2.9
122758,1.948485,0.0902571,0.4906326,1.0062928\PG=C01 [X(C10H19N3)]\@

Model i

1\1\GINC-R37\SP\RM062X\Gen\C10H19Br\ROOT\15-Jun-2017\0\#M062X/gen 6D 10F INT(grid=ultrafine)
Nosymm maxdisk=12GB\CycloI.ext.retry.freq\0,1\C\C,1,2.900697\C,2,1.543409,1,60.983\C,1,1.521749,2,60.
102,3,-28.73,0\C,1,1.521747,4,111.745,3,58.922,0\C,2,1.543418,3,117.976,4,48.461,0\C,6,1.537363,2,113.128,
3,75.227,0\Br,1,1.973675,5,109.419,6,179.733,0\C,6,1.534829,2,107.995,3,-166.113,0\C,3,1.534829,2,107.995,
6,166.111,0\C,3,1.537364,2,113.127,6,-75.229,0\H,1,1.091524,5,111.407,6,66.415,0\H,4,1.098582,1,108.097,5,
-61.407,0\H,4,1.096132,1,110.382,5,-178.322,0\H,5,1.098583,1,108.098,4,61.406,0\H,5,1.096131,1,110.382,4,
178.321,0\H,2,1.099427,6,109.291,5,-174.073,0\H,2,1.100127,6,106.72,5,71.518,0\H,9,1.095492,6,110.788,2,1
77.769,0\H,9,1.095957,6,110.628,2,-62.576,0\H,9,1.095029,6,111.191,2,57.528,0\H,7,1.095523,6,109.794,2,16
9.21,0\H,7,1.091213,6,113.516,2,-70.799,0\H,7,1.095616,6,110.572,2,50.332,0\H,11,1.095523,3,109.794,2,-16
9.213,0\H,11,1.095615,3,110.572,2,-50.334,0\H,11,1.091211,3,113.516,2,70.797,0\H,10,1.09549,3,110.788,2,-
177.772,0\H,10,1.095029,3,111.191,2,-57.531,0\H,10,1.095958,3,110.628,2,62.573,0\Version=ES64L-G09Rev
D.01\HF=-2966.2523004\RMSD=2.429e-09\Dipole=0.078813,-0.3892569,0.9977018\Quadrupole=0.9467992,-
0.1689,-0.7778992,0.2355349,-0.1492246,0.7396182\PG=C01 [X(C10H19Br)]\@

Model k.1

1\1\GINC-R38\FOpt\RM062X\6-31+G(d,p)\C13H22O1\ROOT\11-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Modell.1.freq\0,1\C,0.5923676546,0.2021171614,
-1.3766841724\C,-0.4334995612,1.3239166645,-1.2395157171\C,-0.073138444,-1.1716899438,-1.236343441
3\C,-0.9183369865,-1.3594552497,0.0362171127\C,-1.3198642135,1.2575466502,0.0200837691\C,-1.891308
802,-0.1688096439,0.1675854058\H,-1.0829538443,1.2708140284,-2.1245477092\H,0.0884925399,2.2876008
067,-1.2798732069\H,0.6689979034,-1.9772924195,-1.315226316\H,-0.7300857484,-1.2841046188,-2.110732
0597\C,-0.0313183121,-1.5516444321,1.2775337772\C,-1.7567952223,-2.6360267723,-0.1236322529\C,-2.50
40763355,2.2158882882,-0.1772212378\C,-0.5595773021,1.7302904731,1.2704559233\H,0.6883802177,-0.74
56352686,1.4160124549\H,0.5282358195,-2.4913885601,1.1907647926\H,-0.6511076127,-1.6194909457,2.17
89222317\H,-2.4200117106,-2.5708297354,-0.9931124887\H,-2.3772505015,-2.8041441919,0.7640756813\H,
-1.1113169438,-3.5123364329,-0.2529854176\H,-3.1059085308,1.9331684603,-1.0480280007\H,-2.15125426
41,3.2426354976,-0.3258530072\H,-3.1569531365,2.2093431721,0.7031571859\H,0.3861282017,1.21208987
12,1.4156026278\H,-1.1814185349,1.5961980917,2.1633768727\H,-0.3307423338,2.798294865,1.179052753
6\O,1.626601408,0.4475632073,-0.4264400067\H,1.0447001804,0.2635626816,-2.381738585\C,2.7395656233,-
0.4068237715,-0.5546693548\C,3.8416074917,0.1079261732,0.2628079265\C,4.7590517294,0.5099558443,0.
9336654715\H,3.0586354983,-0.4651578199,-1.6074955044\H,2.4993306439,-1.4266727102,-0.2212136651\
H,5.5664696857,0.8742794382,1.5287841299\H,-2.6490153243,-0.2928382077,-0.621459774\H,-2.430720932
7,-0.2451106511,1.122863801\Version=ES64L-G09RevD.01\State=1-A\HF=-583.5491041\RMSD=3.999e-09\
RMSF=5.928e-06\Dipole=-0.0817076,-0.3568623,-0.4002069\Quadrupole=0.8461638,-1.5915531,0.7453892,-
0.3883586,0.9626266,0.8073518\PG=C01 [X(C13H22O1)]\@

Model k.2

1\1\GINC-R37\SP\RM062X\6-31+G(d,p)\C13H22O1\ROOT\14-Jul-2017\0\#M062X\6-31+G(d,p) INT(grid=u
ltrafine) Nosymm maxdisk=12GB\Cyclo.K3.ext.retry.freq\0,1\C\C,1,2.92359\C,1,1.522568,2,59.132\C,3,1.53
7987,1,113.493,2,-26.983,0\C,2,1.543208,4,117.884,3,-48.064,0\C,1,1.527893,3,110.816,4,-57.458,0\O,1,1.425

436,6,112.533,5,175.33,0\C,7,1.408718,1,115.498,6,67.075,0\C,8,1.474482,7,113.806,1,-92.814,0\C,9,1.20665
8,8,178.386,7,-134.021,0\C,4,1.537862,3,110.773,1,-73.705,0\C,4,1.534935,3,108.733,1,168.738,0\C,5,1.53499
9,6,108.643,1,-168.606,0\C,5,1.538181,6,110.61,1,74.006,0\H,6,1.099458,1,107.275,3,-64.026,0\H,6,1.097464,
1,110.729,3,179.918,0\H,3,1.096977,1,109.25,6,179.015,0\H,3,1.099016,1,107.102,6,63.442,0\H,11,1.09108,4,
113.446,3,51.919,0\H,11,1.095699,4,109.743,3,-67.977,0\H,11,1.095854,4,110.633,3,173.144,0\H,12,1.095097,
4,111.137,3,-60.411,0\H,12,1.096129,4,110.732,3,179.438,0\H,12,1.09563,4,110.753,3,59.711,0\H,13,1.095073,5
,111.114,6,60.649,0\H,13,1.095617,5,110.739,6,-59.446,0\H,13,1.096192,5,110.744,6,-179.199,0\H,14,1.09109
8,5,113.457,6,-52.378,0\H,14,1.095826,5,110.62,6,-173.548,0\H,14,1.095801,5,109.743,6,67.589,0\H,1,1.1032
65,6,109.856,5,-64.658,0\H,8,1.094413,7,106.751,1,147.688,0\H,8,1.100227,7,110.737,1,30.813,0\H,10,1.0672
19,9,179.422,8,138.753,0\H,2,1.099724,4,109.375,3,-173.749,0\H,2,1.10013,4,106.69,3,71.791,0\Version=ES6
4L-G09RevD.01\HF=-583.550469\RMSD=3.697e-09\Dipole=-0.3515225,0.3255912,0.2372311\Quadrupole=-
0.2685255,0.3167382,-0.0482127,2.3527417,1.1330373,-0.9260521\PG=C01 [X(C13H22O1)]\@

Model k.3

1\1\GINC-R114\SP\RM062X\6-31+G(d,p)\C13H22O1\ROOT\14-Jul-2017\0\#M062X\6-31+G(d,p) INT(grid=
ultrafine) Nosymm maxdisk=12GB\Cyclo.K.ext.retry.freq\0,1\C,1,2.920236\C,2,1.543317,1,60.943\C,1,1.5
27746,2,59.507,3,-28.335,0\C,1,1.522078,4,110.762,3,57.633,0\C,5,1.538133,1,113.282,4,-58.044,0\C,6,1.5348
3,5,108.763,1,168.987,0\O,1,1.426946,4,112.369,3,175.573,0\C,8,1.409426,1,115.924,4,60.253,0\C,9,1.474544,8
,113.95,1,53.164,0\C,10,1.206993,9,179.163,8,-110.706,0\C,6,1.537704,5,110.813,1,-73.366,0\C,3,1.534874,4,
108.767,1,-168.775,0\C,3,1.538452,4,110.343,1,73.815,0\H,4,1.100253,1,107.639,5,-63.402,0\H,4,1.09813,1,11
0.824,5,179.387,0\H,5,1.096904,1,109.16,4,178.648,0\H,5,1.0993,1,107.43,4,62.923,0\H,12,1.09093,6,113.422,
5,52.385,0\H,12,1.095674,6,109.749,5,-67.514,0\H,12,1.095934,6,110.587,5,173.632,0\H,7,1.095179,6,111.151,5
,-60.247,0\H,7,1.096156,6,110.753,5,179.58,0\H,7,1.09563,6,110.728,5,59.867,0\H,13,1.095215,3,111.157,4,60.8
34,0\H,13,1.095737,3,110.761,4,-59.372,0\H,13,1.096144,3,110.726,4,-179.045,0\H,14,1.091047,3,113.404,4,-
50.999,0\H,14,1.095817,3,110.613,4,-172.394,0\H,14,1.095769,3,109.718,4,68.673,0\H,1,1.099659,4,109.828,3,-
64.217,0\H,9,1.098556,8,111.289,1,-70.157,0\H,9,1.093033,8,105.776,1,173.23,0\H,11,1.067422,10,179.448,9,
-152.182,0\H,2,1.100269,6,106.697,5,71.842,0\H,2,1.099694,6,109.408,5,-173.693,0\Version=ES64L-G09Rev
D.01\HF=-583.5522629\RMSD=4.086e-09\Dipole=0.4006255,-0.1688962,0.2355698\Quadrupole=-1.0293184,
1.4656063,-0.4362879,-0.4457112,-1.6786763,0.2932779\PG=C01 [X(C13H22O1)]\@

Model k.4

1\1\GINC-R38\FOpt\RM062X\6-31+G(d,p)\C13H22O1\ROOT\11-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\ModellK.4.freq\0,1\C,-0.1215987077,1.1085310412,
-0.7233227597\C,-1.0005799847,0.1305576806,0.0619920507\C,-0.195885462,-0.9597586889,0.7931481433\
C,1.1607781481,-1.2893563404,0.1529906276\C,2.0222139634,-0.0020283976,0.0249691637\C,1.255749605
4,1.3431930303,-0.0916729487\C,0.9469559051,-1.9493085873,-1.2197403799\C,1.8998951284,-2.29408745
7,1.0449319286\C,2.0558689119,2.29955505,-0.9832083649\C,1.0979187472,2.0066858327,1.2869559093\H,
-0.6542554916,2.0607013824,-0.8346106742\H,0.005995098,0.7087626719,-1.7352973373\H,-0.7994723288,
-1.8755809638,0.8434499311\H,-0.030240826,-0.6519166887,1.8327065519\H,0.4216227463,-1.301249421,-
1.9238584929\H,0.3492083083,-2.8616231852,-1.1119345717\H,1.9117621279,-2.2259791115,-1.6597182363
\H,2.0387810105,-1.8949354641,2.0558181384\H,2.8898515318,-2.5207457662,0.632515619\H,1.343583919
3,-3.2352895304,1.12220261\H,2.1447448843,1.9031302297,-2.0004170104\H,3.067301004,2.4430825435,-0.
5858475713\H,1.5723141273,3.281297156,-1.0403919375\H,0.5802800785,1.3665173408,2.0068048788\H,0.
5294137933,2.9397302629,1.1998819506\H,2.0803941236,2.2481357164,1.7075403816\O,-1.9045069179,-0.
431423772,-0.8949469119\H,-1.5924209643,0.6894955628,0.8014486283\C,-3.9813221079,0.1492154844,0.1
69521786\C,-4.6981283041,1.0207878092,0.5972372385\H,-5.3338036612,1.7935793068,0.9685828852\C,-3.
1062591083,-0.919486433,-0.348862642\H,-2.9183300864,-1.6449059476,0.4561402689\H,-3.6187047438,-1.
4469075356,-1.1574581284\H,2.6967676305,0.0681008784,0.8891470007\H,2.6714079015,-0.1203256898,-0.
8529077251\Version=ES64L-G09RevD.01\State=1-A\HF=-583.5444072\RMSD=3.210e-09\RMSF=2.128e-06
\Dipole=0.0280617,-0.0161899,0.431129\Quadrupole=0.9541623,1.3819854,-2.3361477,-0.4283312,-1.927514
1,0.9598604\PG=C01 [X(C13H22O1)]\@

Model k.5

1\1\GINC-R38\FOpt\RM062X\6-31+G(d,p)\C13H22O1\ROOT\11-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\ModellK.5.freq\0,1\C,0.1581843709,0.7174306097,1.0
291301806\C,0.7256303104,-0.640573364,0.5738338243\C,-0.2079327917,-1.3979871278,-0.3760967482\C,-
1.6965374151,-1.1360286548,-0.1184950144\C,-1.9998198428,0.3799347942,-0.2594530263\C,-0.830075831,
1.3576607287,0.0430381517\C,-2.0885678273,-1.6473407468,1.2782158666\C,-2.52384475,-1.9108639266,-1.1
503728837\C,-1.4007435977,2.6342157014,0.6724706927\C,-0.096517495,1.758516735,-1.2482417277\H,0.9
908094658,1.4121512548,1.1995649438\H,-0.338235458,0.597385253,1.9997654861\H,0.0027035231,-2.472

2200566,-0.3103490716\H,0.0434307861,-1.0987686445,-1.3992818934\H,-1.5824838153,-1.1066338132,2.0
829418404\H,-1.8411411134,-2.7102628446,1.3805968331\H,-3.1671657627,-1.5360631588,1.434974862\H,-
2.2376702664,-1.6314274361,-2.1700020234\H,-3.591896381,-1.6973331786,-1.0275410812\H,-2.379940665
1,-2.9915605421,-1.0391894502\H,-1.8958084743,2.4160595269,1.6253438366\H,-2.1389306885,3.09537626
07,0.0063147986\H,-0.6090964421,3.3690434433,0.8580975057\H,0.3469255811,0.9064836883,-1.76695124
22\H,0.7179531255,2.4553926824,-1.0207382363\H,-0.7892685962,2.2577855395,-1.935120372\O,1.9594226
792,-0.4937027382,-0.1294914728\H,0.9146256071,-1.257978966,1.4673477054\C,4.2780379838,-0.1207810
083,-0.0808330111\C,5.2859294149,0.0549590577,-0.718359986\H,6.1724562169,0.2094577128,-1.29186936
98\C,3.0708558796,-0.3324714135,0.7217509345\H,3.2013619747,-1.2277573115,1.3493568185\H,2.9379487
115,0.5259548223,1.3966896494\H,-2.8479790229,0.6164133763,0.3974112746\H,-2.3472793942,0.5809237
452,-1.2815985943\Version=ES64L-G09RevD.01\State=1-A\HF=-583.5422135\RMSD=4.867e-09\RMSF=1.2
25e-05\Dipole=-0.2427436,-0.0103615,0.5113206\Quadrupole=1.3020217,-1.2520364,-0.0499853,0.9772728,0.4
231246,-0.8604814\PG=C01 [X(C13H22O1)]\@

Model I.1

1\1\GINC-R146\SP\RM062X\6-31+G(d,p)\C13H22O2\ROOT\21-Sep-2017\0\#M062X\6-31+G(d,p) INT(grid
=ultrafine) Nosymm maxdisk=12GB\CycloL.GOOD.freq\0,1\C\C,1,2.905063\C,2,1.5443,1,60.958\C,1,1.5203,2
,59.868,3,-28.536,0\C,1,1.524292,4,111.365,3,58.584,0\C,5,1.539392,1,112.356,4,-58.687,0\C,6,1.534723,5,10
8.75,1,168.87,0\O,1,1.443379,4,106.499,3,178.085,0\C,8,1.342997,1,116.844,4,157.921,0\C,9,1.48833,8,110.9
49,1,179.521,0\C,10,1.331224,9,120.035,8,179.889,0\C,6,1.538068,5,110.469,1,-73.548,0\C,3,1.534719,4,108.
657,1,-168.821,0\C,3,1.537626,4,110.695,1,73.59,0\O,9,1.210804,8,124.04,1,-0.734,0\H,4,1.099125,1,107.825,
5,-62.054,0\H,4,1.097143,1,109.781,5,-178.485,0\H,5,1.096174,1,109.724,4,178.593,0\H,5,1.099523,1,107.462,4
,61.669,0\H,12,1.090979,6,113.459,5,50.741,0\H,12,1.095252,6,109.727,5,-68.787,0\H,12,1.095789,6,110.613,
5,172.188,0\H,7,1.095245,6,111.189,5,-60.655,0\H,7,1.096064,6,110.684,5,179.213,0\H,7,1.095451,6,110.72,5,
59.557,0\H,13,1.095155,3,111.164,4,60.371,0\H,13,1.095675,3,110.77,4,-59.831,0\H,13,1.095932,3,110.695,4,
-179.511,0\H,14,1.090933,3,113.495,4,-52.819,0\H,14,1.095672,3,110.51,4,-173.92,0\H,14,1.095711,3,109.8,4,
67.256,0\H,1,1.094455,4,111.39,3,-65.314,0\H,10,1.085018,9,116.975,8,-0.11,0\H,11,1.086287,10,119.956,9,0.
01,0\H,11,1.084494,10,121.515,9,-179.958,0\H,2,1.099507,6,109.316,5,-173.817,0\H,2,1.100276,6,106.7,5,71.
771,0\Version=ES64L-G09RevD.01\HF=-658.8307338\RMSD=2.698e-09\Dipole=0.232185,0.5114959,0.171
4453\Quadrupole=-2.0001961,-2.8350853,4.8352814,-1.4194384,0.5811154,-3.975049\PG=C01 [X(C13H22O
2)]\@

Model I.2

1\1\GINC-R245\SP\RM062X\6-31+G(d,p)\C13H22O2\ROOT\26-Sep-2017\0\#M062X\6-31+G(d,p) SCF=Tig
ht INT(grid=ultrafine) NoSymm maxdisk=12GB\CycloL.GOOD.1.freq\0,1\C\C,1,2.905073\C,2,1.544345,1,60.9
4\C,1,1.520297,2,59.857,3,-28.596,0\C,1,1.524039,4,111.339,3,58.696,0\C,2,1.544232,3,118.056,4,48.117,0\C,
6,1.534741,2,107.872,3,-166.095,0\O,1,1.443441,4,106.463,3,178.244,0\C,8,1.342582,1,116.77,4,158.121,0\C,
9,1.486827,8,113.128,1,179.326,0\C,10,1.331994,9,123.75,8,-0.848,0\C,3,1.534705,2,107.981,6,166.092,0\C,3,
1.537671,2,112.949,6,-75.415,0\C,6,1.538015,2,113.145,3,75.31,0\O,9,1.211453,8,123.911,1,-0.937,0\H,4,1.09
9277,1,107.856,5,-61.907,0\H,4,1.09719,1,109.774,5,-178.396,0\H,5,1.096151,1,109.756,4,178.578,0\H,5,1.09
9567,1,107.472,4,61.653,0\H,14,1.090954,6,113.493,2,-71.632,0\H,14,1.095231,6,109.72,2,168.809,0\H,14,1.0
95813,6,110.593,2,49.807,0\H,7,1.095263,6,111.185,2,57.567,0\H,7,1.096065,6,110.686,2,-62.561,0\H,7,1.095
449,6,110.727,2,177.778,0\H,12,1.095176,3,111.174,2,-57.824,0\H,12,1.095689,3,110.77,2,-178.042,0\H,12,1.
095926,3,110.688,2,62.288,0\H,13,1.090932,3,113.485,2,70.047,0\H,13,1.09565,3,110.516,2,-51.055,0\H,13,1.
095695,3,109.801,2,-169.892,0\H,1,1.094401,4,111.335,3,-65.158,0\H,10,1.085147,9,113.741,8,179.28,0\H,11,
1.085132,10,120.951,9,0.092,0\H,11,1.084975,10,120.969,9,-179.91,0\H,2,1.099517,3,109.225,4,173.763,0\H,2,1
.100313,3,106.698,4,-71.875,0\Version=ES64L-G09RevD.01\HF=-658.8299297\RMSD=5.261e-09\Dipole=0.
3666888,0.7244535,0.3075418\Quadrupole=-1.9665977,-1.2069112,3.1735089,-1.4585956,-0.7590775,-5.4739
191\PG=C01 [X(C13H22O2)]\@

Model I.3

1\1\GINC-R42\SP\RM062X\6-31+G(d,p)\C13H22O2\ROOT\14-Jul-2017\0\#M062X\6-31+G(d,p) INT(grid=u
ltrafine) Nosymm maxdisk=12GB\CycloL.ext.retry.freq\0,1\C\C,1,2.944424\C,2,1.543791,1,61.652\C,1,1.523
918,2,58.69,3,25.994,0\C,1,1.527774,4,112.271,3,-50.123,0\C,2,1.54318,3,118.114,4,-48.588,0\C,6,1.537875,2,
113.002,3,-75.595,0\O,1,1.447224,5,111.344,6,-70.331,0\C,8,1.342661,1,116.988,5,-77.56,0\O,9,1.210417,8,12
4.102,1,-1.537,0\C,6,1.535895,2,107.834,3,166.419,0\C,3,1.537975,2,112.999,6,76.189,0\C,3,1.536026,2,107.7
48,6,-165.868,0\C,9,1.488476,8,110.797,1,178.442,0\C,14,1.331259,9,120.096,8,-179.345,0\H,5,1.099326,1,10
6.062,4,-69.405,0\H,5,1.096044,1,109.393,4,176.103,0\H,4,1.097103,1,109.337,5,-175.1,0\H,4,1.098935,1,106.
133,5,70.035,0\H,1,1.094541,5,108.813,6,172.331,0\H,14,1.085552,9,116.983,8,0.483,0\H,15,1.086293,14,119.
926,9,-0.193,0\H,15,1.084467,14,121.529,9,179.857,0\H,2,1.099743,6,109.297,5,174.72,0\H,2,1.10079,6,106.7
09,5,-70.984,0\H,12,1.096085,3,110.177,2,52.042,0\H,12,1.088326,3,113.181,2,-69.791,0\H,12,1.09617,3,109.

616,2,170.529,0\H,13,1.095955,3,110.634,2,-62.684,0\H,13,1.095878,3,110.777,2,177.751,0\H,13,1.095423,3,111.322,2,57.435,0\H,11,1.096029,6,110.667,2,62.27,0\H,11,1.095406,6,111.291,2,-57.872,0\H,11,1.095749,6,110.742,2,-178.101,0\H,7,1.096141,6,110.18,2,-54.655,0\H,7,1.096322,6,109.689,2,-173.155,0\H,7,1.088787,6,113.269,2,66.774,0\Version=ES64L-G09RevD.01\HF=-658.8286329\RMSD=4.342e-09\Dipole=0.3996629,0.2437118,0.3896614\Quadrupole=-2.8419777,5.3043411,-2.4623634,0.6775718,-1.9138105,-2.9493945\PG=C01 [X(C13H22O2)]\@

Model I.4

1\1\GINC-R148\SP\RM062X\6-31+G(d,p)\C13H22O2\ROOT\16-Jul-2017\0\#M062X/6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloL.2.ext.retry.freq\0,1\C,1,2.945701\C,2,1.543895,1,61.475\C,1,1.527972,2,58.586,3,-26.577,0\C,1,1.523596,4,112.176,3,50.714,0\C,2,1.543311,3,118.091,4,49.055,0\C,6,1.535841,2,107.941,3,-165.772,0\O,1,1.447611,4,111.621,3,-70.201,0\C,8,1.342158,1,116.823,4,-76.796,0\O,9,1.211185,8,123.974,1,-1.239,0\C,3,1.536001,2,107.706,6,166.316,0\C,3,1.538476,2,113.234,6,-75.695,0\C,6,1.536925,2,112.71,3,76.294,0\C,9,1.486943,8,113.001,1,178.717,0\C,14,1.332191,9,123.788,8,1.868,0\H,4,1.099397,1,106.009,5,-69.312,0\H,4,1.095832,1,109.483,5,176.212,0\H,5,1.097104,1,109.344,4,-175.282,0\H,5,1.098903,1,106.129,4,69.864,0\H,1,1.094531,4,108.778,3,172.302,0\H,14,1.085143,9,113.773,8,-178.271,0\H,15,1.085705,14,121.102,9,0.42,0\H,15,1.08494,14,121.,9,-179.979,0\H,2,1.099766,3,109.299,4,174.602,0\H,2,1.100758,3,106.706,4,-71.106,0\H,13,1.096037,6,110.135,2,55.117,0\H,13,1.088158,6,112.909,2,-66.186,0\H,13,1.096325,6,109.814,2,173.797,0\H,7,1.095881,6,110.665,2,-62.,0\H,7,1.09594,6,110.778,2,178.392,0\H,7,1.095386,6,111.293,2,58.111,0\H,11,1.096065,3,110.662,2,62.679,0\H,11,1.095397,3,111.297,2,-57.469,0\H,11,1.095676,3,110.739,2,-177.704,0\H,12,1.096157,3,110.303,2,-52.54,0\H,12,1.096274,3,109.573,2,-171.024,0\H,12,1.089252,3,113.387,2,69.171,0\Version=ES64L-G09RevD.01\HF=-658.8284687\RMSD=4.852e-09\Dipole=-0.4480236,-0.4472562,0.6013804\Quadrupole=-2.3744804,5.9093202,-3.5348398,-1.5987973,1.800037,2.3018758\PG=C01 [X(C13H22O2)]\@

Model I.5

1\1\GINC-R39\FOpt\RM062X\6-31+G(d,p)\C13H22O2\ROOT\11-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\Modell.5.freq\0,1\C,-0.0183344546,0.7106532964,-0.8998047083\C,-0.5108098023,-0.6548584098,-0.3968934826\C,0.5095879931,-1.4032069649,0.4644941096\C,1.9622631799,-1.1243398614,0.0563800566\C,2.2623179688,0.3960934298,0.1599696085\C,1.0577996123,1.361622583,-0.0203909482\C,2.2167505307,-1.6390762799,-1.3706022915\C,2.8968879707,-1.885331571,1.0034093889\C,1.5460249951,2.6438262188,-0.7049471037\C,0.4590605362,1.7556026804,1.3406576144\H,-0.8805739889,1.3796837628,-0.9995794\H,0.3764466927,0.5853280044,-1.9146254977\H,0.3082031795,-2.4801982729,0.4172774733\H,0.3671941079,-1.1078190353,1.5094657321\H,1.6239701735,-1.1114134413,-2.1228710181\H,1.9758885048,-2.705919425,-1.4421643746\H,3.2721582959,-1.5137394858,-1.6360487549\H,2.7140244935,-1.6015794383,2.0454829057\H,3.9445939174,-1.6631340609,0.7710373463\H,2.7529213016,-2.9679470231,0.9132444549\H,1.9391614579,2.429862724,-1.7048576225\H,2.3458067314,3.1126978977,-0.1202409566\H,0.7315101276,3.3697633506,-0.8065075559\H,0.095123428,0.8963486641,1.9083608071\H,-0.3882330116,2.4362548224,1.1994738971\H,1.2103956084,2.2712328382,1.9492453381\O,-1.6821298998,-0.4993676551,0.4391555158\H,-0.8128315439,-1.2591581892,-1.2570327468\C,-2.8500777498,-0.2925365823,-0.1898051565\O,-2.9695753068,-0.2347436986,-1.3933852788\C,-3.962925286,-0.146252257,0.7876718622\C,-5.2038779521,0.0706069089,0.357251321\H,-3.7075985294,-0.2239151207,1.8394085209\H,-5.4039455102,0.1400137686,-0.7081982442\H,-6.0325221322,0.1807911817,1.0481591319\H,2.7161059083,0.6047930791,1.1380616604\H,3.0322084524,0.6376915618,-0.5851416041\Version=ES64L-G09RevD.01\State=1-A\HF=-658.8228804\RMSD=9.794e-09\RMSF=2.756e-06\Dipole=0.2461063,-0.0064456,0.5980213\Quadrupole=4.0256457,-1.1301829,-2.8954629,-1.1684018,-5.142774,0.0495096\PG=C01 [X(C13H22O2)]\@

Model I.6

1\1\GINC-R39\FOpt\RM062X\6-31+G(d,p)\C13H22O2\ROOT\11-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\Modell.6.freq\0,1\C,0.4549251264,1.0081245886,-1.1487016249\C,-0.5481156626,-0.082993632,-0.7635909483\C,-0.0051005215,-1.0957706154,0.2544137987\C,1.509596889,-1.3181294372,0.1364911493\C,2.2699673478,0.0241858462,0.316143508\C,1.5053542938,1.3197363586,-0.0736082774\C,1.8398703891,-1.9596184078,-1.2223115798\C,1.9508077938,-2.294054465,1.233325467\C,2.5026433239,2.3383485694,-0.6377255975\C,0.8330293196,1.9516508929,1.1567564668\H,-0.1062077041,1.9159959526,-1.3999117246\H,0.9715307757,0.7017294055,-2.0653885773\H,-0.5368918629,-2.0459349756,0.1384936035\H,-0.234750032,-0.7288502548,1.2617298111\H,1.6003595596,-1.3083914556,-2.0676107654\H,1.2803546743,-2.8929082881,-1.3507382744\H,2.9082703749,-2.1948403474,-1.2811246334\H,1.6844422893,-1.9139575055,2.2255102293\H,3.0369954715,-2.4382254472,1.2064029518\H,1.4756955231,-3.2727335769,1.1032469016\H,2.9759170604,1.9610308707,-1.5509631716\H,3.2940677342,2.5470992388,0.0910813072\H,2.0052095227,3.2852730447,-0.8763334094\H,0.1231830497,1.2787207729,1.6426112555\H,0.2

823909202,2.8541002482,0.8686438515\H,1.5908843186,2.2359065152,1.8954095635\O,-1.7051229841,0.58671651,-0.2050417522\H,-0.8915585251,-0.6069071291,-1.6611684826\C,-2.8493703372,-0.1143534648,-0.1764992259\O,-2.9591640809,-1.2476018111,-0.5884886661\C,-3.9522655088,0.6890814904,0.4184253831\C,-5.1710672714,0.1659076089,0.5324910742\H,-3.70845714,1.6952743386,0.7433117944\H,-5.3599859893,-0.8477862825,0.1907983517\H,-5.992299663,0.7295355333,0.9615023816\H,2.5808684302,0.1219530999,1.3649112099\H,3.1987630948,-0.0351737898,-0.2672233489\Version=ES64L-G09RevD.01\State=1-A\HF=-658.8229338\RMSD=4.205e-09\RMSF=2.770e-06\Dipole=0.221462,0.5330286,0.2194211\Quadrupole=3.652456,-2.4619313,-1.1905247,-4.2555251,-3.2151358,-0.3540688\PG=C01 [X(C13H22O2)]\@

Model m.1

1\1\GINC-R37\SP\RM062X\6-31+G(d,p)\C11H20O2\ROOT\14-Jul-2017\0\#M062X\6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloM.lined.ext.retry.freq\0,1\C\C,1,2.922664\C,2,1.543709,1,61.006\C,1,1.537473,2,59.237,3,28.792,0\C,1,1.537474,4,110.106,3,-58.834,0\C,2,1.543709,3,118.102,4,-48.41,0\C,6,1.536908,2,113.056,3,-75.293,0\C,1,1.509286,5,110.725,6,-178.384,0\O,8,1.207734,1,125.723,5,118.789,0\C,6,1.534991,2,107.878,3,166.193,0\C,3,1.536909,2,113.056,6,75.293,0\C,3,1.534991,2,107.878,6,-166.193,0\O,8,1.351866,1,112.468,5,-61.211,0\H,5,1.09817,1,108.111,4,-61.839,0\H,5,1.098074,1,110.223,4,-178.605,0\H,4,1.098074,1,110.223,5,178.605,0\H,4,1.09817,1,108.111,5,61.839,0\H,1,1.094053,5,110.257,6,-63.043,0\H,13,0.96932,8,107.156,1,180.,0\H,2,1.100256,6,106.7,5,-71.611,0\H,2,1.099614,6,109.252,5,174.033,0\H,11,1.095661,3,110.583,2,50.301,0\H,11,1.090977,3,113.455,2,-70.838,0\H,11,1.095664,3,109.813,2,169.189,0\H,12,1.096008,3,110.686,2,-62.313,0\H,12,1.095677,3,110.792,2,178.027,0\H,12,1.095147,3,111.182,2,57.798,0\H,10,1.096008,6,110.687,2,62.313,0\H,10,1.095148,6,111.182,2,-57.798,0\H,10,1.095677,6,110.792,2,-178.027,0\H,7,1.095661,6,110.583,2,-50.301,0\H,7,1.095664,6,109.813,2,-169.189,0\H,7,1.090978,6,113.455,2,70.838,0\Version=ES64L-G09RevD.01\HF=-581.4746497\RMSD=8.460e-09\Dipole=-0.0691806,-0.3455003,0.7317477\Quadrupole=0.9238278,1.303699,-2.2275268,0.0792556,0.8346786,4.1657977\PG=C01 [X(C11H20O2)]\@

Model m.2

1\1\GINC-R37\SP\RM062X\6-31+G(d,p)\C11H20O2\ROOT\15-Jun-2017\0\#M062X\6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloM.ext.retry.freq\0,1\C\C,1,2.920397\C,2,1.5438,1,60.89\C,1,1.52791,2,59.337,3,-28.58,0\C,1,1.541032,4,110.753,3,57.981,0\C,2,1.543529,3,118.059,4,48.497,0\C,6,1.534965,2,107.936,3,-166.342,0\C,1,1.51033,5,109.073,6,179.87,0\O,8,1.351434,1,111.905,5,-70.118,0\C,3,1.534805,2,107.837,6,166.415,0\C,3,1.537333,2,112.986,6,-75.194,0\C,6,1.536894,2,113.076,3,75.046,0\O,8,1.207411,1,126.137,5,108.627,0\H,4,1.098113,1,107.931,8,58.144,0\H,4,1.097087,1,110.185,8,-57.497,0\H,5,1.096484,1,110.126,8,56.951,0\H,5,1.09994,1,107.943,8,-59.898,0\H,1,1.097337,8,106.222,13,-134.302,0\H,9,0.96948,8,107.215,1,178.13,0\H,2,1.100232,3,106.685,4,-71.495,0\H,2,1.099675,3,109.331,4,174.12,0\H,11,1.095703,3,109.768,2,-168.964,0\H,11,1.09577,3,110.684,2,-50.06,0\H,11,1.091277,3,113.452,2,71.093,0\H,10,1.095621,3,110.743,2,-177.99,0\H,10,1.095082,3,111.143,2,-57.905,0\H,10,1.096095,3,110.766,2,62.277,0\H,12,1.095628,6,109.843,2,177.899,0\H,7,1.095972,6,110.672,2,-62.425,0\H,7,1.095149,6,111.176,2,57.638,0\Version=ES64L-G09RevD.01\HF=-581.4756431\RMSD=8.152e-09\Dipole=-0.3105374,-0.5421487,0.2983255\Quadrupole=0.4815078,-3.6801043,3.1985965,-1.9780699,1.877575,1.21013\PG=C01 [X(C11H20O2)]\@

Model m.3

1\1\GINC-R41\FOpt\RM062X\6-31+G(d,p)\C11H20O2\ROOT\10-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\ModelM.3.freq\0,1\C,-0.5970640317,0.8139253399,-0.9885745459\C,-1.1444644557,-0.5905096476,-0.6113814558\C,-0.1684058192,-1.4218315276,0.2362076407\C,1.3055035665,-1.1169033117,-0.0602532074\C,1.6022460721,0.3860411083,0.1934697868\C,0.4144660425,1.3717331024,0.021597965\C,1.6457954268,-1.5079822251,-1.5080217594\C,2.1820516448,-1.9619895707,0.8712059834\C,0.9483023676,2.7085722978,-0.5061514389\C,-0.2804419526,1.6380968423,1.3674264403\H,-1.4293657629,1.5171324626,-1.1054370738\H,-0.1146423497,0.7542194672,-1.969878655\H,-0.3619937686,-2.4889631143,0.0708626977\H,-0.3697405344,-1.244836305,1.2971235075\H,1.093642952,-0.9197582846,-2.2462450084\H,1.4156898337,-2.5654240937,-1.6824113514\H,2.7139143291,-1.3602360838,-1.7018475179\H,1.9366812508,-1.7683924611,1.9208905499\H,3.2422559814,-1.7275037401,0.7218662012\H,2.0422690735,-3.0319413732,0.679807786\H,1.4016142021,2.5878405393,-1.4962218123\H,1.7129453642,3.110346941,0.1683962975\H,0.1449860061,3.4497586508,-0.5855230304\H,-0.6606667227,0.7289212292,1.8395696453\H,-1.1287666162,2.3193972699,1.2300194922\H,0.4184642812,2.1106685058,2.0663646871\C,-2.4893065901,-0.4826005171,0.079686936\H,-1.3579450088,-1.1137600113,-1.5516998844\O,-2.7519037938,-0.8310263638,1.2058360983\O,-3.4246266946,0.0628144123,-0.7292530467\H,-4.2507955972,0.1038572124,-0.2238736905\H,2.418427434,0.686117856,-0.4777753452\H,1.9924738697,0.5068253935,1.2128571083\Version=ES64L-G09RevD.01\State=1-A\HF=-581.4682473\RMSD=9.364e-09\RMSF=3.694e-06\Dipole=0.1814572,0.2

250792,-0.5292103\Quadrupole=2.8205023,0.0951631,-2.9156654,-1.8035855,2.1615939,1.986216\PG=C01 [X(C11H20O2)]\@

Model m.4

1\1\GINC-R41\FOpt\RM062X\6-31+G(d,p)\C11H20O2\ROOT\10-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\ModellM.4.freq\0,1\C,-1.1892712374,0.232634143
6,-1.0925454549\C,-0.5538318744,-1.1676133316,-1.1205054744\C,-0.1272301786,1.3402219142,-1.1026498
402\C,1.0224481841,1.1904281327,-0.0827815324\C,0.505576407,-1.4037496719,-0.0310597607\C,1.542303
8128,-0.2631131118,-0.090408175\H,-0.0642809774,-1.2748443002,-2.0981017515\H,-1.3306114488,-1.93768
83978,-1.0650204484\H,-0.6084311413,2.3159010368,-0.9722759435\H,0.3166549339,1.3316381272,-2.1073
605418\C,0.6193313031,1.6677583607,1.3222206274\C,2.173763579,2.0999635886,-0.5403005688\C,1.2323
397162,-2.7194337362,-0.3424193088\C,-0.143980508,-1.5594117871,1.3526038795\H,-0.2485787184,1.1569
090499,1.7329465564\H,0.3700398365,2.7338712939,1.2938421976\H,1.4582979375,1.5319748468,2.014759
0572\H,2.5323132807,1.8181652059,-1.536353421\H,3.0180143383,2.0343835354,0.1553503184\H,1.849522
7863,3.1459869904,-0.5781664265\H,1.7210594992,-2.6794737093,-1.3219626697\H,0.5301152508,-3.56062
0365,-0.3464679743\H,2.0009024255,-2.9252024814,0.4112060412\H,-0.7821160525,-0.7213628629,1.63496
46634\H,0.6268412108,-1.6580343439,2.1252696222\H,-0.7661760283,-2.460949767,1.3725839752\C,-2.247
8282479,0.4259568646,-0.0255674535\H,-1.7770273246,0.3290369162,-2.0181108023\O,-2.4381307421,1.43
27928804,0.6145524286\O,-3.0565694943,-0.6503118546,0.0939760461\H,-3.7391624178,-0.4202772974,0.7
428699488\H,2.269901765,-0.389295991,0.7246422392\H,2.1053101251,-0.4007698719,-1.0262700534\Vers
ion=ES64L-G09RevD.01\State=1-A\HF=-581.4722868\RMSD=9.411e-09\RMSF=3.055e-06\Dipole=0.053203
6,-0.5322712,-0.3147452\Quadrupole=1.9511114,-3.0749624,1.123851,2.5219456,-0.0896776,-2.1215953\PG=
C01 [X(C11H20O2)]\@

Model n

CycloN.r1.ext.retry11\1\GINC-R48\SP\RM062X\6-31+G(d,p)\C10H17N1O1\ROOT\14-Jul-2017\0\#M062X\6
-31+G(d,p) INT(grid=ultrafine) Symmetry=None maxdisk=12GB\CycloN.r1.ext.retry1.freq\0,1\X\C,1,2.2811
35\C,2,2.552323,1,77.115\H,3,1.095557,2,91.187,1,-82.637,0\C,3,2.502547,2,60.912,1,77.627,0\C,2,1.553592,
3,33.951,5,33.328,0\C,6,1.52314,2,101.318,3,119.587,0\C,1,0.668815,7,179.999,6,1.011,0\C,8,1.511557,1,113.
076,7,0.346,0\C,9,1.533267,2,111.921,6,136.92,0\C,9,1.537558,2,112.536,6,-99.78,0\C,7,1.492905,1,125.802,2,1
75.797,0\N,12,1.368076,7,116.011,1,-25.393,0\O,12,1.222283,7,122.211,1,153.482,0\H,8,1.089447,1,125.333,2,-
176.743,0\H,13,1.006748,12,120.816,7,-18.216,0\H,13,1.009168,12,116.726,7,-175.15,0\H,2,1.096922,9,108.8
55,10,18.832,0\H,2,1.09604,9,112.017,10,-99.646,0\H,5,1.095951,6,109.653,2,64.654,0\H,5,1.094179,6,111.29
1,2,-55.011,0\H,5,1.092329,6,110.347,2,-175.33,0\H,3,1.09577,6,109.925,2,-60.583,0\H,3,1.093373,6,110.692,
2,179.604,0\H,10,1.095629,9,110.305,2,62.39,0\H,10,1.094606,9,110.962,2,-57.451,0\H,10,1.095808,9,111.083,2
,178.053,0\H,11,1.095571,9,110.16,2,-66.404,0\H,11,1.095616,9,110.81,2,174.132,0\H,11,1.093196,9,111.395,2
,53.837,0\Version=ES64L-G09RevD.01\HF=-521.0858619\RMSD=7.378e-09\Dipole=-0.969945,-1.0494292,-
0.0394158\Quadrupole=-3.9659726,-1.2408006,5.2067733,-3.6742161,0.5815837,4.4698903\PG=Unknown\@

Model o.1

CycloO.ext.retry11\1\GINC-R111\SP\RM062X\6-31+G(d,p)\C10H16O2\ROOT\14-Jul-2017\0\#M062X\6-31+
G(d,p) INT(grid=ultrafine) Symmetry=None maxdisk=12GB\CycloO.ext.retry1.freq\0,1\C,0,0,0,2.282908\C,
0,1.274682,0,1.391195\C,0,2.086796,-1.296718,1.540869\C,0,0.663274,0.085275,0.00075\C,0,-0.663268,-0.08
5304,-0.000744\C,0,-1.221757,-0.324262,1.380776\C,0,1.486277,0.256601,-1.214101\O,0,2.697578,0.283499,-
1.232891\C,0,2.174317,1.199963,1.712512\C,0,-2.413172,0.595434,1.672682\C,0,-1.669201,-1.790379,1.5089
1\O,0,0.755277,0.378335,-2.34397\H,0,1.38464,0.472442,-3.074736\H,0,-1.282341,-0.095374,-0.894826\H,0,0,0
90251,-0.704661,3.11748\H,0,-0.13191,0.999017,2.715273\H,0,2.479002,1.161909,2.764475\H,0,1.640037,2.1
41732,1.547704\H,0,3.07196,1.194588,1.089472\H,0,2.486301,-1.371861,2.558266\H,0,2.925257,-1.305469,0.
838693\H,0,1.466754,-2.178521,1.351371\H,0,-2.06055,-1.976706,2.515008\H,0,-0.836574,-2.476848,1.33121
\H,0,-2.460751,-2.021982,0.788017\H,0,-2.753538,0.45812,2.704909\H,0,-3.254262,0.372898,1.007026\H,0,-2.1
38287,1.646369,1.539795\Version=ES64L-G09RevD.01\HF=-540.9544335\RMSD=7.236e-09\Dipole=-0.821
1145,-0.1088385,0.1608704\Quadrupole=-4.6227232,-0.2886552,4.9113784,0.0706804,-0.1452941,-0.6219521
\PG=Unknown\@

Model o.2

1\1\GINC-R38\FOpt\RM062X\6-31+G(d,p)\C10H16O2\ROOT\10-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\ModellO.2.freq\0,1\C,0.0307530046,0.0074411482,0.0
032691657\C,0.0027551312,0.0078466176,2.3820042817\C,0.9961004495,0.0044255629,1.1833612142\C,-1.
2374449234,-0.2096971297,0.3680032774\C,-1.3971266067,-0.4053119678,1.8543579722\C,-2.5109563908,0.4
816569625,2.423053797\C,0.3901216777,0.1563006332,-1.4267700446\O,1.7255404148,0.202426356,-1.6370

955689\C,-1.7225095222,-1.8793646695,2.1503749119\C,1.8988335258,1.2442542506,1.2276108173\C,1.8702499263,-1.2604980812,1.1705391286\O,-0.3984316766,0.2252000223,-2.3418779284\H,1.8540133323,0.2923847769,-2.5939411291\H,-2.0650602155,-0.2786880069,-0.334704019\H,0.3455572134,-0.6458995195,3.1922646307\H,-0.0574947979,1.0241011694,2.7893904167\H,2.446488111,1.2659268879,2.1765616235\H,1.3041116723,2.1611707795,1.1582389644\H,2.6247249319,1.2378359098,0.4111690755\H,2.5166543691,-1.2757380199,2.0550371601\H,2.5054288274,-1.2834453272,0.2806304302\H,1.2573918545,-2.1669946503,1.1796012546\H,-1.8224403211,-2.0318379745,3.2306092439\H,-0.9356789923,-2.5428298953,1.7806408389\H,-2.651048843,-2.173664212,1.676591407\H,-2.5558774809,0.3808467614,3.5130557679\H,-3.4869722716,0.1958676935,2.0163196751\H,-2.3340163584,1.5346539225,2.1832936354\Version=ES64L-G09RevD.01\State=1-A\HF=-540.9528925\RMSD=9.299e-09\RMSF=7.915e-06\Dipole=0.2642708,-0.1301884,0.7192401\Quadrupole=1.8279744,-0.3695168,-1.4584576,0.9460601,-5.1553555,0.0913521\PG=C01 [X(C10H16O2)]\@

Model p

CycloP.GOOD.retry1\1\GINC-R37\SP\RM062X\6-31+G(d,p)\C9H16O2\ROOT\17-Oct-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) NoSymm maxdisk=8GB\CycloP.GOOD.retry.freq\0,1\O\C,1,2.887395\C,2,1.548477,1,60.153\C,1,1.349426,2,63.83,3,8.106,0\C,1,1.429143,4,121.239,3,-5.659,0\C,5,1.524024,1,112.473,4,-35.363,0\C,6,1.529667,5,108.704,1,-178.845,0\O,4,1.205613,1,118.24,5,176.607,0\C,6,1.533407,5,110.428,1,-58.51,0\C,3,1.541419,4,105.342,1,-105.464,0\C,3,1.536293,4,107.621,1,138.665,0\H,5,1.094005,1,104.956.4,-156.942,0\H,5,1.098702,1,108.927,4,87.104,0\H,9,1.093861,6,112.613,5,57.103,0\H,9,1.095217,6,110.38,5,-62.853,0\H,9,1.09516,6,110.19,5,177.78,0\H,7,1.095456,6,111.362,5,-57.029,0\H,7,1.094876,6,110.304,5,-176.806,0\H,7,1.09533,6,111.039,5,63.67,0\H,10,1.09545,3,111.297,4,61.724,0\H,10,1.092759,3,110.474,4,-58.97,0\H,10,1.095048,3,109.348,4,-178.918,0\H,11,1.094245,3,111.456,4,-68.497,0\H,11,1.094819,3,109.077,4,172.242,0\H,11,1.091347,3,110.565,4,52.175,0\H,2,1.097395,6,110.05,5,-175.503,0\H,2,1.09802,6,107.556,5,68.954,0\Version=ES64L-G09RevD.01\HF=-502.8610949\RMSD=3.794e-09\Dipole=-1.1437106,0.2287374,1.455147\Quadrupole=-2.6334977,0.2218617,2.411636,1.4545936,1.9791791,-0.5027794\PG=C01 [X(C9H16O2)]\@

Model r

1\1\GINC-R37\SP\RM062X\6-31+G(d,p)\C9H18O1\ROOT\15-Jun-2017\0\#M062X\6-31+G(d,p) INT(grid=ultrafine) Nosymm maxdisk=12GB\CycloR.ext.retry.freq\0,1\O\C,1,2.829926\C,2,1.54354,1,59.77\C,1,1.41427,2,61.415,3,-30.237,0\C,1,1.414276,4,111.435,3,65.161,0\C,2,1.543553,3,116.352,4,45.471,0\C,6,1.531986,2,108.79,3,-163.481,0\C,6,1.534985,2,113.119,3,75.726,0\C,3,1.534987,2,113.118,6,-75.728,0\C,3,1.531992,2,108.79,6,163.479,0\H,5,1.104604,1,109.32,4,56.753,0\H,5,1.095325,1,106.543,4,173.562,0\H,4,1.095327,1,106.543,5,-173.564,0\H,4,1.104601,1,109.319,5,-56.755,0\H,2,1.099398,6,109.768,5,-170.859,0\H,2,1.100502,6,107.044,5,74.132,0\H,7,1.095955,6,110.941,2,177.072,0\H,7,1.095749,6,110.448,2,-63.528,0\H,7,1.095429,6,111.459,2,56.484,0\H,8,1.095864,6,109.887,2,166.329,0\H,8,1.090901,6,111.934,2,-74.35,0\H,8,1.095668,6,111.048,2,47.085,0\H,9,1.095862,3,109.888,2,-166.336,0\H,9,1.095668,3,111.047,2,-47.092,0\H,9,1.090903,3,111.935,2,74.342,0\H,10,1.095954,3,110.941,2,-177.08,0\H,10,1.09543,3,111.458,2,-56.492,0\H,10,1.095747,3,110.447,2,63.519,0\Version=ES64L-G09RevD.01\HF=-428.8464477\RMSD=9.606e-09\Dipole=-0.0341659,0.1850931,0.5209476\Quadrupole=1.0970307,-0.7915976,-0.3054332,0.360641,0.0178527,-0.0973893\PG=C01 [X(C9H18O1)]\@

Cation 1.1

1\1\GINC-R40\FOpt\RM062X\6-31+G(d,p)\C9H16N1O3(+)\ROOT\06-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide.1.freq\1,1\C,-0.6649605043,-1.2588687498,0.1511544165\N,0.5638563301,-0.3805937496,0.1487883294\C,0.2949539994,1.0762470474,0.445821511\C,-1.1597637426,1.0170141092,0.9177918896\C,-0.5523699748,-2.0736729372,1.4556084932\C,-0.6460768655,-2.1467801208,-1.0858840477\C,0.4597553659,1.7842962745,-0.9135075773\C,1.3084325571,1.5659177622,1.4725086235\H,-1.6846858013,1.9446104483,0.6818772079\H,-1.2187105746,0.8726920031,2.0008652437\H,-0.2440706155,1.4137076847,-1.6637088147\H,1.4807344725,1.6711980183,-1.2849815297\H,0.258887667,2.8455916108,-0.7494999356\H,1.2496573853,0.9834822804,2.3957957665\H,1.0678779298,2.6053974954,1.7083079356\H,2.3255882118,1.5254757736,1.0777104472\H,0.3611220712,-2.672246783,1.4454470028\H,-1.4112314358,-2.7485659321,1.4928503125\H,-0.5700343679,-1.4404312191,2.3468408562\H,-0.5984391649,-1.5498111298,-2.0008992171\H,-1.5778801963,-2.7169368141,-1.0947917153\H,0.1963204539,-2.8407145768,-1.0586656361\C,-1.7782801133,-0.1873269047,0.1968905128\C,-3.020461993,-0.7015585054,0.906687225\H,-2.066652689,0.0622165385,-0.8308523745\O,-3.4121319419,-0.2974254751,1.9670598657\O,-3.6021003463,-1.6808400929,0.2004672222\H,-4.4030813083,-1.975159035,0.6670216929\O,1.6432951912,-0.8023350211,-0.0689437059\Version=ES64L-G09RevD.01\State=1-A\HF=-632.4842042\RMSD=5.254e-09\RMSF=1.159e-05\Dipole=0.8866947,0.1622395,-0.6526013\Quadrupole=0.9773906,5.2680992,-6.2454898,7.605887,2.4339621,-1.5228205\PG=C01 [X(C9H16N1O3)]\@

Cation 1.2

1\1\GINC-R40\FOpt\RM062X\6-31+G(d,p)\C9H16N1O3(1+)\ROOT\06-Dec-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide.1b.freq\1,1\C,-0.6777774358,-1.25
69403101,0.1021927703\N,0.5413080507,-0.3709076561,0.0519975442\C,0.290735199,1.0660449519,0.4618
682125\C,-1.1658728851,0.9966377142,0.9355943016\C,-0.498987756,-2.0488451374,1.4176364107\C,-0.70
26336249,-2.1717284753,-1.1122237412\C,0.4644591402,1.8832062038,-0.8311835709\C,1.3155224527,1.45
23797558,1.523250411\H,-1.6905673779,1.9313075057,0.7320949665\H,-1.2131777539,0.817643016,2.0141
738338\H,-0.2540299395,1.5955052362,-1.6035507146\H,1.4789385376,1.7740349733,-1.2210388406\H,0.29
51105542,2.9321337547,-0.577535829\H,1.2506222813,0.7971402234,2.3960347903\H,1.0947270146,2.4734
690301,1.8437920106\H,2.330290119,1.4260278076,1.1210189295\H,0.4312350161,-2.6200275199,1.377159
4091\H,-1.3424316565,-2.7361804506,1.495607538\H,-0.4897012117,-1.4020303163,2.299200947\H,-0.7036
584586,-1.5970360842,-2.0427335034\H,-1.6260072985,-2.7533373865,-1.0560087291\H,0.14799915,-2.8559
200348,-1.108648376\C,-1.777392301,-0.1810062743,0.1576426809\C,-3.0934412679,-0.7028303875,0.70479
72722\H,-2.0021017317,0.1395412051,-0.8697276858\O,-3.4163878832,-1.8622861521,0.6947636161\O,-3.8
555457681,0.2968038493,1.151213924\H,-4.7123040859,-0.0610441139,1.4404750824\O,1.6049709206,-0.76
33549278,-0.2721836603\Version=ES64L-G09RevD.01\State=1-A\HF=-632.4840327\RMSD=6.383e-09\RM
SF=7.194e-06\Dipole=0.8216399,0.9732558,-0.012115\Quadrupole=2.5836161,-0.183161,-2.400455,0.818593
9,-1.3201105,0.3392997\PG=C01 [X(C9H16N1O3)]\@

Cation 1.3

1\1\GINC-R40\FOpt\RM062X\6-31+G(d,p)\C9H16N1O3(1+)\ROOT\06-Dec-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide.1c.freq\1,1\C,-0.8471834433,-1.22
07262463,-2.482064249\N,-1.5117145224,-2.4644812478,-1.9534463608\C,-3.0047667696,-2.5209434725,-2.
2036534417\C,-3.2835372113,-1.0971239945,-2.7264504189\C,-0.4868343731,-1.5366309679,-3.9516615376
\C,0.4075141994,-0.9178173669,-1.6762220571\C,-3.6943979787,-2.8840387145,-0.8837890089\C,-3.231323
0511,-3.6291155832,-3.2442298289\H,-4.1782429594,-0.6827629754,-2.2564215494\H,-3.4589399627,-1.114
0287562,-3.804472754\H,-3.5087841493,-2.1364973593,-0.1128508986\H,-3.3569883124,-3.8629940153,-0.5
365120179\H,-4.7668867905,-2.9402690742,-1.084613569\H,-2.6935886393,-3.4431238579,-4.1763141216\H,-
4.3013696678,-3.6524024237,-3.4649191672\H,-2.9393335936,-4.6012709006,-2.8408393715\H,0.144936892,-
2.4264161063,-4.007960637\H,0.0853557552,-0.6835704506,-4.3241210663\H,-1.3623128951,-1.6659039524,-
4.5894110663\H,0.2057663606,-0.8927031201,-0.6052628591\H,0.7820544486,0.0591417309,-1.9935296431\
H,1.1806294968,-1.6609643921,-1.8808791737\C,-2.0262627933,-0.2337560654,-2.4105131525\C,-2.1678378
919,0.3341180366,-1.0118306346\O,-0.9184217325,-3.3338664551,-1.4245595731\H,-1.9024413781,0.57066
65392,-3.1377756087\O,-2.0555862861,-0.3542708201,-0.0225876646\O,-2.4702438341,1.6250631868,-1.007
1047324\H,-2.5905389169,1.9284488246,-0.0904838365\Version=ES64L-G09RevD.01\State=1-A\HF=-632.4
853751\RMSD=6.563e-09\RMSF=1.046e-05\Dipole=-0.1900812,-0.1198799,-1.1282778\Quadrupole=1.49158
73,2.1320338,-3.6236211,2.9475767,-2.4383174,4.9085579\PG=C01 [X(C9H16N1O3)]\@

Nitroxide 1.1

1\1\GINC-R38\FOpt\UM062X\6-31+G(d,p)\C9H16N1O3(2)\ROOT\04-Dec-2017\0\#M062X\6-31+G(d,p) SC
F=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide.1.freq\0,2\C,-0.6347966131,-1.2582
101086,0.1768199338\N,0.5469738751,-0.3718032896,0.1120190369\C,0.2993503535,1.0590821528,0.39742
42284\C,-1.1565566428,1.024992624,0.8813439916\C,-0.5604653118,-2.0856424837,1.4652694195\C,-0.666
7103342,-2.1623598828,-1.0493486061\C,0.4707754506,1.8541402941,-0.9012361598\C,1.2779844743,1.545
3060914,1.4613868163\H,-1.6940778329,1.944671743,0.6358785757\H,-1.2023312421,0.8942119217,1.9671
040178\H,-0.264408863,1.5474377121,-1.6524246689\H,1.4711745414,1.6808924664,-1.30696585\H,0.34634
25403,2.9241506874,-0.7086719698\H,1.1921260519,0.9385259864,2.3675589323\H,1.0646061892,2.588242
4263,1.7142516168\H,2.3030343765,1.4702243621,1.0905582257\H,0.386908956,-2.6306325028,1.47646216
99\H,-1.3823479827,-2.8075257788,1.5063635785\H,-0.6083973112,-1.4487690701,2.3539997623\H,-0.6619
914142,-1.5645973268,-1.9658224792\H,-1.5678314286,-2.7806706463,-1.0329121214\H,0.2168517824,-2.80
50675599,-1.0531158938\C,-1.7715016512,-0.2020140793,0.1988095508\C,-3.0096628248,-0.704919244,0.89
75719522\H,-2.046947014,0.0204663315,-0.8390831155\O,-3.413032216,-0.3394211945,1.9738123476\O,-3.
6353071477,-1.6598593832,0.1779066905\H,-4.4077797396,-1.9488917029,0.6886362921\O,1.7075669786,-0.8
27380546,-0.1058362738\Version=ES64L-G09RevD.01\State=2-A\HF=-632.7465987\S2=0.755238\S2-1=0\ S
2A=0.750018\RMSD=8.631e-09\RMSF=1.219e-05\Dipole=-0.9195991,0.2026617,-0.2472091\Quadrupole=-3.
7100291,5.3208315,-1.6108024,5.490355,4.2726782,-1.9152245\PG=C01 [X(C9H16N1O3)]\@

Nitroxide 1.2

1\1\GINC-R51\FOpt\UM062X\6-31+G(d,p)\C9H16N1O3(2)\ROOT\04-Dec-2017\0\#M062X\6-31+G(d,p) SC
F=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide.1b.freq\0,2\C,-0.6503213741,-1.253

957997,0.1175637847\N,0.5213122478,-0.3564835362,-0.0059250653\C,0.2938073919,1.050392321,0.4031946491\C,-1.1673137119,1.0085505886,0.8796293995\C,-0.5190435743,-2.0558469494,1.4187565355\C,-0.7151347552,-2.1841477817,-1.0863824917\C,0.4848861621,1.9489204785,-0.8219682492\C,1.2747545732,1.4296335492,1.5090107999\H,-1.7017331459,1.9349786989,0.6580099901\H,-1.2113681438,0.8522056062,1.9627706533\H,-0.2568274014,1.7237089617,-1.5951945744\H,1.4808896498,1.7860664804,-1.2424639356\H,0.3862777861,3.0013904109,-0.5390311\H,1.1785913469,0.7479031526,2.3594319696\H,1.0740847672,2.449735048,1.8504469249\H,2.3000916392,1.3725326066,1.1362284801\H,0.4511340216,-2.559823,1.414740803\H,-1.3142572597,-2.8002375433,1.4917240173\H,-0.562308514,-1.4046408087,2.2985290327\H,-0.7485899284,-1.607741061,-2.0161215008\H,-1.6087049208,-2.8093279255,-1.0162994703\H,0.1739377249,-2.8189627951,-1.1085282625\C,-1.7748478029,-0.2008305942,0.1491506383\C,-3.0858458527,-0.6993688917,0.7037610335\H,-1.9963297298,0.0869176497,-0.8896754168\O,-3.4827517708,-1.8381309168,0.6509832604\O,-3.8214360106,0.294608544,1.2397724582\H,-4.6627846939,-0.0926484303,1.5283900339\O,1.6837312795,-0.8069958651,-0.2248243975\Version=ES64L-G09RevD.01\State=2-A\HF=-632.744731\S2=0.755189\S2-1=0.\S2A=0.750018\RMSD=7.220e-09\RMSF=3.730e-06\Dipole=-0.984075,1.0074008,0.3783878\Quadrupole=-2.7621087,0.1293737,2.632735,-0.4277692,0.5593776,-0.5424424\PG=C01 [X(C9H16N1O3)]\@

Nitroxide 1.3

1\1\GINC-R51\FOpt\UM062X\6-31+G(d,p)\C9H16N1O3(2)\ROOT\04-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide.1c.freq\0,2\C,-0.928368747,-1.2205349845,-2.4489026765\N,-1.533827872,-2.4867512255,-1.9864149878\C,-2.9924097114,-2.6119720941,-2.2187705667\C,-3.3679478293,-1.1962332291,-2.7050180821\C,-0.4083110213,-1.3992941695,-3.8814466574\C,0.2159926534,-0.8466402469,-1.5138618481\C,-3.6639272443,-3.0076133962,-0.9029206454\C,-3.245239769,-3.6826518237,-3.2826309704\H,-4.2628157741,-0.8284693454,-2.1976261804\H,-3.5712058283,-1.2125362987,-3.7798291661\H,-3.5264739771,-2.2290246445,-0.1504704103\H,-3.2263742021,-3.9428206617,-0.5426192462\H,-4.7356494701,-3.1600384865,-1.0654438692\H,-2.7286867283,-3.4416460457,-4.2168292681\H,-4.3181679668,-3.7558054435,-3.4855592402\H,-2.883271399,-4.6504664077,-2.9274966019\H,0.2809247995,-2.2475767783,-3.9088585705\H,0.1212437298,-0.4981549718,-4.204864284\H,-1.2261800046,-1.5916660538,-4.5827021464\H,-0.1278555312,-0.7836124953,-0.4771555719\H,0.6482022802,0.1134719851,-1.80636921\H,0.9822831617,-1.6232026607,-1.5673871508\C,-2.158590622,-0.2737581417,-2.4356801541\C,-2.2855559423,0.4605522442,-1.1200877851\O,-0.8134365315,-3.505153136,-1.7683581038\H,-2.0397987241,0.4832248439,-3.2156676952\O,-2.9412444799,0.1090955816,-0.1692089406\O,-1.5560999575,1.5939786004,-1.1093804687\H,-1.6584872914,1.9970594854,-0.232919502\Version=ES64L-G09RevD.01\State=2-A\HF=-632.7439177\S2=0.755139\S2-1=0.\S2A=0.750017\RMSD=5.989e-09\RMSF=1.873e-05\Dipole=-0.2842181,1.1479306,-0.7841636\Quadrupole=0.1749742,-0.7351175,0.5601432,4.5894057,1.883655,2.6807666\PG=C01 [X(C9H16N1O3)]\@

Cation 4b.1

1\1\GINC-R80\FOpt\RM062X\6-31+G(d,p)\C13H16N1O3(1+)\ROOT\05-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat9.freq\1,1\C,0.2154589158,0.4729129724,0.0272874792\C,0.6813730652,-0.840987297,0.0369462467\C,2.1848795105,-0.9222499443,0.0019829764\N,2.5259901304,0.555117672,-0.0297285566\C,1.3295012232,1.4859841834,-0.0156795444\C,-1.145634637,0.7477559627,0.0557280739\C,-2.0327340206,-0.3289958056,0.0942376922\C,-1.5679829143,-1.6476812629,0.1040017665\C,-0.2024554047,-1.9144421092,0.0753197274\C,1.3897930103,2.3161155445,-1.3047412321\C,1.4512057454,2.3565704104,1.2419810825\C,2.7610229228,-1.5445786208,-1.2768168468\C,2.8224472667,-1.504059485,1.2706717813\H,-1.5284602363,1.7639153797,0.0487964413\C,-3.516019833,-0.1182820301,0.1266460175\H,-2.2965947877,-2.4514194911,0.1343460672\H,0.1560478146,-2.9396119205,0.0829732142\H,1.3571229409,1.6785495976,-2.1913901767\H,2.2869419174,2.9392933693,-1.3209522076\H,0.5103232006,2.9643744749,-1.3176172183\H,1.4617905826,1.7474968381,2.1489658468\H,0.5728768744,3.005577411,1.2766354793\H,2.3476136249,2.9792657868,1.1951484635\H,2.3349218606,-1.0840849163,-2.1712834104\H,2.4918255238,-2.6034517236,-1.276287118\H,3.8500069488,-1.4582894547,-1.2903827576\H,2.4395873357,-1.0150435758,2.1695425149\H,3.9107539112,-1.4182192384,1.2290006157\H,2.5543445759,-2.5622070278,1.3167654413\O,-4.3152437781,-1.0170774478,0.160205094\O,-3.848254711,1.181741436,0.1139811892\H,-4.8167163467,1.2456881891,0.136310598\O,3.6360477677,0.9486621229,-0.0628347404\Version=ES64L-G09RevD.01\State=1-A\HF=-784.8644807\RMSD=5.569e-09\RMSF=1.627e-05\Dipole=2.6001526,0.6851207,-0.0735645\Quadrupole=5.4736482,3.4902851,-8.9639332,-8.1856588,-0.2179134,-0.0006977\PG=C01 [X(C13H16N1O3)]\@

Cation 4b.2

1\1\GINC-R44\FOpt\RM062X\6-31+G(d,p)\C13H16N1O3(1+)\ROOT\06-Dec-2017\0\#M062X/6-31+G(d,p) SCF=XQC INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat9.b.freq\1,1\C,-0.0577151097,0.432760

9534,0.0014349655\C,-0.4204907878,-0.914730897,0.0018884811\C,-1.9138503431,-1.1103885604,0.002188
8342\N,-2.3677724046,0.3371065537,0.0018389784\C,-1.2466653274,1.3570234129,0.0013579229\C,1.27655
01283,0.8084546691,0.0011078045\C,2.2465879896,-0.1952768927,0.0012437437\C,1.888306903,-1.5462434
736,0.0016975449\C,0.5439535789,-1.9153520421,0.0020244202\C,-1.4018539655,2.1988983636,1.27506305
71\C,-1.4022686826,2.1981525027,-1.2727893078\C,-2.4733472913,-1.7566281534,1.2766690099\C,-2.47376
20975,-1.7573741745,-1.2717305539\H,1.5976108252,1.8469624186,0.0007515312\C,3.6789180651,0.246355
6783,0.0008813175\H,2.6653660968,-2.3023910287,0.0017924174\H,0.2657924163,-2.9652362696,0.002377
041\H,-1.3424925953,1.5784755241,2.1724218251\H,-2.3439197806,2.7517146474,1.2592645022\H,-0.57424
42806,2.9119970237,1.2976131306\H,-1.3431993849,1.5772043763,-2.1698039526\H,-0.5746664505,2.91123
7759,-1.2960263047\H,-2.3443293574,2.7509780312,-1.2570077379\H,-2.1051118726,-1.252887911,2.17350
07556\H,-2.1256790517,-2.7921748358,1.2990626412\H,-3.5656760627,-1.7521336773,1.2625226857\H,-2.1
058187032,-1.2541591325,-2.1689769055\H,-3.5660862062,-1.7528713127,-1.2572312649\H,-2.1261010678,-
2.7929338237,-1.2936310669\O,4.0126094246,1.4042646428,0.0004880347\O,4.5333473901,-0.7831067003,
0.0010436069\H,5.4376823658,-0.4300263748,0.000793046\O,-3.5054993285,0.6436998608,0.0019344152\|
Version=ES64L-G09RevD.01\State=1-A\HF=-784.8653439\RMSD=7.447e-09\RMSF=8.725e-05\Dipole=-2.3
472467,-0.566778,0.000548\Quadrupole=9.7449737,0.3935614,-10.138535,-3.9178759,-0.0020895,-0.0024455
\PG=CS [SG(C9H4N1O3),X(C4H12)]\@

Nitroxide 4b.1

1\1\GINC-R48\FOpt\UM062X\6-31+G(d,p)\C13H16N1O3(2)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide9.freq\0,2\C,0.2266069113,0.4783
73512,0.0255544579\C,0.6929733118,-0.8377872955,0.0350398024\C,2.200112542,-0.8943685787,-0.002498
6189\N,2.5193930614,0.5517525119,-0.034273797\C,1.3602574619,1.4742097904,-0.0195476919\C,-1.13519
32956,0.7470261766,0.055942373\C,-2.0279390645,-0.3285595061,0.0962059088\C,-1.5621898442,-1.64786
3027,0.1057591017\C,-0.1957931954,-1.9086270879,0.0751230673\C,1.365091069,2.3200050134,-1.2955148
496\C,1.4295752644,2.3607886069,1.2265127796\C,2.7419354693,-1.564683269,-1.267991015\C,2.80630741
92,-1.5234743853,1.2549273001\H,-1.5125343579,1.7651858528,0.0490260625\C,-3.5002456197,-0.1161954
314,0.1303287007\H,-2.2891487295,-2.4527629493,0.1373902286\H,0.1671382417,-2.9327427581,0.0825011
006\H,1.3033313092,1.6820359586,-2.1813102961\H,2.2901448145,2.9008774314,-1.3401606277\H,0.51268
87168,3.0058756067,-1.2962527537\H,1.413717174,1.7518225693,2.1344576482\H,0.5777360323,3.0470013
08,1.2486619057\H,2.3552050435,2.9420616231,1.2050307717\H,2.2928613729,-1.1222603741,-2.16129852
79\H,2.5170843253,-2.6352460828,-1.254354798\H,3.8257756509,-1.4283914498,-1.310884018\H,2.4030170
985,-1.0517381431,2.1550539067\H,3.8908138281,-1.3867824043,1.2380222182\H,2.5819176711,-2.5937178
933,1.2877398351\O,-4.3237030675,-1.0002761005,0.1657123395\O,-3.8466709756,1.1873844248,0.1179910
838\H,-4.8148113345,1.2226467063,0.1421276792\O,3.7113456954,0.9731896437,-0.0714612776\|Version=E
S64L-G09RevD.01\State=2-A\HF=-785.1293564\S2=0.755263\S2-1=0.\S2A=0.750018\RMSD=7.282e-09\RM
SF=2.288e-06\Dipole=-0.3922242,0.0574865,0.0091571\Quadrupole=-9.0226728,7.0520086,1.9706641,-11.17
75593,0.4630448,0.2030565\PG=C01 [X(C13H16N1O3)]\@

Nitroxide 4b.2

1\1\GINC-R44\FOpt\UM062X\6-31+G(d,p)\C13H16N1O3(2)\ROOT\06-Dec-2017\0\#M062X\6-31+G(d,p) S
CF=XQC INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide9.b.freq\0,2\C,0.0613450343,0.440
4342612,0.0004132457\C,0.4258444574,-0.9085893181,0.0003164349\C,1.9249009541,-1.0795433241,0.0003
147667\N,2.3537253724,0.3380082969,0.0004275854\C,1.26866838,1.3466921657,0.0004894562\C,-1.27560
47597,0.8089172333,0.000429205\C,-2.2492659561,-0.1943839003,0.0003491444\C,-1.8873505335,-1.54611
26005,0.0002503091\C,-0.5420912831,-1.9077669071,0.0002352096\C,1.3714330715,2.2076557912,-1.26107
36743\C,1.3714101996,2.2074760436,1.2621768151\C,2.4477543009,-1.7711482181,-1.2617791401\C,2.4477
354253,-1.7713431856,1.2623094624\H,-1.5905777521,1.8489965572,0.0005046193\C,-3.6753439535,0.2306
739299,0.0003756133\H,-2.6621632854,-2.3045126132,0.0001885144\H,-0.2582892194,-2.9566519065,0.000
1603351\H,1.2860257432,1.5888901982,-2.1584839797\H,2.3383306331,2.7176491026,-1.272109466\H,0.57
28813259,2.955314566,-1.272474972\H,1.2859889215,1.5885824452,2.1594975196\H,0.5728571733,2.95513
20155,1.2736711648\H,2.338306637,2.7174695465,1.2733020594\H,2.0575450957,-1.2830347736,-2.158939
5853\H,2.1419070731,-2.821529316,-1.2711065497\H,3.5395549631,-1.7173971445,-1.2748026615\H,2.0575
100922,-1.283370096,2.1595392483\H,3.5395357528,-1.717591504,1.2753590742\H,2.1418908965,-2.821726
5348,1.2714683342\O,-4.0495694718,1.3803448143,0.0003527325\O,-4.5381044251,-0.8051037498,0.000162
4184\H,-5.4317303881,-0.4297748414,0.0000997823\O,3.5755195249,0.6665829663,0.0004569785\|Version=
ES64L-G09RevD.01\State=2-A\HF=-785.1294491\S2=0.755268\S2-1=0.\S2A=0.750018\RMSD=3.811e-09\RM
SF=8.507e-05\Dipole=-0.6724516,-0.951452,-0.0000531\Quadrupole=-5.447639,4.5243451,0.9232939,1.779
3883,0.0001197,0.0004076\PG=C01 [X(C13H16N1O3)]\@

Cation 4c.1

I\1\GINC-R51\FOpt\RM062X\6-31+G(d,p)\C14H16N1O5(1+)\ROOT\05-Dec-2017\0\#M062X/6-31+G(d,p)
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat10.a.freq\1,1\C,-0.9366186754,-0.6973
605543,0.0000691129\C,-0.9363694847,0.6958108298,0.0273947274\C,-2.3250363797,1.2784150475,0.02800
17437\N,-3.1408531967,0.0001337266,-0.0127353687\C,-2.325354539,-1.2788361082,-0.033534346\C,0.2552
567314,-1.4065012776,0.0137083224\C,1.4601917925,-0.702938161,0.0489726785\C,1.4609283419,0.699437
6727,0.0349584409\C,0.2560711836,1.4039826764,0.041785657\C,-2.6737921251,-2.0149924833,-1.3342606
125\C,-2.7138257108,-2.0835231436,1.213463346\C,-2.6829695712,2.083911423,-1.2275902849\C,-2.703760
0472,2.0143974879,1.3203434986\H,0.2854448598,-2.4928567879,0.0041622337\C,2.6989192503,-1.5479345
699,0.1720858657\C,2.7028902487,1.5434252227,-0.0589323333\H,0.2869180608,2.4903137702,0.05190724
73\H,-2.4419907987,-1.4066593746,-2.2116838721\H,-3.7275131245,-2.3030378692,-1.3424707954\H,-2.060
3269477,-2.9183596485,-1.3735310785\H,-2.505019427,-1.5261029281,2.1296277618\H,-2.1071304572,-2.99
22059492,1.219183288\H,-3.768566182,-2.3654324449,1.1757954883\H,-2.4528658173,1.5265334282,-2.138
6746365\H,-2.0755994484,2.9920983208,-1.2185930881\H,-3.7380892432,2.3666297021,-1.2149311989\H,-2.4
933600046,1.4057111982,2.2028923355\H,-3.7571316284,2.3033436018,1.3036188605\H,-2.090635075,2.91
72508344,1.3744008914\O,2.8121110834,-2.61998355,-0.3628910231\O,3.5927226872,-1.0160607082,1.0097
305648\H,4.3617814146,-1.6076403403,1.0549842696\O,2.8041603777,2.6155444254,0.4782937751\O,3.615
9293605,1.0106308618,-0.8749571209\H,4.3862829737,1.6016313918,-0.9021022869\O,-4.3187504824,0.000
6142777,-0.0269220631\Version=ES64L-G09RevD.01\State=1-A\HF=-973.3705299\RMSD=5.602e-09\RMS
F=1.382e-05\Dipole=-3.1602851,0.001228,-0.0370889\Quadrupole=20.313473,-7.0420372,-13.2714358,0.0550
57,0.3939849,-5.5909587\PG=C01 [X(C14H16N1O5)]\@

Cation 4c.2

I\1\GINC-R51\FOpt\RM062X\6-31+G(d,p)\C14H16N1O5(1+)\ROOT\05-Dec-2017\0\#M062X/6-31+G(d,p)
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat10.b.freq\1,1\C,0.9286079798,0.692205
7728,0.031273552\C,0.9300109702,-0.7004277776,0.0206085752\C,2.3187810246,-1.2819254068,-0.0025723
487\N,3.1339417423,-0.0032185042,0.0071708649\C,2.3175144653,1.2751913374,0.0261933779\C,-0.265236
2534,1.4009986024,0.0287166885\C,-1.4681943262,0.6925565872,0.023508741\C,-1.4654324051,-0.7101896
839,0.046497296\C,-0.2614000529,-1.4122517745,0.0278490404\C,2.6783153726,2.0596245281,-1.24206313
3\C,2.6950951444,2.0320591418,1.3065084016\C,2.6703713622,-2.0309135146,-1.2954640282\C,2.70353015
33,-2.0746382017,1.253160507\H,-0.2875811983,2.4866979863,0.0146338235\C,-2.7591112439,1.439664078,-
0.1498027195\C,-2.7141522383,-1.5514770055,0.1176946083\H,-0.2859536637,-2.4986909173,0.0172630606
\H,2.4491562277,1.4874334197,-2.1441398626\H,3.7336141666,2.341903802,-1.2324666087\H,2.071640936,
2.9682674331,-1.2494684913\H,2.4828557083,1.4380021965,2.1985413286\H,2.083156851,2.9364597021,1.3
447546761\H,3.7487403033,2.3198954128,1.2870154138\H,2.4401185785,-1.4315014245,-2.1793856573\H,2.0
572576573,-2.9347844005,-1.3273461692\H,3.7242150274,-2.3186515835,-1.2982163358\H,2.4922431175,-1.5
082676956,2.1632516893\H,3.7582721482,-2.3572197165,1.2212167529\H,2.0965525664,-2.9830282237,1.2
660160225\O,-3.7227831436,0.9803505999,-0.7016320629\O,-2.6837228824,2.6909306438,0.3260073992\H,-
3.5310145705,3.1316617301,0.1499283368\O,-2.8719737973,-2.5296321015,-0.5641496557\O,-3.5395740186,-
1.1456833637,1.0835095153\H,-4.3354968445,-1.7021078041,1.0631952726\O,4.311975136,-0.0023438743,0.0
00421289\Version=ES64L-G09RevD.01\State=1-A\HF=-973.3700545\RMSD=4.348e-09\RMSF=1.345e-05\
Dipole=3.6135932,0.7983807,0.6043751\Quadrupole=11.6591202,2.4850514,-14.1441716,-5.6167452,-6.3021
581,-3.5144457\PG=C01 [X(C14H16N1O5)]\@

Cation 4c.3

I\1\GINC-R48\FOpt\RM062X\6-31+G(d,p)\C14H16N1O5(1+)\ROOT\05-Dec-2017\0\#M062X/6-31+G(d,p)
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat10.c.freq\1,1\C,0.9333247133,0.679886
7472,0.0011496609\C,0.944453157,-0.7118094022,-0.0039607801\C,2.3378681222,-1.2833876559,-0.002414
2058\N,3.1435665875,0.0016203517,0.0089136645\C,2.317404451,1.2736056007,0.0125266304\C,-0.265716
4289,1.3820903252,-0.0109668111\C,-1.4615747267,0.6662890314,-0.0250583545\C,-1.450500749,-0.736392
314,-0.0000351823\C,-0.2433028151,-1.433037314,-0.0029397553\C,2.6890505917,2.0569894014,-1.2531951
862\C,2.6713919055,2.037312944,1.2956697691\C,2.7159290251,-2.0411335442,-1.282203378\C,2.71018967
73,-2.060920416,1.2667188588\H,-0.2939272074,2.4679894639,-0.0197407355\C,-2.7537427917,1.41404487
11,-0.2112067904\C,-2.7322683362,-1.5046494468,0.174131516\H,-0.254290959,-2.5192482975,0.005689597
9\H,2.4768471613,1.4801315737,-2.1564607026\H,3.7417589584,2.3480130153,-1.2301805712\H,2.0751056
501,2.960570698,-1.2718627524\H,2.4509993624,1.4445449798,2.1865784089\H,2.0522930587,2.937223287,
1.3227038315\H,3.7230388783,2.3329763408,1.2896696875\H,2.4944367047,-1.451837189,-2.1751373028\H,2
.1115076439,-2.9507803931,-1.3149916399\H,3.7720466489,-2.3200360649,-1.2664181262\H,2.4803938089,
-1.4876299156,2.1679517319\H,3.7675864317,-2.3350629781,1.2535014594\H,2.1106285394,-2.9742062601,
1.2797062799\O,-3.6299575377,1.0445626676,-0.9439056256\O,-2.7623048158,2.5671403157,0.4709019787\

H,-3.6044362799,3.0169921634,0.2915683452\O,-3.6211561085,-1.1491109042,0.898413701\O,-2.715970537
5,-2.657834176,-0.5076930501\H,-3.552466087,-3.1210512573,-0.3361820801\O,4.3215443032,0.011003751
2,0.0144579084\Version=ES64L-G09RevD.01\State=1-A\HF=-973.3685333\RMSD=5.893e-09\RMSF=5.813
e-06\Dipole=3.9449996,0.0313965,0.0184399\Quadrupole=5.1193667,10.2357408,-15.3551075,-0.0416269,0.0
916874,0.2749528\PG=C01 [X(C14H16N1O5)]\@

Nitroxide 4c.1

1\1\GINC-R60\FOpt\UM062X\6-31+G(d,p)\C14H16N1O5(2)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide10.a.freq\0,2\C,-0.9503152559,-0.6
980054271,-0.005224994\C,-0.950257677,0.6964633257,0.0316175131\C,-2.3508620255,1.2567747399,0.02
94793741\N,-3.1347502301,0.0000640231,-0.0149140618\C,-2.3509392001,-1.2572471553,-0.0391214056\C,
0.2456927528,-1.4038210634,0.0044581867\C,1.4524755134,-0.7039245895,0.0440303716\C,1.4530081267,0.7
005380901,0.0445101549\C,0.2461426248,1.4013603117,0.0528717106\C,-2.6545721214,-2.0262344229,-1.3
276397745\C,-2.6909875098,-2.0956528114,1.1958435583\C,-2.6584045061,2.095518074,-1.2137326194\C,-
2.6869426026,2.0259098762,1.3098481623\H,0.2699733187,-2.4901898961,-0.0034326334\C,2.688699907,-1.5
339985824,0.1820886191\C,2.6930255797,1.5296649446,-0.0615112215\H,0.2710435539,2.4877102167,0.06
13948809\H,-2.397632506,-1.4267094708,-2.205055421\H,-3.7209535038,-2.2643411761,-1.3605663972\H,-2.0
79615751,-2.9564200736,-1.3567765389\H,-2.4556847641,-1.5472826559,2.1120160864\H,-2.1211991962,-3.
0294617864,1.1872472465\H,-3.7587077421,-2.3298211,1.1870787774\H,-2.4000703982,1.5470535295,-2.12
3622786\H,-2.0883264335,3.028898693,-1.1904396352\H,-3.725820345,2.330513539,-1.2323963228\H,-2.45
30964779,1.4261005004,2.1935052331\H,-3.7536296569,2.2648388455,1.3153602834\H,-2.112183331,2.955
6339725,1.3538164535\O,2.8451224136,-2.6095043208,-0.3421344837\O,3.5788176995,-0.9983597173,1.035
2618054\H,4.3431017439,-1.5942930417,1.0672671369\O,2.8366471202,2.6050628774,0.4665832975\O,3.60
45214566,0.9933269671,-0.8913524714\H,4.3698309291,1.5886781585,-0.9035679177\O,-4.3991015052,0.00
05466059,-0.0312201675\Version=ES64L-G09RevD.01\State=2-A\HF=-973.6383667\S2=0.755259\S2-1=0.\S
2A=0.750018\RMSD=4.468e-09\RMSF=3.825e-06\Dipole=0.7125086,-0.000273,0.0092015\Quadrupole=-0.84
63135,-0.0694905,0.915804,0.071808,-0.0242991,-5.5260578\PG=C01 [X(C14H16N1O5)]\@

Nitroxide 4c.2

1\1\GINC-R60\FOpt\UM062X\6-31+G(d,p)\C14H16N1O5(2)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide10.b.freq\0,2\C,0.9411627142,0.69
13969063,0.0330139972\C,0.9428383013,-0.702843736,0.0142629455\C,2.3439636689,-1.26099442,-0.00313
13048\N,3.1268693858,-0.0034452644,0.0389447033\C,2.3415563977,1.253192925,0.0316865917\C,-0.25592
09034,1.3958637356,0.0328229265\C,-1.4621833367,0.6913056757,0.0260266308\C,-1.4587298525,-0.71301
55892,0.0366936236\C,-0.2528118865,-1.4114054788,0.0144936411\C,2.6638711214,2.0513033085,-1.23472
01739\C,-2.6632742001,2.0634105963,1.2896918275\C,2.6634343937,-2.0227745451,-1.2925879993\C,2.6692
434771,-2.1059036451,1.230928108\H,-0.2727395138,2.481503366,0.0187515593\C,-2.74630783,1.43354165
88,-0.1353791671\C,-2.705535325,-1.5408907932,0.1276870647\H,-0.2712012572,-2.4979260268,0.00573624
45\H,2.4177620647,1.4731293555,-2.1294610965\H,3.7309673428,2.2880813456,-1.2479415005\H,2.091460
3648,2.9835089182,-1.2495040146\H,2.4178650565,1.4927853341,2.1893825513\H,2.089844227,2.99510497
43,1.2961257774\H,3.7300940985,2.3017630321,1.300653295\H,2.4174004902,-1.4185927632,-2.169932057
8\H,2.0883885694,-2.9523698293,-1.3343097346\H,3.7301060841,-2.2608340804,-1.3134482516\H,2.420796
3076,-1.5632173998,2.1469875016\H,3.737477648,-2.3379794791,1.2347420383\H,2.1019899972,-3.0410304
326,1.2093966387\O,-3.7409929997,0.9809778633,-0.6466280513\O,-2.6700268982,2.7041722932,0.3059186
323\H,-3.5248513346,3.1212257548,0.1183416142\O,-2.921427844,-2.5077287938,-0.5595530645\O,-3.5046
345237,-1.1541972253,1.134115669\H,-4.2997676316,-1.7084717675,1.1031172059\O,4.3911052258,-0.0016
957739,0.0149256291\Version=ES64L-G09RevD.01\State=2-A\HF=-973.6383375\S2=0.755256\S2-1=0.\S2A
=0.750018\RMSD=7.245e-09\RMSF=2.993e-06\Dipole=-0.2586299,0.7764099,0.5808705\Quadrupole=-9.384
1802,9.236899,0.1472812,-5.6095968,-5.970388,-3.6093853\PG=C01 [X(C14H16N1O5)]\@

Nitroxide 4c.3

1\1\GINC-R60\FOpt\UM062X\6-31+G(d,p)\C14H16N1O5(2)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) S
CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide10.c.freq\0,2\C,0.9451466344,0.68
08630002,0.0041377232\C,0.9562547601,-0.7125975775,-0.0077450811\C,2.3613906959,-1.2618709986,-0.0
06893488\N,3.1354586535,0.001477722,0.0059135034\C,2.3413593831,1.2523797533,0.0138002957\C,-0.25
74387798,1.3785003736,-0.0029410687\C,-1.4569848908,0.6669694855,-0.0181384538\C,-1.4458971476,-0.7
368253638,-0.0026895212\C,-0.235135879,-1.4292305327,-0.009241833\C,2.6629751673,2.0698760468,-1.23
99444156\C,2.6515141082,2.0480113751,1.2845367075\C,2.6934907638,-2.053236476,-1.2746633452\C,2.68
66604387,-2.0734179926,1.2498535906\H,-0.2806753242,2.4644238517,-0.0130396282\C,-2.7388006079,1.4
164127675,-0.2011086011\C,-2.7168895079,-1.5066002319,0.1712518795\H,-0.2412295132,-2.5153876331,0.

0007182511\H,2.4232250718,1.5026124107,-2.1433403426\H,3.7287411833,2.3129817394,-1.2461402081\H,2.08571825,2.9991734752,-1.2437447209\H,2.4069835927,1.4635527972,2.1755414687\H,2.0701599416,2.9745843263,1.3013472077\H,3.716336462,2.2945652151,1.3029092591\H,2.4463713707,-1.4732966538,-2.1679141837\H,2.1270589664,-2.9889443772,-1.2952063154\H,3.7621880064,-2.2829763234,-1.2850368687\H,2.4312025262,-1.5094470201,2.1509914349\H,3.7560862881,-2.2994564471,1.2640609027\H,2.1242204108,-3.0117573788,1.249986028\O,-3.6407035384,1.0639118331,-0.9175462875\O,-2.746407879,2.5843383581,0.4690296892\H,-3.5863760264,3.0235569108,0.2639729614\O,-3.6291040306,-1.1688376766,0.8817028467\O,-2.7013812697,-2.6741716858,-0.4993586291\H,-3.5356393338,-3.1267829532,-0.3001858547\O,4.3998710535,0.0115058809,0.010825097\Version=ES64L-G09RevD.01\State=2-A\HF=-973.6370577\S2=0.755257\S2-1=0.\S2A=0.750018\RMSD=7.839e-09\RMSF=8.447e-06\Dipole=0.0606046,0.0006262,0.000196\Quadrupole=-15.5881277,16.6724983,-1.0843706,-0.2576448,-0.0495127,0.0257815\PG=C01 [X(C14H16N1O5)]\@

Cation 4d.1

1\1\GINC-R51\FOpt\RM062X\6-31+G(d,p)\C12H16N1O2(1+)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat11.a.freq\1,1\C,-0.0379694767,-0.8319286031,0.0452090151\C,0.3521505845,0.5067460748,0.0419281992\C,-0.8210261802,1.4501268032,-0.002069436\N,-1.9594987385,0.4488754436,-0.0239041045\C,-1.5326154555,-1.0070163482,0.0041017326\C,0.9233921422,-1.835898574,0.0836995879\C,2.2688327931,-1.4855133818,0.118628358\C,2.651651402,-0.1367686478,0.1150324439\C,1.686406018,0.8758191801,0.076278369\C,-2.0722977312,-1.6552741324,-1.2776403834\C,-2.1454884561,-1.6278222862,1.2663807852\C,-0.9265279202,2.2792285741,-1.2885088791\C,-0.9997175538,2.3069739418,1.2578325187\H,0.6416427407,-2.8850750791,0.0869765511\H,2.0114892136,1.9116732286,0.0743770263\H,-1.6745284036,-1.1646830627,-2.1690848205\H,-3.1646200094,-1.6377239807,-1.2924410626\H,-1.7375775341,-2.6954058392,-1.2831327203\H,-1.7992581453,-1.1179138823,2.1684271294\H,-1.812345132,-2.6674110812,1.3135039775\H,-3.2368436662,-1.6105894588,1.2180042401\H,-0.8489448536,1.6474756989,-2.176490367\H,-0.0894190556,2.9812006417,-1.2949954666\H,-1.8611188374,2.8446504208,-1.3079521828\H,-0.9736539909,1.6947375709,2.1623341439\H,-1.9335179886,2.8721139182,1.2112513553\H,-0.1639172356,3.0094410247,1.2971041026\H,3.028716306,-2.2608119439,0.1489200154\O,3.9374646114,0.2621914438,0.1478408332\H,4.546110161,-0.4867155893,0.1722192092\O,-3.0904896079,0.7775179254,-0.0599001707\Version=ES64L-G09RevD.01\State=1-A\HF=-671.5508847\RMSD=4.000e-09\RMSF=2.890e-06\Dipole=-0.8501478,-0.3841089,-0.0211883\Quadrupole=5.7197683,4.2974726,-10.0172409,-4.3725917,0.4923285,-0.2802314\PG=C01 [X(C12H16N1O2)]\@

Cation 4d.2

1\1\GINC-R48\FOpt\RM062X\6-31+G(d,p)\C12H16N1O2(1+)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat11.b.freq\1,1\C,-0.0373624647,-0.8152625112,0.0412775685\C,0.3432276778,0.521676855,0.0364248727\C,-0.8357937531,1.4587215136,-0.0044471335\N,-1.9679441535,0.4492699124,-0.0226439907\C,-1.5304428551,-1.0025121137,0.0044986617\C,0.9315882047,-1.8179197079,0.0774743913\C,2.2704480003,-1.4624633263,0.1082548724\C,2.648678861,-0.1098524239,0.103166994\C,1.681170547,0.8985137572,0.0670080485\C,-2.0679005945,-1.6560672975,-1.2755996797\C,-2.1341431879,-1.6287112822,1.2685619035\C,-0.9529815208,2.2863753889,-1.2907385831\C,-1.0188647822,2.3144780648,1.2554653196\H,0.6527821838,-2.8678724901,0.0817858713\H,1.9745952591,1.9455264934,0.0631464793\H,-1.6773394752,-1.1620467379,-2.1683368819\H,-3.1603761606,-1.6491867067,-1.2870643963\H,-1.7229370569,-2.6928461151,-1.2817917862\H,-1.7904176004,-1.1153886743,2.169635601\H,-1.7904610988,-2.6648981804,1.3150329284\H,-3.2257304689,-1.6223164527,1.22300448\H,-0.8708553936,1.6551368618,-2.1786565996\H,-0.1247975737,2.998816043,-1.30027422\H,-1.8936834768,2.8417115571,-1.3083517718\H,-0.9832167402,1.7030544057,2.1601736049\H,-1.9588467187,2.8696241141,1.212151535\H,-0.1918063469,3.027354341,1.2921501224\H,3.0528392417,-2.2125410062,0.1368020003\O,3.9715676702,0.1396187481,0.1348442073\H,4.16458416,1.0850668867,0.1287529697\O,-3.1008523857,0.7713600835,-0.0554073888\Version=ES64L-G09RevD.01\State=1-A\HF=-671.5493637\RMSD=6.849e-09\RMSF=7.185e-06\Dipole=-1.1313971,0.665705,-0.0372608\Quadrupole=1.8180782,7.0046291,-8.8227072,5.9555777,0.2070398,-0.0203515\PG=C01 [X(C12H16N1O2)]\@

Nitroxide 4d.1

1\1\GINC-R68\FOpt\UM062X\6-31+G(d,p)\C12H16N1O2(2)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat11.a.freq\0,2\C,-0.0490047214,-0.8281800507,0.0393083086\C,0.3399125438,0.5129148665,0.0349552103\C,-0.8527409218,1.4372298874,-0.0059459535\N,-1.9550855847,0.4475409213,-0.024330527\C,-1.5505513612,-0.9780029972,0.0019350739\C,0.9137982309,-1.8285554943,0.0751088806\C,2.2638571308,-1.4800954582,0.1064312794\C,2.64133876,-0.1341543627,0.1017449681\C,1.6785443056,0.876255188,0.0658274315\C,-2.0577365387,-1.6723204465,-1.2647801802\C,-2.1231915137,-1.6444956252,1.2556457757\C,-0.9093796153,2.2864858772,-1.2783635642\C,-0.

9751999633,2.3129751202,1.243710281\H,0.6283160621,-2.8773667129,0.0789834811\H,2.0000392346,1.9136396783,0.0629919548\H,-1.6399010307,-1.197587448,-2.1566703303\H,-3.1484037842,-1.606092731,-1.3043341424\H,-1.7648373839,-2.7267035816,-1.258744134\H,-1.7519254175,-1.1499734441,2.1573307021\H,-1.8309631614,-2.6985819999,1.2880629328\H,-3.2144006595,-1.578022451,1.2370658035\H,-0.8074116794,1.6565198355,-2.1661820251\H,-0.1007516508,3.0234047162,-1.2759550823\H,-1.86877874,2.8090043652,-1.3215451161\H,-0.9200171106,1.7018279447,2.1486572303\H,-1.935259586,2.8357540121,1.2258061789\H,-0.167122517,3.0500986839,1.2680016717\H,3.0269674201,-2.2539278793,0.1345758151\O,3.9473060661,0.2566228554,0.1314088979\H,4.5247315007,-0.5145945095,0.1549554179\O,-3.1698683136,0.7993512401,-0.0594862401\Version=ES64L-G09RevD.01\State=2-A\HF=-671.808714\S2=0.755269\S2-1=0.\S2A=0.750018\RMSD=3.703e-09\RMSF=2.652e-06\Dipole=1.2775419,-0.8625669,0.0428962\Quadrupole=-3.9646191,5.6718396,-1.7072205,-2.30241,-0.0336459,-0.1391035\PG=C01 [X(C12H16N1O2)]\@

Nitroxide 4d.2

1\1\GINC-R68\FOpt\UM062X\6-31+G(d,p)\C12H16N1O2(2)\ROOT\05-Dec-2017\0\#M062X/6-31+G(d,p) S CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide11.b.freq\0,2\C,-0.0491153653,-0.8162487643,0.041676429\C,0.3311277113,0.5234748298,0.0367342547\C,-0.8649020013,1.4433684793,-0.0063885274\N,-1.9621276757,0.4484162192,-0.024884432\C,-1.5496838382,-0.974943514,0.0025535125\C,0.9214189413,-1.8140574768,0.0795614488\C,2.26696339,-1.4634137392,0.1122681939\C,2.6386982235,-0.1150068067,0.1069795036\C,1.6721919797,0.8910641767,0.0691081144\C,-2.0509685466,-1.6729462251,-1.2644219298\C,-2.1197476475,-1.6442803384,1.2558460437\C,-0.9258207283,2.2911697561,-1.2797501256\C,-0.9945273102,2.3200093375,1.2420839494\H,0.6382990986,-2.8635499063,0.0838428455\H,1.9667362801,1.9391616813,0.0651593697\H,-1.6355290807,-1.1957400188,-2.156117252\H,-3.1420515455,-1.6146412447,-1.3050605048\H,-1.7504419067,-2.7251027869,-1.2577694999\H,-1.7532074588,-1.1467128934,2.1577936296\H,-1.8200351376,-2.6961518601,1.289483266\H,-3.2113843207,-1.5856696054,1.2356072452\H,-0.8173132608,1.6612406727,-2.1667680422\H,-0.1239662392,3.0357852622,-1.2770912233\H,-1.8892662906,2.8060101929,-1.3250813646\H,-0.934838809,1.7105628501,2.1478398336\H,-1.9587097647,2.8351184555,1.2231220038\H,-0.1932762764,3.0648913334,1.2660657255\H,3.0483263787,-2.2148795064,0.1421873578\O,3.9745600389,0.1557806981,0.1403483302\H,4.1215389461,1.1081909735,0.1333961218\O,-3.1781877844,0.7955197681,-0.0620242772\Version=ES64L-G09RevD.01\State=2-A\HF=-671.8085599\S2=0.755266\S2-1=0.\S2A=0.750018\RMSD=8.163e-09\RMSF=2.113e-06\Dipole=0.9998135,0.1792507,0.0251185\Quadrupole=-7.8669158,8.3805292,-0.5136134,7.720278,-0.2891405,0.1087725\PG=C01 [X(C12H16N1O2)]\@

Cation 4e.1

1\1\GINC-R99\FOpt\RM062X\6-31+G(d,p)\C13H18N1O2(1+)\ROOT\05-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat12.a.freq\1,1\C,-0.5210567271,-0.8660876727,0.0397610184\C,0.0953172716,0.3769923782,0.0246534338\C,-0.8946875196,1.5120498613,-0.0198536761\N,-2.1911866563,0.7250177868,-0.02826061\C,-2.0229528239,-0.7814373937,0.0081656967\C,0.252799028,-2.0285487602,0.0806184864\C,1.6306738575,-1.9167489852,0.105432634\C,2.2534930007,-0.6524706774,0.0899828718\C,1.4815313609,0.5146297883,0.0490667823\C,-2.6752510193,-1.3357670525,-1.2655949571\C,-2.7256296265,-1.2798991597,1.27821007\C,-0.8650940228,2.3394129952,-1.3114269485\C,-0.9155097167,2.3952239105,1.234402526\H,-0.2098279073,-3.011397825,0.0930540711\H,1.9425344024,1.4959896207,0.0366422885\H,-2.2056570808,-0.9254347483,-2.1626763881\H,-3.7487024237,-1.1324752668,-1.2733932955\H,-2.522003961,-2.4176703206,-1.2659102765\H,-2.2915424465,-0.8301965368,2.1743026849\H,-2.5734691606,-2.360614953,1.3320634072\H,-3.7983697762,-1.0773829875,1.234596683\H,-0.9029886488,1.697628223,-2.1948167909\H,0.0794099169,2.8882106596,-1.3284923065\H,-1.6888128085,3.0569191662,-1.3299193043\H,-0.9888961836,1.7927178615,2.1428638773\H,-1.7386879535,3.1121415106,1.1888310531\H,0.0280604359,2.9450516262,1.2647775753\H,2.2676328107,-2.7936920819,0.1373055315\O,3.5945504042,-0.6725329729,0.1169744665\C,4.2978447631,0.5624686027,0.1036363081\H,5.3536933584,0.3019922475,0.1301516587\H,4.045478194,1.162118183,0.9846970636\H,4.0808475495,1.1225661641,-0.8121909817\O,-3.2476098912,1.2462668092,-0.0606346532\Version=ES64L-G09RevD.01\State=1-A\HF=-710.8331281\RMSD=4.042e-09\RMSF=9.239e-05\Dipole=-1.2237927,0.7787783,-0.0413584\Quadrupole=8.7065998,2.0051146,-10.7117143,6.0845653,0.2501538,-0.1589598\PG=C01 [X(C13H18N1O2)]\@

Cation 4e.2

1\1\GINC-R97\FOpt\RM062X\6-31+G(d,p)\C13H18N1O2(1+)\ROOT\05-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat12.b.freq\1,1\C,-0.5367265156,-0.8804488424,0.0852173865\C,0.0870572302,0.3687622302,0.0691890172\C,-0.8982790032,1.504613183,-0.0166019539\N,-2.1966041228,0.7215014794,-0.0478118618\C,-2.0372879748,-0.7867161122,0.0130448882\C,0.2302996841,-2.0348396994,0.1617972947\C,1.6192389778,-1.935301041,0.2219516761\C,2.2385238634,-0.6754122646,0.2051411919\C,1.4620275048,0.4922825955,0.1278724717\C,-2.6596506537,-1.3528128465,-1.2700

527729\C,-2.7762870856,-1.2627323074,1.2705686631\C,-0.8301595999,2.3130769018,-1.3184555837\C,-0.9462823611,2.4046635272,1.2245812364\H,-0.2343802685,-3.0169497173,0.1757165129\H,1.9681569376,1.4528897115,0.1168556482\H,-2.1633815921,-0.9582661093,-2.1597656451\H,-3.7308504143,-1.1414226182,-1.3098441068\H,-2.5153178547,-2.435739679,-1.2517462284\H,-2.3622475741,-0.8046503599,2.1718314213\H,-2.6344145841,-2.3437699846,1.3421637448\H,-3.8459421779,-1.0525449373,1.1971265502\H,-0.8498449943,1.659504007,-2.1937062332\H,0.1191413622,2.8537546812,-1.3179587703\H,-1.6480553084,3.035650277,-1.368329729\H,-1.0477164147,1.8155485718,2.1390569138\H,-1.7629448142,3.1262683843,1.147798573\H,0.00087523,2.9470422794,1.271698746\H,2.2117039828,-2.8395118892,0.2817582352\O,3.5651199741,-0.4817822258,0.2589942686\C,4.4201258194,-1.6162494588,0.3393378482\H,5.4324702421,-1.219512501,0.3713612743\H,4.3027400445,-2.2541586271,-0.5425223509\H,4.2202772181,-2.1892565953,1.2504260276\O,-3.2499447571,1.2455999868,-0.1142343537\Version=ES64L-G09RevD.01\State=1-A\HF=-710.8341661\RMSD=7.728e-09\RMSF=2.926e-05\Dipole=-1.1570824,-0.0168582,-0.0524602\Quadrupole=8.6183382,3.2548562,-11.8731945,-5.0552086,1.1285575,-0.7774499\PG=C01 [X(C13H18N1O2)]\@\

Nitroxide 4e.1

1\1\GINC-R68\FOpt\UM062X\6-31+G(d,p)\C13H18N1O2(2)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) S CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide12.a.freq\0,2\C,-0.5318262109,-0.8655371315,0.0395382002\C,0.0858501991,0.3792314821,0.0244450016\C,-0.9230098417,1.5020018342,-0.0201778673\N,-2.1834299111,0.7240679635,-0.0281013617\C,-2.0361465967,-0.7500675206,0.0072022181\C,0.2433006965,-2.0242756342,0.080332754\C,1.6265957439,-1.9191273871,0.1054195486\C,2.2436627139,-0.6586829674,0.0899680549\C,1.4742080022,0.5067136611,0.0491452988\C,-2.6618248914,-1.3531144037,-1.2532431842\C,-2.711754351,-1.2977485233,1.2671463695\C,-0.8345701337,2.3394615195,-1.2987406533\C,-0.884549877,2.3947558277,1.2229642333\H,-0.223871112,-3.005734847,0.0926262604\H,1.9328348299,1.489690372,0.0366589073\H,-2.1715628102,-0.9633321924,-2.1494798958\H,-3.724722416,-1.0991088378,-1.289854945\H,-2.5561117591,-2.4422277238,-1.2414110097\H,-2.2570170473,-0.8685770372,2.1641153435\H,-2.6066030361,-2.386239149,1.3073264638\H,-3.7750465275,-1.0433043017,1.2504687203\H,-0.8473344408,1.6949757094,-2.181900883\H,0.090064577,2.9246761943,-1.3041026393\H,-1.6877949806,3.0216738986,-1.3439464278\H,-0.9328474463,1.7895738455,2.1323150654\H,-1.7382991189,3.0775572252,1.2044043737\H,0.0396590394,2.9804395229,1.239299242\H,2.2617062323,-2.7978132513,0.1372875207\O,3.6034186645,-0.6739103295,0.1172502645\C,4.2766209129,0.5673574514,0.1030717512\H,5.3402600252,0.3339111145,0.1291198766\H,4.013818774,1.1705628341,0.9803287226\H,4.0489723179,1.1310445547,-0.809580056\O,-3.3167202204,1.2861462269,-0.0628752679\Version=ES64L-G09RevD.01\State=2-A\HF=-711.0900848\S2=0.755269\S2-1=0.\S2A=0.750018\RMSD=4.589e-09\RMSF=5.278e-05\Dipole=1.2702272,-0.0461538,0.0260724\Quadrupole=-3.1076954,4.0414566,-0.9337613,9.6218334,-0.25565,0.0815432\PG=C01 [X(C13H18N1O2)]\@\

Nitroxide 4e.2

1\1\GINC-R80\FOpt\UM062X\6-31+G(d,p)\C13H18N1O2(2)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) S CF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide12.b.freq\0,2\C,-0.5449080962,-0.8744275585,0.0847824196\C,0.0768574175,0.3782881875,0.0684034484\C,-0.9319670257,1.4978785413,-0.018028042\N,-2.1918700546,0.7185840446,-0.0474975554\C,-2.0477209637,-0.7555160895,0.0116632769\C,0.2248261387,-2.0243818361,0.1613047011\C,1.6186841613,-1.9276743562,0.2216780897\C,2.229659214,-0.6692228272,0.2044596861\C,1.4545152271,0.4953334884,0.1273426383\C,-2.6424005629,-1.3739816513,-1.2562971331\C,-2.7577461414,-1.2841809124,1.2607655148\C,-0.8097106581,2.3167973944,-1.305600072\C,-0.9248515237,2.4076740547,1.2130522883\H,-0.2421583024,-3.0060633543,0.1751640004\H,1.957971001,1.4578261153,0.1159675258\H,-2.1269552109,-0.9991584416,-2.1447025009\H,-3.7027189465,-1.1159241868,-1.3246499121\H,-2.5417513165,-2.4632275615,-1.2258821055\H,-2.3243773758,-0.8454285202,2.1636097328\H,-2.658285447,-2.3724971694,1.3172232486\H,-3.8190328628,-1.0253825928,1.2134614301\H,-0.8021124157,1.6599871684,-2.1796849248\H,0.1170089833,2.898218668,-1.2953834104\H,-1.6596733524,3.0002568879,-1.3817757523\H,-0.9990586642,1.8154595125,2.1291618359\H,-1.7759941268,3.0920094853,1.1621145401\H,0.0008237888,2.9899406716,1.2455017606\H,2.2110096434,-2.8324340284,0.2814558617\O,3.5748690617,-0.4744239244,0.2593423193\C,4.4053364292,-1.6143114495,0.3382866152\H,5.427695758,-1.2398659011,0.3712970121\H,4.2803083988,-2.2573334407,-0.5409510795\H,4.1988900091,-2.192816493,1.2465220827\O,-3.3237221845,1.2790780751,-0.1196475403\Version=ES64L-G09RevD.01\State=2-A\HF=-711.0900613\S2=0.755271\S2-1=0.\S2A=0.750018\RMSD=6.901e-09\RMSF=3.561e-05\Dipole=1.3412002,-1.0225203,0.0979712\Quadrupole=-2.9289411,4.7481503,-1.8192091,0.6947519,-0.0745896,-0.2047107\PG=C01 [X(C13H18N1O2)]\@\

Cation 4f.1

1\1\GINC-R53\FOpt\RM062X\6-31+G(d,p)\C14H20N1O3(1+)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat13.b.freq\1,1\C,0.3248039933,0.693021

0801,0.0896996339\C,0.3353773383,-0.6872733844,0.0917600122\C,1.724496526,-1.2658841598,0.1280396548\N,2.5297934195,0.0198079816,0.1469693554\C,1.7048953176,1.2929502727,0.1242200591\C,-0.8792158745,1.4065538215,0.0579792861\C,-2.0747171115,0.7000099159,0.0283183523\C,-2.0637537125,-0.7312040374,0.0304547386\C,-0.8575695566,-1.4192588715,0.0621974027\C,2.1068736642,2.0649753412,-1.1388928482\C,2.0418286807,2.0682732191,1.4042254308\C,2.1382836121,-2.0354277796,-1.1327721387\C,2.0732386285,-2.0321299017,1.4103461403\H,-0.8809419924,2.4908092342,0.0565290912\H,-0.8426852028,-2.5034129872,0.0639840127\H,1.9153400758,1.4778048684,-2.0401281406\H,3.1578319566,2.3609629567,-1.0969443158\H,1.4904663098,2.9660891405,-1.1821511247\H,1.8044352726,1.4834279077,2.2960099695\H,1.4240756402,2.9694552466,1.4135805677\H,3.0935768899,2.3642207846,1.4152899183\H,1.9377979592,-1.4539534248,-2.035751878\H,1.5357541831,-2.9460039975,-1.1733260888\H,3.193651993,-2.3151539743,-1.089964233\H,1.826893156,-1.4483303856,2.3003862321\H,3.1293969263,-2.3118961464,1.4222700011\H,1.4693635136,-2.9426378914,1.4224056036\O,-3.2938528311,1.2503172389,-0.0035769432\O,-3.274315211,-1.3002160774,0.0002302613\C,-3.3519875519,-2.7174693229,0.0000815195\H,-4.4132905196,-2.9547929782,-0.0267555215\H,-2.9054473951,-3.1314590709,0.9108538144\H,-2.8594998305,-3.1337886811,-0.8855966571\C,-3.3932276455,2.6662075092,-0.0079547445\H,-4.4580411316,2.8871635256,-0.0354758638\H,-2.9071552632,3.087376857,-0.8948830482\H,-2.9531028278,3.0897064672,0.9015674234\O,3.7077309336,0.0288761847,0.1770855403\Version=ES64L-G09RevD.01\State=1-A\HF=-825.3134905\RMSD=3.795e-09\RMSF=3.678e-05\Dipole=2.0038718,0.0154266,0.0512327\Quadrupole=3.5005155,10.1329813,-13.6334968,-0.0501547,0.4385873,-0.0321174\PG=C02V [C2(N1O1),SGV(C10H4O2),X(C4H16)]\@

Cation 4f.2

1\1\GINC-R102\FOpt\RM062X\6-31+G(d,p)\C14H20N1O3(1+)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat13.c.freq\1,1\N,2.79793478,0.1212489337,0.0614462011\C,2.15365209,2.0285760454,1.4622247479\C,1.8788924798,1.327427585,0.1259634675\C,2.241672711,2.216949718,-1.0751567164\C,0.5452071781,0.6332997689,0.0372863216\C,2.0917371327,-1.2155314434,-0.0618910626\C,2.4963919326,-2.0523341419,1.158247477\C,2.5598008466,-1.8508015673,-1.377709903\C,0.6629314368,-0.743607164,-0.0623675007\C,-0.4748504944,-1.5445572417,-0.1519975327\C,-1.7285587076,-0.9503535927,-0.1479139695\C,-1.8477247924,0.4657610878,-0.0660496864\C,-0.7026048045,1.256838951,0.0383590797\O,-3.1010107083,0.9448155,-0.1179893534\C,-3.2918332092,2.3526658759,-0.0961718057\O,-2.8157038542,-1.736542225,-0.3112243469\C,-3.752858657,-1.7791892763,0.7736770416\H,-0.7810585826,2.3366505498,0.1009346987\H,-0.4254852376,-2.6262698304,-0.2362087835\H,2.0760610835,1.6855467217,-2.0181682348\H,3.25134337,2.5827053531,-1.005100408\H,1.5452700594,3.0727794635,-1.0557047566\H,1.9577546818,1.3637121373,2.3067436423\H,1.4715637801,2.8792065818,1.5323967657\H,3.1809748757,2.3982725171,1.5033324332\H,2.3192792655,-1.215149345,-2.2330887456\H,2.021191355,-2.7944351689,-1.4934562994\H,3.6321473555,-2.0582554105,-1.3501789496\H,2.2096367878,-1.559557875,2.0902348506\H,3.569960063,-2.255140069,1.1528772992\H,1.9589811111,-3.0015932802,1.0950396745\H,-4.5039547005,-2.5112148714,0.4823539267\H,-4.2191103684,-0.8053825674,0.9281035923\H,-3.2482250061,-2.1117995287,1.6866984571\H,-4.3662650355,2.5068151487,-0.1697202385\H,-2.7948443053,2.823578924,-0.9508873744\H,-2.9222293127,2.7814432091,0.8414837518\O,3.9715388401,0.2177705274,0.1033822392\Version=ES64L-G09RevD.01\State=1-A\HF=-825.3100853\RMSD=3.832e-09\RMSF=4.615e-06\Dipole=1.932701,0.8050845,0.4852963\Quadrupole=9.3735976,3.8410466,-13.2146442,-4.8804482,-3.8703936,-1.3484987\PG=C01 [X(C14H20N1O3)]\@

Nitroxide 4f.1

1\1\GINC-R44\FOpt\UM062X\6-31+G(d,p)\C14H20N1O3(2)\ROOT\08-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat13.b.freq\0,2\C,0.,0.69117,-0.36753\C,0.,-0.69117,-0.36753\C,0.,-1.25624,-1.76704\N,0.,0.,-2.55321\C,0.,1.25624,-1.76704\C,0.,1.40659,0.83432\C,0.,0.71031,2.03662\C,0.,-0.71031,2.03662\C,0.,-1.40659,0.83432\C,-1.26066,2.0604,-2.09549\C,1.26066,2.0604,-2.09549\C,-1.26066,-2.0604,-2.09549\C,1.26066,-2.0604,-2.09549\H,0.,2.49129,0.82376\H,0.,-2.49129,0.82376\H,-2.15747,1.48506,-1.85024\H,-1.27205,2.30003,-3.16229\H,-1.27377,2.99218,-1.52161\H,2.15747,1.48506,-1.85024\H,1.27377,2.99218,-1.52161\H,1.27205,2.30003,-3.16229\H,-2.15747,-1.48506,-1.85024\H,-1.27377,-2.99218,-1.52161\H,-1.27205,-2.30003,-3.16229\H,2.15747,-1.48506,-1.85024\H,1.27205,-2.30003,-3.16229\H,1.27377,-2.99218,-1.52161\O,0.,1.28475,3.26443\O,0.,-1.28475,3.26443\C,0.,-2.69488,3.32108\H,0.,-2.95248,4.37941\H,0.89532,-3.11086,2.84321\H,-0.89532,-3.11086,2.84321\C,0.,2.69488,3.32108\H,0.,2.95248,4.37941\H,-0.89532,3.11086,2.84321\H,0.89532,3.11086,2.84321\O,0.,0.,-3.81864\Version=ES64L-G09RevD.01\State=2-B1\HF=-825.5674936\S2=0.755266\S2-1=0.\S2A=0.750018\RMSD=2.649e-09\RMSF=8.160e-06\Dipole=0.,0.,1.1944592\Quadrupole=-1.1923196,14.1730917,-12.9807721,0.,0.,0.\PG=C02V [C2(N1O1),SGV(C10H4O2),X(C4H16)]\@

Nitroxide 4f.2

I\1\GINC-R155\FOpt\UM062X\6-31+G(d,p)\C14H20N1O3(2)\ROOT\05-Dec-2017\0\#M062X\6-31+G(d,p)
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide13.c.freq\0,2\N,2.776853284,0.11
662249,0.0884338296\C,2.0996674973,2.0502727863,1.4460577025\C,1.8933688055,1.3055864987,0.124696
1508\C,2.2102897235,2.2115281717,-1.0683742511\C,0.543428064,0.6375131843,0.0210734038\C,2.097567
1386,-1.1926124436,-0.0577819937\C,2.4379785892,-2.0777677896,1.1435658064\C,2.5403040474,-1.85373
42846,-1.3658418913\C,0.6575195216,-0.7421312073,-0.078399695\C,-0.4858587018,-1.532828168,-0.18151
31576\C,-1.7355896194,-0.9300458525,-0.1889558833\C,-1.8508881198,0.476528061,-0.0991878654\C,-0.70
38757929,1.2621358478,0.0125427696\O,-3.1182654447,0.965181157,-0.13912743\C,-3.2796524477,2.36854
61001,-0.104366065\O,-2.8520226568,-1.7045206026,-0.3440179124\C,-3.6619507837,-1.8122425593,0.8225
610018\H,-0.7728954352,2.3426142535,0.0821968302\H,-0.4382534061,-2.6151957603,-0.2664043074\H,2.0
501802041,1.6780728486,-2.0092253058\H,3.2545433308,2.5308847251,-1.0138104425\H,1.5660700179,3.0
960342876,-1.0524013086\H,1.8595237291,1.4022898607,2.2933532011\H,1.456086225,2.9345116812,1.485
8881008\H,3.1433097297,2.3666913415,1.5248924835\H,2.289179979,-1.2202578846,-2.2208649695\H,2.04
00641838,-2.8193518984,-1.4867087766\H,3.6219621647,-2.012142291,-1.345703504\H,2.111167449,-1.604
8007958,2.0736447746\H,3.5192552224,-2.2347428351,1.1851147281\H,1.9406963194,-0.832777462,1.129600024\H,-3.089
034817\H,-4.496463774,-2.4614085916,0.5565684692\H,-4.0389940436,-0.832777462,1.129600024\H,-3.089
5685477,-2.2662794735,1.6402873925\H,-4.351758901,2.549334905,-0.1699047971\H,-2.7762285285,2.8438
141911,-0.9543046811\H,-2.8938652516,2.7889843184,0.8320024598\O,4.0372162287,0.2179300343,0.1353
116275\Version=ES64L-G09RevD.01\State=2-A\HF=-825.565874\S2=0.755263\S2-1=0.\S2A=0.750018\RM
SD=6.441e-09\RMSF=3.053e-06\Dipole=-1.3112033,0.6067652,0.4449407\Quadrupole=-8.5594749,9.208490
2,-0.6490152,-5.4333545,-4.3608654,-1.6957219\PG=C01 [X(C14H20N1O3)]\@

Cation 9.1

I\1\GINC-R39\FOpt\RM062X\6-31+G(d,p)\C10H20N1O2(1+)\ROOT\14-Dec-2017\0\#M062X\6-31+G(d,p)
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat.OMe.freq\1,1\C,-0.0574586512,0.0268
663389,-0.0550359827\C,-0.082308963,0.0335885963,1.4782589401\C,2.396403641,0.0063032824,1.6908026
542\C,2.6376552834,-0.0059745536,0.1780800114\N,1.3462806078,0.4176010184,-0.5252135341\O,1.439652
5252,1.0490591805,-1.5215984345\C,-1.0312177506,1.0462950998,-0.6387699129\C,-0.3284297523,-1.36930
18331,-0.6539993955\H,-1.0284565839,-0.4346546651,1.7680952059\H,3.2532498528,-0.4861645853,2.1606
139125\C,2.9734749225,-1.4101132005,-0.3669214398\C,3.7229881912,0.9870919621,-0.2260220809\H,-0.7
576446085,2.0670329589,-0.3595537674\H,-2.0154540499,0.830048714,-0.2171911573\H,-1.0981064591,0.9
767507318,-1.7253568806\H,0.2284283338,-2.1661505149,-0.1629635699\H,-0.1254053896,-1.3847318463,-
1.7280717238\H,-1.3941291128,-1.563488354,-0.5086189609\H,2.3202529422,-2.1914490838,0.0189649668\
H,3.9919695612,-1.6301013375,-0.0371789851\H,2.9608052236,-1.4236206703,-1.4599601097\H,3.43015496
96,2.0152165789,0.0017538018\H,3.9773616892,0.9114779557,-1.2840503423\H,4.6120966994,0.748393194,
0.3620050372\C,1.1070709481,-0.6677528919,2.1404778722\O,1.0727962144,-0.5237698487,3.5328856596\
H,1.1156898949,-1.7398110539,1.8808132037\C,0.1190380435,-1.3377847825,4.1972504499\H,-0.10771157
66,1.0674666297,1.8441367801\H,2.3816255928,1.0400602011,2.0566285268\H,0.2993075321,-1.217006967
3,5.2643918507\H,-0.9083525597,-1.0261955312,3.975510955\H,0.2504746484,-2.3925621143,3.9246427956
\Version=ES64L-G09RevD.01\State=1-A\HF=-597.7419578\RMSD=4.557e-09\RMSF=6.591e-06\Dipole=-0.
1681001,-0.3373976,-0.9801375\Quadrupole=5.3285099,-3.5629452,-1.7655647,0.7458209,-2.4859638,-2.406
2662\PG=C01 [X(C10H20N1O2)]\@

Cation 9.2

I\1\GINC-R39\FOpt\RM062X\6-31+G(d,p)\C10H20N1O2(1+)\ROOT\14-Dec-2017\0\#M062X\6-31+G(d,p)
SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Cat.OMe.2.freq\1,1\C,-0.0016055951,0.01
82183765,0.0251584787\C,0.0517860348,-0.0196477063,1.5613307556\C,1.4445731535,-0.0462584991,2.177
2651616\C,2.2345229411,-1.2340051745,1.6205679311\C,2.3656772697,-1.282139452,0.0902616322\N,1.001
4565527,-0.988515335,-0.5304082481\O,0.7251096269,-1.5434614141,-1.5395439874\C,0.4002201642,1.384
5056718,-0.5736348985\C,-1.3821658281,-0.3884695602,-0.4847304126\H,-0.4992044065,-0.9006572929,1.9
099654774\H,-0.4870793512,0.8636512689,1.9167336997\H,1.7535075531,-2.1572738011,1.9648290954\H,3.2
531836789,-1.2504686,2.0210054965\C,2.7908704559,-2.6697410292,-0.3834236545\C,3.324309767,-0.2128
932198,-0.4770928102\H,1.3087235361,1.7858560869,-0.1320518552\H,-0.4194604573,2.0686153314,-0.338
4891389\H,0.4855113583,1.3165555054,-1.661495315\H,-1.6200584626,-1.4235780687,-0.2251898577\H,-1.
4761214814,-0.2584126856,-1.5634725966\H,-2.1099374938,0.2624141848,0.0054226416\H,2.0394862697,-3.4
264038472,-0.142236754\H,3.7123157767,-2.9230375429,0.1459676479\H,2.9924148943,-2.693962246,-1.45
50185062\H,3.1303071623,0.7788247354,-0.0749535281\H,3.2856691069,-0.2016076217,-1.5696479471\H,4.
3310438589,-0.5176730328,-0.177894497\H,1.3294075134,-0.1999935492,3.2608364391\O,2.0589537814,1.2
01052073,1.9456313931\C,3.1830527844,1.4681293755,2.7718665308\H,3.4556768698,2.5095437505,2.6046
229806\H,2.9291177619,1.3254966083,3.82867638\H,4.0379394019,0.830380071,2.5140185724\Version=ES

64L-G09RevD.01\State=1-A\HF=-597.7473253\RMSD=5.847e-09\RMSF=5.708e-06\Dipole=0.0166312,-0.424682,0.0723115\Quadrupole=3.8779222,-2.7600291,-1.1178931,-1.6921109,2.378564,0.9404906\PG=C01 [X(C10H20N1O2)]\@

Nitroxide 9.1

1\1\GINC-R94\FOpt\UM062X\6-31+G(d,p)\C10H20N1O2(2)\ROOT\14-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide.OMe.freq\0,2\C,-0.0155744612,0.0242216678,-0.0480825638\C,-0.0630180177,0.0385953339,1.4850366522\C,2.4030750386,0.0179789765,1.6829646636\C,2.6073533306,-0.0019842794,0.1647486223\N,1.3466553589,0.404370254,-0.5207717599\O,1.449044768,0.6561681745,-1.7660516292\C,-0.9911797184,1.0676347905,-0.5964950021\C,-0.3836976485,-1.356853666,-0.615204681\H,-1.011938907,-0.4176969035,1.7888910608\H,3.2653143354,-0.4575013627,2.1625861424\C,3.0343232096,-1.3910400325,-0.3368972064\C,3.6795479768,1.0205403103,-0.216937922\H,-0.6843582624,2.0722705278,-0.2921747229\H,-1.9914700018,0.8687673645,-0.1998759858\H,-1.022560801,1.0305032821,-1.6863135501\H,0.1907860163,-2.16536653,-0.1565263767\H,-0.2009555801,-1.3650005705,-1.6930671002\H,-1.4455870561,-1.5537655903,-0.4373401552\H,2.3743440629,-2.1864284509,0.018004685\H,4.0467537369,-1.6108175641,0.0157295024\H,3.0338396633,-1.3968875584,-1.4301934386\H,3.3472799804,2.031768866,0.0341600784\H,3.8880413206,0.9799454677,-1.2869459002\H,4.5969695186,0.8030282919,0.3382766753\C,1.1244778263,-0.6647469605,2.1349689164\O,1.0940722776,-0.572494218,3.5470047476\H,1.1371889193,-1.7317750144,1.8541164956\C,0.0922489893,-1.3505739085,4.1603338509\H,-0.0666585693,1.075891122,1.8448291751\H,2.3647790717,1.0564414793,2.0358141883\H,0.2814191427,-1.3233108579,5.2343583956\H,-0.9138512363,-0.9555161074,3.9707772835\H,0.1354375761,-2.3937477255,3.8150832047\Version=ES64L-G09RevD.01\State=2-A\HF=-598.0016151\S2=0.754868\S2-1=0.\S2A=0.750014\RMSD=2.869e-09\RMSF=5.514e-06\Dipole=-0.4250156,-0.7253309,0.8202104\Quadrupole=4.8009826,1.3602702,-6.1612528,0.3775949,-1.5934185,0.6663714\PG=C01 [X(C10H20N1O2)]\@

Nitroxide 9.2

1\1\GINC-R52\FOpt\UM062X\6-31+G(d,p)\C10H20N1O2(2)\ROOT\14-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\Nitroxide.OMe.2.freq\0,2\C,0.0221622085,0.050862789,0.0114204417\C,0.0365694216,-0.0034114669,1.5477754151\C,1.4151225125,-0.0310679337,2.1911370651\C,2.2132552878,-1.2080238473,1.6304914133\C,2.3340732083,-1.2464644353,0.1016473364\N,1.0010275289,-0.9906336914,-0.5122490021\O,0.9016941221,-1.2651345569,-1.7533272698\C,0.337436241,1.3919829055,-0.5719069274\C,-1.363611578,-0.4346281124,-0.4697673217\H,-0.5027445117,-0.89324843,1.8958694506\H,-0.513662495,0.8739662628,1.9043868227\H,1.7041771083,-2.121643777,1.9635814228\H,3.2214153969,-1.2435223473,2.0591261898\C,2.7659937049,-2.6518041136,-0.3259510401\C,3.3511798353,-0.2253403589,-0.4336735661\H,1.252839965,1.8116734299,-0.1556681627\H,-0.4847277739,2.0760305321,-0.3374043953\H,0.4250180504,1.3096885506,-1.658835054\H,-1.5636980928,-1.4681093847,-0.1717395222\H,-1.4328501547,-0.3688810988,-1.5563358485\H,-2.1214283198,0.215467092,-0.0215497174\H,2.0014678936,-3.3863635019,-0.056482121\H,3.6998375517,-2.9110951858,0.1826594454\H,2.92138885,-2.6959940404,-1.4046175783\H,3.1398630741,0.7848265256,-0.0809474934\H,3.3279114877,-0.2383969037,-1.5268655414\H,4.3573072817,-0.5067304953,-0.1036930089\H,1.291257224,-0.187060691,3.2764881356\O,2.0258191735,1.2347869296,1.9984891321\C,3.227515054,1.413585716,2.7115268557\H,3.4751228759,2.474970892,2.6600381068\H,3.1079166929,1.123395208,3.7653438539\H,4.0545553733,0.8371374103,2.2759087899\Version=ES64L-G09RevD.01\State=2-A\HF=-598.001483\S2=0.754886\S2-1=0.\S2A=0.750014\RMSD=4.999e-09\RMSF=4.690e-06\Dipole=0.4463977,0.185133,1.4493891\Quadrupole=3.7293993,-0.84351,-2.8858893,-0.3081399,0.1061954,-2.5487591\PG=C01 [X(C10H20N1O2)]\@

Model 1.1

1\1\GINC-R43\FOpt\RM062X\6-31+G(d,p)\C10H18O2\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\1.a.freq\0,1\C,-3.2041622317,1.0120450997,0.2065908085\C,-2.8997680931,-0.4409482614,-0.1451752602\C,-1.3813277616,-0.6407650224,0.2173159085\C,-0.8185612775,0.8133038836,0.2341338597\C,-1.9392140275,1.7732967639,-0.2230279903\H,-3.3466998141,1.094724177,1.291478504\H,-4.1149193039,1.3867086253,-0.2735148503\H,-3.0206407558,-0.6125243505,-1.2209446403\C,-3.796686458,-1.429336054,0.5507500038\C,-0.6883617183,-1.5210709392,-0.8253194395\C,-1.214649727,-1.2734825032,1.6054629358\H,0.0745737424,0.9057577611,-0.3958943929\H,-0.5162756402,1.0735352028,1.2560550956\C,-1.9055618612,1.9608952935,-1.7462370868\C,-1.8384738726,3.1407930721,0.451337246\H,-0.7282934296,-1.0609233173,-1.8187489997\H,-1.1687180252,-2.5033647485,-0.8833006785\H,0.3653356875,-1.6677356088,-0.5640305972\H,-1.7665769859,-0.7144938636,2.3688030907\H,-0.1559465176,-1.2750185569,1.8848622439\H,-1.5661647867,-2.311153712,1.6175940844\H,-1.9304263676,1.0071499485,-2.2829216686\H,-0.9894203661,2.481823825,-2.0451492059\H,-2.7601425609,2.5587505811,-2.08224718

12\H,-1.8809179744,3.0435214414,1.5413010562\H,-2.6604020507,3.7932241367,0.1359977338\H,-0.897194
2524,3.637380451,0.190280024\O,-4.4875665455,-1.2109899062,1.5167089795\O,-3.7318313123,-2.6557885
06,-0.0166182336\H,-4.3092057125,-3.2398949125,0.4992686506\Version=ES64L-G09RevD.01\State=1-A\H
F=-542.1748067\RMSD=9.663e-09\RMSF=1.281e-05\Dipole=0.4783798,-0.0635431,-0.4413134\Quadrupole=
-1.4885027,3.7365338,-2.2480311,1.3243377,2.9897392,-0.7813832\PG=C01 [X(C10H18O2)]\@

Model 1.2

1\1\GINC-R43\FOpt\RM062X\6-31+G(d,p)\C10H18O2\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight
INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\1.b.freq\0,1\C,-3.192378585,1.0194273703,0.2400
808493\C,-2.8982038534,-0.4283818705,-0.1467827319\C,-1.3852429035,-0.6397543993,0.2208250084\C,-0.
8002577779,0.8051963774,0.18662768\C,-1.9330401168,1.7804577486,-0.2123293537\H,-3.3015899712,1.09
57548367,1.3287390013\H,-4.1112983266,1.4082313179,-0.2127654481\H,-3.003813249,-0.5610437567,-1.2
286023051\C,-3.7737831256,-1.4946419956,0.4558489095\C,-0.7169345329,-1.572415413,-0.7907079818\C,-
1.2298367556,-1.2273982325,1.6304584394\H,0.0490152453,0.8770286299,-0.5034837005\H,-0.423925174,1.0
698596788,1.1823173973\C,-1.9441764224,2.0012182249,-1.73150564\C,-1.804945895,3.1330022359,0.4875
36922\H,-0.7494470381,-1.1445903661,-1.7988434728\H,-1.2255201892,-2.5420377698,-0.8146869833\H,0.3
333105474,-1.7379722074,-0.5268095692\H,-1.7559304209,-0.6230597411,2.3773582504\H,-0.1696736535,-
1.2544164309,1.902660712\H,-1.6151737457,-2.252015603,1.6812852888\H,-1.9784385699,1.0591211113,-2.
2878685338\H,-1.0385218416,2.5324649655,-2.0436722614\H,-2.8098068669,2.6025884835,-2.0310088485\
H,-1.8127969965,3.0126106019,1.5761196161\H,-2.6332845132,3.7955072259,0.2122886342\H,-0.87004605
37,3.6311862385,0.2075646175\O,-3.8997817,-2.6104674622,0.0061278213\O,-4.3937775856,-1.1144759069,
1.5926131643\H,-4.8957199291,-1.881373892,1.9098545184\Version=ES64L-G09RevD.01\State=1-A\HF=-5
42.1734101\RMSD=3.381e-09\RMSF=9.187e-06\Dipole=0.1945471,0.6537686,0.3056622\Quadrupole=2.2514
024,-4.0013919,1.7499895,-0.9447774,-2.0008016,-3.4981032\PG=C01 [X(C10H18O2)]\@

Model 1.3

1\1\GINC-R37\FOpt\RM062X\6-31+G(d,p)\C10H18O2\ROOT\20-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight
INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\1.c.freq\0,1\C,-0.1632170179,1.14617627,0.21066
3799\C,-0.9449933977,0.2045938427,-0.7254808205\C,-1.0463086514,-1.1811292354,-0.0375086578\C,0.050
9628689,-1.1386897755,1.0701094543\C,-1.0585653596,1.7440389613,1.3052369907\C,0.4972570899,2.2922
173026,-0.5582895069\C,-0.7738086013,-2.303170674,-1.0467133496\C,-2.4335380675,-1.4131977998,0.577
1174342\H,0.7034820881,-2.015691493,1.0189856873\H,-0.4114587812,-1.1385187034,2.0630433503\H,0.23
08376708,-2.2087947929,-1.4663071953\H,-1.501882265,-2.2645194876,-1.8653269032\H,-0.86126236,-3.28
46344858,-0.5663561868\H,-2.7219300346,-0.6096629594,1.2615862548\H,-2.4522108635,-2.355713471,1.1
361961884\H,-3.1954877461,-1.4741603211,-0.2076981878\H,-1.8931761151,2.2932524691,0.8564592877\H,
-0.4856337009,2.4428953895,1.9244204917\H,-1.474776605,0.9788476849,1.965542784\H,1.1187192069,1.9
219445748,-1.3806735899\H,1.1262238054,2.9017676612,0.0989404282\H,-0.2725147018,2.9400447768,-0.9
911769808\C,0.8483515376,0.1680526119,0.8918440895\C,2.0577920369,-0.0275772011,0.0130615239\H,1.
1975956121,0.5857009882,1.8414044794\O,2.1424674811,-0.7937181074,-0.9193558208\O,3.075065685,0.7
923719003,0.3508673923\H,3.7931888093,0.6333384913,-0.2815726866\H,-1.9300091426,0.6169461632,-0.9
776241828\H,-0.3858504806,0.0993294196,-1.6634755669\Version=ES64L-G09RevD.01\State=1-A\HF=-54
2.1736086\RMSD=5.111e-09\RMSF=1.223e-05\Dipole=-0.0760235,0.4684733,0.3737273\Quadrupole=2.5993
451,-1.2705335,-1.3288116,1.1647398,0.0053985,-2.1729477\PG=C01 [X(C10H18O2)]\@

Model 3a

1\1\GINC-R45\FOpt\RM062X\6-31+G(d,p)\C17H20\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight
INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\3.freq\0,1\C,-1.7740338871,1.158448735,0.93900264
52\C,-2.8587005532,0.834471993,-0.0828480611\C,-2.5225529076,0.2430302026,-1.3466810141\C,-1.180410
2954,-0.1168139709,-1.7057467912\C,-0.0180908264,0.1469818332,-0.7538185236\C,-0.5435811997,0.27423
4603,0.6844609518\C,-2.2382275112,0.8504475569,2.3739571662\C,-1.4518269395,2.6651894384,0.8664908
517\C,0.980348989,-1.0249462958,-0.746385151\C,0.7434027276,1.4034192452,-1.2235336754\H,0.2766519
922,0.6145947505,1.3315261185\H,-0.8041166974,-0.7393152666,1.0208191582\H,-2.5888155948,-0.182476
0995,2.461952724\H,-3.042019362,1.5153537821,2.7008182937\H,-1.3999751851,0.9901086097,3.06574526
51\H,-1.2709744974,3.004166255,-0.1541406051\H,-0.5703589828,2.8997449839,1.4747605546\H,-2.298477
0093,3.2420006672,1.2528284276\H,0.4756851743,-1.9712777325,-0.5288913781\H,1.7383255229,-0.852899
3122,0.0260716944\H,1.5059912968,-1.1269361234,-1.6994411977\H,0.0806831317,2.2500310071,-1.405519
0907\H,1.2615665491,1.1905378134,-2.1642560809\H,1.4919742006,1.6989928456,-0.4790572895\C,-3.5705
773763,0.0059606255,-2.2914243504\C,-4.9084758366,0.3523104389,-1.9682568225\C,-5.2041408668,0.920
0090495,-0.7579564288\C,-4.1729116387,1.1580654505,0.1778108098\C,-0.9430751816,-0.6657018294,-2.94
78064442\C,-1.9811464836,-0.8953375543,-3.8777958265\C,-3.2709403279,-0.5696036029,-3.5535191682\H,-

5.6882055491,0.1610962404,-2.7004466561\H,-6.2263245115,1.1880616901,-0.5093012866\H,-4.4348537609,1.6124651594,1.1282272375\H,0.0702750039,-0.933474385,-3.2305855215\H,-1.7487377253,-1.3328123899,-4.8437889789\H,-4.083133881,-0.7416784137,-4.2545015565\Version=ES64L-G09RevD.01\State=1-A\HF=-659.6237896\RMSD=6.239e-09\RMSF=4.663e-05\Dipole=0.1888227,0.0771284,0.1495984\Quadrupole=2.6747453,-4.2555512,1.5808059,-1.1610348,0.3493593,3.0541724\PG=C01 [X(C17H20)]\@

Model 3b

1\1\GINC-R37\FOpt\RM062X\6-31+G(d,p)\C17H19N1O2\ROOT\04-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=20GB\4.freq\0,1\C,-2.469015717,0.923109525,0.0320185563\C,-1.0016153885,1.2846491524,-0.1526071301\C,-0.0080658862,0.2509409946,-0.0616297595\C,-0.3780167242,-1.1307445283,0.0387653023\C,-1.8149536095,-1.6073063867,-0.1697693383\C,-2.7197415508,-0.4460264779,-0.6127838929\C,-3.4124068208,1.9230299278,-0.6514523992\C,-2.7707601989,0.9350635172,1.5444895188\C,-1.8398441526,-2.6489589022,-1.3081138727\C,-2.350228314,-2.2999543148,1.0995898414\H,-3.7668511946,-0.7361447748,-0.4535824932\H,-2.5954386181,-0.311649752,-1.6961381653\H,-3.1693727332,-2.0387666135,-1.7125260302\H,-3.3815032195,2.9085448648,-0.1790816854\H,-4.4426847375,1.560308078,-0.5731879275\H,-2.0289218372,0.3708543187,2.1142502807\H,-3.7632992758,0.5149337346,1.7450372623\H,-2.7496521494,1.9646650652,1.9153839585\H,-1.3751373856,-2.2489341278,-2.2142419259\H,-2.87830782,-2.910710519,-1.5398568447\H,-1.3176309915,-3.568951896,-1.0317953275\H,-2.3428844467,-1.6485399326,1.9736928802\H,-1.7504472864,-3.1832052649,1.3386270695\H,-3.3797692267,-2.6325770393,0.9279659603\C,1.379772453,0.6220212421,-0.0502781201\C,1.7387213253,1.9920487109,-0.1807099579\C,0.7651857315,2.9453257953,-0.3107079163\C,-0.6011736319,2.5927041262,-0.2885480329\C,0.6009146004,-2.073998376,0.2790831299\C,1.9563209946,-1.7245652825,0.36533261\C,2.3256152983,-0.4220390301,0.1570593927\H,2.7809039132,2.2773249016,-0.181948798\H,1.0460905743,3.9887454059,-0.4128401976\H,-1.3417347667,3.3817764895,-0.357784852\H,0.3334342039,-3.1210940786,0.3761341501\H,2.7189102502,-2.4709820378,0.5541689511\N,3.7741993775,-0.1670778045,0.159080355\O,4.2156677753,0.6782826308,-0.6015773862\O,4.459291186,-0.8467105682,0.9048408344\Version=ES64L-G09RevD.01\State=1-A\HF=-864.0530096\RMSD=4.389e-09\RMSF=3.419e-06\Dipole=-2.3273307,-0.2080688,-0.0201917\Quadrupole=-11.250034,11.5386554,-0.2886214,-0.3173228,-0.4278131,0.5650841\PG=C01 [X(C17H19N1O2)]\@

Model 3c

1\1\GINC-R46\FOpt\RM062X\6-31+G(d,p)\C17H18N2O4\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\5.freq\0,1\C,-1.7286396726,1.0265491175,1.006840995\C,-2.7778495504,0.9001225828,-0.0971812037\C,-2.5075499382,0.2291718935,-1.336888934\C,-1.1736115081,-0.1843571381,-1.685388455\C,-0.0090897595,0.2847725224,-0.8267525895\C,-0.4486253235,0.2564216736,0.6425493317\C,-2.2806727753,0.3870838219,2.2982248398\C,-1.4359774079,2.5090803615,1.3145886138\C,1.2212836899,-0.6241773917,-0.9524266657\C,0.3838282448,1.6966177342,-1.3092833237\H,0.3728645039,0.6227447799,1.2718236922\H,-0.5962744194,-0.7993967317,0.9080808221\H,-2.6046711768,-0.6422431172,2.1184209624\H,-3.1271988851,0.9479491907,2.7032512223\H,-1.4945048882,0.3731137349,3.0610562191\H,-1.0629790797,3.0576659806,0.4493806542\H,-0.6873088628,2.5752567824,2.11129602\H,-2.3401780892,3.0155902126,1.6646951043\H,0.9735147625,-1.6663021907,-0.7269858668\H,1.9867294876,-0.2936444133,-0.2430918444\H,1.6673400958,-0.5797914424,-1.9496469512\H,-0.4813997058,2.3578965656,-1.3935857698\H,0.842876639,1.6332533724,-2.3007249412\H,1.1072171838,2.1487075587,-0.6213316839\C,-3.5795977202,-0.0162290682,-2.2549762484\C,-4.8233356352,0.6167013027,-1.9902498637\C,-5.0614887063,1.2938604644,-0.8256471963\C,-4.0445165985,1.393235343,0.1359921565\C,-0.9655159116,-0.9001302056,-2.8401474508\C,-2.0414063544,-1.2890743166,-3.661567743\C,-3.3056879834,-0.8707962886,-3.3618945443\N,-5.863500546,0.7474356242,-3.0240325895\H,-6.030237171,1.7558755272,-0.6734724662\H,-4.2671297431,1.8975567094,1.0703605654\H,0.0336810214,-1.2108717909,-3.1203650022\H,-1.8905407656,-1.9358991983,-4.5183461901\N,-4.3865358576,-1.5060817171,-4.1338049366\O,-5.4007154108,-1.7967278875,-3.5222489202\O,-4.1720917881,-1.7644712572,-5.3009657709\O,-5.4817637894,0.8861514206,-4.1737713276\O,-7.0213206049,0.7837698784,-2.6591127202\Version=ES64L-G09RevD.01\State=1-A\HF=-1068.4740987\RMSD=4.566e-09\RMSF=4.542e-06\Dipole=2.9756064,0.743804,2.5301\Quadrupole=-2.7778677,3.8566041,-1.0787364,-5.7297116,-11.4612544,1.5079909\PG=C01 [X(C17H18N2O4)]\@

Model 4a

1\1\GINC-R46\FOpt\RM062X\6-31+G(d,p)\C13H18\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\8.freq\0,1\C,-0.6606864258,-0.2634187835,1.4504642592\C,-0.6269877672,0.1111240432,0.1064425382\C,0.7930777879,0.3590225982,-0.3729440146\C,1.5845294547,0.3888648474,0.9639116768\C,0.7322166088,-0.3174173249,2.0544151139\C,-1.8725445236,-0.5602512524,2.0698215101\C,-3.0540222713,-0.4744593485,1.3321265979\C,-3.0203012064,-0.0996674882,-0.0127887631\C,-1.8047825785,0.192887047,-0.6327645786\C,0.813031324,0.4249662526,3.392441029\C,1.1621229

429,-1.7786296727,2.2655929638\C,0.9264023594,1.6850255489,-1.1291969333\C,1.251240677,-0.78813303
56,-1.2887375419\H,1.736299394,1.4345901557,1.2591326172\H,2.5772492636,-0.0655194038,0.862177431
2\H,-1.9034709537,-0.851706736,3.1171924032\H,-4.0051233651,-0.6976376088,1.8057889184\H,-3.945373
1802,-0.0335458007,-0.5772598306\H,-1.7831875307,0.4851801041,-1.6801360282\H,0.4538343859,1.45365
42211,3.2903695517\H,1.8485483229,0.4538479008,3.749905543\H,0.2092083276,-0.0731618929,4.1587677
508\H,1.1290052306,-2.3463028866,1.3316710195\H,0.497257337,-2.2742713902,2.9812339829\H,2.183470
0904,-1.822410275,2.6602665013\H,0.5495458466,2.5174366545,-0.5269421007\H,0.3653772576,1.6625734
42,-2.0698016553\H,1.9769615888,1.88109366,-1.3716697869\H,1.1820862357,-1.7563354957,-0.785387248
3\H,2.290318677,-0.6348445592,-1.6012331276\H,0.6268547693,-0.8338642465,-2.1875700897\Version=ES
64L-G09RevD.01\State=1-A\HF=-506.0368351\RMSD=4.243e-09\RMSF=1.103e-05\Dipole=0.1965358,-0.00
02044,0.0048708\Quadrupole=1.5040406,-3.0320404,1.5279998,0.4625717,0.1188478,-1.3642808\PG=CS [S
G(C1H2),X(C12H16)]\@

Model 4b.1

1\1\GINC-R47\FOpt\RM062X\6-31+G(d,p)\C14H18O2\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\9.freq\0,1\C,-0.6600778043,-0.3077158265,1.4186
601474\C,-0.6158015326,0.0827314371,0.0784285386\C,0.8049648677,0.3623989872,-0.3770724051\C,1.577
886567,0.3925098335,0.970509039\C,0.7247181686,-0.3411661743,2.0422569371\C,-1.8714249944,-0.63240
42392,2.0186798002\C,-3.0433018666,-0.5562148672,1.2580858764\C,-3.0001291125,-0.1651727061,-0.0847
858161\C,-1.7837240011,0.1539290958,-0.6800312554\C,0.770200906,0.3896325378,3.3882035115\C,1.1786
971541,-1.7961755502,2.2452710357\C,0.9214766835,1.6981239748,-1.1190887423\C,1.2922842375,-0.7686
820279,-1.2984166339\H,1.7071454905,1.4374576548,1.2783881255\H,2.5795332022,-0.0430081824,0.8767
012291\H,-1.924537084,-0.9372261521,3.0598732634\C,-4.3712335909,-0.881315603,1.8403142458\H,-3.931
0943705,-0.115955431,-0.6401744231\H,-1.7516877976,0.4589043878,-1.7228593133\H,0.3939564639,1.412
6036242,3.2907079169\H,1.7994348143,0.4338709119,3.7612893187\H,0.1644916231,-0.1271888121,4.1403
225624\H,1.1725539808,-2.3551680266,1.3056008533\H,0.5125490698,-2.3117806372,2.945239608\H,2.194
0094022,-1.8234688699,2.656074326\H,0.5213425164,2.5178835249,-0.5146180118\H,0.3748906648,1.6739
544911,-2.0679126276\H,1.9714579563,1.9153687785,-1.3441662303\H,1.2343889866,-1.7429535279,-0.805
7221868\H,2.3321793219,-0.5932361357,-1.5951214838\H,0.6806573537,-0.8155967819,-2.2057142936\O,-5.4
212496043,-0.8357148626,1.2414206288\O,-4.3077130491,-1.2454612334,3.1392321566\H,-5.215344623,-1.
434343592,3.4206943024\Version=ES64L-G09RevD.01\State=1-A\HF=-694.5597823\RMSD=4.460e-09\RM
SF=5.359e-06\Dipole=1.0963725,0.0508016,0.209274\Quadrupole=-4.2689387,-0.748251,5.0171897,0.929610
7,-4.3786635,-2.3782682\PG=C01 [X(C14H18O2)]\@

Model 4b.2

1\1\GINC-R85\FOpt\RM062X\6-31+G(d,p)\C14H18O2\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\9.b.freq\0,1\C,-0.6684285897,-0.2987369491,1.409
7158479\C,-0.61839389,0.0944001436,0.0695260466\C,0.8056148728,0.3653250418,-0.3813059129\C,1.5749
953602,0.387632973,0.9686083912\C,0.7141487014,-0.3422066247,2.0368157124\C,-1.8831810181,-0.61584
6188,2.0032177523\C,-3.053355209,-0.5309647478,1.24152901\C,-3.0061734992,-0.1374532116,-0.10065289
83\C,-1.7834790352,0.1747099385,-0.6907405189\C,0.7594524234,0.3857995042,3.3842676994\C,1.1571789
805,-1.8007684995,2.2387008663\C,0.9337988458,1.7014720356,-1.1205879743\C,1.2880915164,-0.7676100
29,-1.3029324394\H,1.7105815321,1.4310954377,1.278849664\H,2.5739532866,-0.0543658714,0.876507504
8\H,-1.9572097746,-0.9242621636,3.0429175582\C,-4.337371073,-0.8689339907,1.9085757966\H,-3.9264924
14,-0.0762944895,-0.6707977351\H,-1.7469079302,0.4815794238,-1.7328796658\H,0.3910440414,1.4116696
923,3.287081914\H,1.7874659923,0.421914158,3.7615607334\H,0.14649715,-0.1278096353,4.1325064711\H,
1.1493189635,-2.3584595761,1.2981994487\H,0.4856254437,-2.3122560101,2.936369796\H,2.1713284476,-1.8
357035038,2.6517576915\H,0.5371663188,2.5228998845,-0.5160769946\H,0.3905925649,1.6826518338,-2.0
715087864\H,1.986059517,1.911957449,-1.3414265482\H,1.2205532636,-1.7422876738,-0.812286169\H,2.33
0649074,-0.5996548915,-1.5945570316\H,0.6801556383,-0.8079366418,-2.2130682495\O,-4.4473985416,-1.2
141149051,3.0629155947\O,-5.4078829951,-0.7565071538,1.0936928759\H,-6.1854879645,-0.9967447595,1.
6193045489\Version=ES64L-G09RevD.01\State=1-A\HF=-694.5598743\RMSD=5.504e-09\RMSF=1.645e-05
\Dipole=0.592101,0.2494274,-0.705983\Quadrupole=5.1410248,-2.59539,-2.5456348,-0.1699729,3.5064605,0.
374777\PG=C01 [X(C14H18O2)]\@

Model 4c.1

1\1\GINC-R48\FOpt\RM062X\6-31+G(d,p)\C15H18O4\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\10.a.freq\0,1\C,-0.6564735368,-0.2804500602,1.42
80341239\C,-0.5950189602,0.0538297836,0.0751372118\C,0.8296104747,0.319854547,-0.375388284\C,1.584
1088457,0.4079047471,0.9807097749\C,0.717812938,-0.2811322985,2.0720510866\C,-1.8752879444,-0.5961

264046,2.0194894949\C,-3.0421896288,-0.5652594893,1.2543129724\C,-2.9847778683,-0.1939481487,-0.0993176798\C,-1.75523017,0.0996867838,-0.6910097437\C,0.7374325526,0.507832848,3.3855463207\C,1.1706095449,-1.7254468501,2.344188384\C,0.9511492565,1.6241707944,-1.1702567248\C,1.330185696,-0.8476399851,-1.2424504364\H,1.7093178661,1.4648174891,1.2460128009\H,2.5863615466,-0.0312485872,0.9184894425\H,-1.9474087547,-0.8798604667,3.0663017865\C,-4.2870825006,-1.0366856885,1.9319587528\C,-4.1926968698,0.0135659823,-0.9534866594\H,-1.7372263219,0.379454152,-1.7411325724\H,0.3605117857,1.5243790475,3.23773676\H,1.7603812256,0.5714929446,3.7722807935\H,0.1206581442,0.0223597732,4.1492267726\H,1.1783517768,-2.3252131323,1.4300453176\H,0.4978486945,-2.2114340879,3.058752774\H,2.180520112,-1.7304328604,2.7683185792\H,0.5408431492,2.4670225586,-0.605644531\H,0.4184165851,1.5585547408,-2.124821355\H,2.003456916,1.8354352575,-1.3893214597\H,1.2715609823,-1.8002566402,-0.7090947693\H,2.3723266431,-0.680117192,-1.5352874866\H,0.7283623294,-0.9361044608,-2.1530563937\O,-4.5468014746,-0.8406619328,3.0947032308\O,-5.0591151218,-1.7949501743,1.1319626672\H,-5.8383601168,-2.0533285783,1.6476333787\O,-4.2382847294,-0.2183173958,-2.1375408751\O,-5.2120428361,0.5820121,-0.2837115631\H,-5.9471002302,0.6776208842,-0.9085918915\Version=ES64L-G09RevD.01\State=1-A\HF=-883.0698369\RMSD=4.303e-09\RMSF=2.707e-06\Dipole=0.7802819,0.0650017,0.0489029\Quadrupole=10.334346,-0.7615685,-9.5727775,1.4148994,1.8289927,-3.6868272\PG=C01 [X(C15H18O4)]\@

Model 4c.2

1\GINC-R49\FOpt\RM062X\6-31+G(d,p)\C15H18O4\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Ti ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\10.b.freq\0,1\C,-0.6399743893,-0.2923350038,1.4406929837\C,-0.5919596255,0.1094941506,0.106269177\C,0.8302542843,0.3717722865,-0.3532568058\C,1.6079818529,0.3713233321,0.9925477129\C,0.7445431127,-0.3574461583,2.0599627393\C,-1.8589368264,-0.585389403,2.0436255214\C,-3.0374650913,-0.4819045766,1.3000971438\C,-2.9843860608,-0.105253605,-0.0520409473\C,-1.7608691399,0.2034708064,-0.6439281198\C,0.8076609766,0.3568584242,3.414009803\C,1.1679955683,-1.824422239,2.2438081578\C,0.9622433845,1.7157972278,-1.0773829573\C,1.2953633173,-0.7547836971,-1.2913176034\H,1.7597083847,1.4097516013,1.3115027427\H,2.5996100717,-0.084180213,0.890165017\H,-1.9172517464,-0.8696056355,3.0902379516\C,-4.3537249226,-0.6281555539,1.9837441027\C,-4.1864826319,-0.0652746793,-0.9446581883\H,-1.7452734663,0.5090429752,-1.6869971856\H,0.4487147105,1.3872386247,3.3307237371\H,1.8395283701,0.3795615467,3.7810908587\H,0.1985974805,-0.1591153163,4.1639326008\H,1.1476532351,-2.3717344876,1.2975306925\H,0.4941255275,-2.3346803209,2.9402581925\H,2.1838713953,-1.8764360383,2.6502935051\H,0.5784078601,2.5332586071,-0.459613725\H,0.4096073555,1.713590761,-2.0227887484\H,2.0141828962,1.9194085295,-1.3053917518\H,1.2248225873,-1.7347627257,-0.8116093677\H,2.3365493864,-0.5910393627,-1.5895553604\H,0.6805005215,-0.7796042506,-2.1972203691\O,-5.376241386,-0.0891292326,1.6353340965\O,-4.2843786975,-1.3972880905,3.0894404435\H,-5.1670873338,-1.3927804878,3.4897610504\O,-4.4305620527,0.8350706639,-1.7096976022\O,-4.9101620062,-1.1954200579,-0.8841896911\H,-5.6841669022,-1.0724384016,-1.4549998069\Version=ES64L-G09RevD.01\State=1-A\HF=-883.0697589\RMSD=7.486e-09\RMSF=3.920e-06\Dipole=1.2562936,-0.6965143,0.6510061\Quadrupole=1.6997515,-4.7241196,3.0243681,7.3128372,-3.7152249,1.5701299\PG=C01 [X(C15H18O4)]\@

Model 4c.3

1\GINC-R39\FOpt\RM062X\6-31+G(d,p)\C15H18O4\ROOT\06-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Ti ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\10.c.freq\0,1\C,0.4606134933,1.4988009241,0.2431564939\C,-0.6623621808,1.0585492404,-0.4547127434\C,-1.6935323302,2.1604607645,-0.6169615588\C,-1.1620487406,3.2441223806,0.3623899768\C,0.3389344215,2.9569974035,0.6465513475\C,1.5338123688,0.6397273675,0.4656272676\C,1.4741843181,-0.6709294123,-0.0081527408\C,0.3314626646,-1.1222738352,-0.6880816145\C,-0.7324719053,-0.2511308805,-0.922843745\C,0.6818672274,3.1761916868,2.1238465498\C,1.2681082349,3.8225602835,-0.2208394549\C,-3.1016645491,1.6972514662,-0.2290376129\C,-1.7084232096,2.6534034283,-2.0736686506\H,-1.7188989107,3.1706937773,1.3045507175\H,-1.3169063681,4.2567847522,-0.0272551619\H,2.4245628759,0.9732807892,0.9908432126\C,2.6927382917,-1.5307653318,0.0872016331\C,0.1706619193,-2.5679976819,-1.0309508786\H,-1.6096947973,-0.6162997362,-1.4496775999\H,0.0804709665,2.52598529,2.7663942385\H,0.4875851154,4.2166399841,2.4063203899\H,1.7390138831,2.9684814741,2.3208902572\H,1.0528751931,3.7031471378,-1.2861074194\H,2.3151786598,3.5460103409,-0.0575013936\H,1.1498874235,4.8802376588,0.0384724578\H,-3.1117877488,1.2773445386,0.7814388978\H,-3.4734216124,0.9343244067,-0.9213216258\H,-3.7984076492,2.5420549831,-0.258677729\H,-0.7227800493,3.0044816543,-2.3908464469\H,-2.420826936,3.4779097022,-2.186005907\H,-2.0096417526,1.8462800835,-2.7498553654\O,3.0881287744,-2.2621657789,-0.7854200473\O,3.3631682103,-1.3438501288,1.2416727881\H,4.1552763365,-1.9014524709,1.1996458332\O,0.5317489613,-3.4842056492,-0.3360735058\O,-0.5026574806,-2.7489571031,-2.1847641773\H,-0.599693119,-3.7060735093,-2.3055866824\Version=ES64L-G09RevD.01\State=1-A\HF=-883.0684621\RMSD=7.389e-09\RMSF=2.358e-05\Dipole=-0.6372945,1.4121075,0.1328525\Quadrupole=4.5452114,-2.5409202,-2.0042911,3.1682253,5.8910517,2.4941816\PG=C01 [X(C15H18O4)]\@

Model 4d.1

I\1\GINC-R51\FOpt\RM062X\6-31+G(d,p)\C13H18O1\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\11.a.freq\0,1\C,-0.6444768906,-0.3006948919,1.43
74580919\C,-0.5907393733,0.0532673127,0.0875297284\C,0.8315695373,0.3464037424,-0.3577376015\C,1.5
84044735,0.4293426148,0.9992440124\C,0.7320063456,-0.2935910565,2.0795390063\C,-1.8651833209,-0.62
92830916,2.0172392726\C,-3.0278904432,-0.5983647656,1.2461903662\C,-2.9610734867,-0.2430374642,-0.1
032837521\C,-1.7395975001,0.0841897918,-0.6938658674\C,0.7506463399,0.4727657719,3.4064228443\C,1.
2166477842,-1.7317349825,2.3269517648\C,0.9353961587,1.6628456531,-1.1347346911\C,1.3554913937,-0.
7992753591,-1.2395135086\H,1.6850265,1.4850721585,1.280226445\H,2.5969328348,0.0148111976,0.93103
12806\H,-1.9273348441,-0.9063578731,3.0669834135\H,-1.7212529778,0.358420634,-1.7449834995\H,0.357
3578849,1.4857884698,3.2772524504\H,1.7740533439,0.5448838963,3.7918043435\H,0.1442260941,-0.0348
789143,4.1646851391\H,1.2301940052,-2.315466379,1.4025204267\H,0.5543246562,-2.2427318765,3.03429
98351\H,2.228539782,-1.7279222766,2.7478306562\H,0.5104199516,2.4906082323,-0.5586843271\H,0.4024
778344,1.6024461603,-2.089758682\H,1.9843529338,1.89447699,-1.3511857828\H,1.3060650846,-1.7605563
955,-0.7208691007\H,2.3971988769,-0.6137489995,-1.5243732527\H,0.7595146909,-0.8823585529,-2.15462
7449\H,-3.9880262295,-0.8469616316,1.6922997302\O,-4.0702910054,-0.1952592368,-0.8999011958\H,-4.85
17806958,-0.4356888783,-0.3901900971\Version=ES64L-G09RevD.01\State=I-A\HF=-581.2379443\RMSD
=7.514e-09\RMSE=1.332e-05\Dipole=-0.0549081,-0.1407857,0.4597101\Quadrupole=5.5031041,-3.5516054,-
1.9514986,2.2093448,-3.4009026,-0.9966923\PG=C01 [X(C13H18O1)]\@

Model 4d.2

I\1\GINC-R41\FOpt\RM062X\6-31+G(d,p)\C13H18O1\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\11.b.freq\0,1\C,-0.6422315184,-0.2938322436,1.43
56980724\C,-0.5873582114,0.0624488728,0.0901531624\C,0.8349277862,0.3504168734,-0.3584476649\C,1.5
896691485,0.4261652348,0.9977481673\C,0.7342941327,-0.2933823616,2.0776420363\C,-1.8668475616,-0.6
217397035,2.0160157733\C,-3.029120069,-0.5864027103,1.2509685177\C,-2.9627509301,-0.2270363352,-0.0
9805813\C,-1.7413669227,0.0979665195,-0.6893239017\C,0.7560470222,0.4727469553,3.4046584197\C,1.21
22677563,-1.733739586,2.3248757614\C,0.9443475274,1.6687181276,-1.1316477123\C,1.3535552744,-0.794
9889882,-1.2436995529\H,1.6977173679,1.4807206543,1.2803608852\H,2.5997975604,0.005385175,0.92701
03028\H,-1.9263208666,-0.9015802049,3.0652291942\H,-1.6999901569,0.3782238388,-1.7411550065\H,0.36
75781995,1.4876313499,3.2754994923\H,1.7795523871,0.5397950348,3.790709704\H,0.1465656038,-0.0320
464831,4.1622180852\H,1.2254633075,-2.3167304896,1.3999075505\H,0.5459466268,-2.242558981,3.02990
40666\H,2.223091825,-1.734810454,2.7483192301\H,0.5224470144,2.4965705598,-0.5534974467\H,0.41279
1039,1.613492722,-2.0881448766\H,1.9941105245,1.8970538492,-1.3473934214\H,1.3009819293,-1.7570036
47,-0.7268932787\H,2.3954859188,-0.6129018315,-1.5298531298\H,0.7567936689,-0.8744211952,-2.158887
696\H,-3.9970936097,-0.8292300936,1.6759365544\O,-4.1392092802,-0.208411602,-0.7927764492\H,-3.9769
924942,0.0536311432,-1.7056867091\Version=ES64L-G09RevD.01\State=I-A\HF=-581.2378712\RMSE=3.9
40e-09\RMSE=1.386e-05\Dipole=0.5292213,0.1589158,-0.3839127\Quadrupole=-3.2041044,-2.5501704,5.754
2748,-0.4732072,1.8062776,-2.0762826\PG=C01 [X(C13H18O1)]\@

Model 4e.1

I\1\GINC-R47\FOpt\RM062X\6-31+G(d,p)\C14H20O1\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti
ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\12.a.freq\0,1\C,-0.620533209,-0.303064467,1.4804
461622\C,-0.5899093238,0.0485513042,0.1362357928\C,0.8242893171,0.340987467,-0.3363408537\C,1.6015
092788,0.4219815883,1.0067388864\C,0.7645924799,-0.2950104605,2.1025888772\C,-1.836955504,-0.63592
51987,2.0805902045\C,-3.0050643072,-0.6074914622,1.3311238169\C,-2.9660055572,-0.251130304,-0.02501
65977\C,-1.7538931137,0.0784070389,-0.6354488393\C,0.8025912088,0.4778173264,3.4254175752\C,1.2509
500576,-1.7325596973,2.3501451253\C,0.9171580955,1.6582866586,-1.1135835976\C,1.3326204573,-0.8039
881327,-1.2280579582\H,1.7132435605,1.4774742924,1.2843931814\H,2.6107300667,0.0017329933,0.92094
36194\H,-1.881096253,-0.9133081363,3.1312648242\H,-1.706987672,0.3572614959,-1.683082987\H,0.40898
06335,1.4908148543,3.2965965096\H,1.8312177031,0.5502871121,3.7966660708\H,0.2055067966,-0.025049
6114,4.1940986906\H,1.2550942113,-2.3194172464,1.4274829844\H,0.5954062916,-2.2410359753,3.065532
2132\H,2.2669164517,-1.7280979667,2.7612050263\H,0.5036775552,2.4861611728,-0.5293469481\H,0.3686
612842,1.600156406,-2.0602818915\H,1.9625019081,1.8885041908,-1.3482602536\H,1.2928138355,-1.76499
23887,-0.7081234986\H,2.3687559488,-0.6184995373,-1.5327069157\H,0.7203321869,-0.887907986,-2.1325
495644\H,-3.9673366083,-0.8532903718,1.7676884219\O,-4.1697317434,-0.2524943154,-0.6650361104\C,-4.
1857900712,0.0972891266,-2.0317553781\H,-5.2265692579,0.0343039085,-2.3477913042\H,-3.5812240652,-
0.5979303654,-2.6268926451\H,-3.8193426429,1.1197166871,-2.1844826392\Version=ES64L-G09RevD.01\

State=1-A\HF=-620.5190903\RMSD=8.577e-09\RMSF=6.370e-06\Dipole=0.2942369,0.144837,-0.46346\Quadrupole=-1.0387137,-3.415656,4.4543697,-0.4132793,3.1403511,-1.7459233\PG=C01 [X(C14H20O1)]\@

Model 4e.2

1\1\GINC-R48\FOpt\RM062X\6-31+G(d,p)\C14H20O1\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\12.b.freq\0,1\C,-0.6191261055,-0.2933677583,1.5023262716\C,-0.5908975419,0.0599581355,0.1491571905\C,0.8244100092,0.3422788285,-0.3252039527\C,1.6048807014,0.4214300006,1.0161968906\C,0.7708836045,-0.295367768,2.1145480451\C,-1.828497963,-0.6108958643,2.1042595078\C,-3.014338627,-0.5740572824,1.3624870489\C,-2.9731871982,-0.2198341124,0.010317722\C,-1.7547137597,0.098090553,-0.6028145735\C,0.8231521193,0.470819772,3.4405909106\C,1.2508961408,-1.7368238212,2.3518682933\C,0.9224969847,1.6567988604,-1.1061517519\C,1.3226098351,-0.8081329558,-1.2156557054\H,1.7181708108,1.4767301644,1.2942067536\H,2.613546125,0.0004415844,0.927792854\H,-1.8706918322,-0.8865956319,3.1555586137\H,-1.7597609387,0.3711477263,-1.6546197268\H,0.4354860774,1.4869770327,3.3192114124\H,1.8547673457,0.5345639062,3.8050647204\H,0.2279834461,-0.0318672232,4.2109513917\H,1.2399933638,-2.3209496987,1.4276698702\H,0.6005588272,-2.242904019,3.0736643613\H,2.2719101998,-1.7398920929,2.7502340851\H,0.5173743657,2.4888455651,-0.5220353529\H,0.3676699311,1.5992637802,-2.0488046174\H,1.9683184295,1.8791488809,-1.3463371093\H,1.2751016191,-1.7687537078,-0.6956541233\H,2.3602670535,-0.6313698072,-1.5203035577\H,0.7085256538,-0.886682761,-2.119112929\H,-3.9524437263,-0.8176741665,1.8463258233\O,-4.0715574189,-0.1528661649,-0.7948912166\C,-5.3245227638,-0.4647176936,-0.2257981274\H,-6.0555707078,-0.3539696352,-1.02607956\H,-5.5719782737,0.2230785309,0.591844354\H,-5.345935787,-1.4957311567,0.147546184\Version=ES64L-G09RevD.01\State=1-A\HF=-620.5190419\RMSD=6.921e-09\RMSF=1.016e-05\Dipole=-0.2081106,-0.1233148,0.3068759\Quadrupole=6.2949362,-4.2734421,-2.0214941,1.8180592,-1.6358227,-0.8800655\PG=C01 [X(C14H20O1)]\@

Model 4f.1

1\1\GINC-R47\FOpt\RM062X\6-31+G(d,p)\C15H22O2\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\13.b.freq\0,1\C,-0.5422047772,-0.2596644932,1.4479585543\C,-0.5107044368,0.0927536829,0.1114143807\C,0.9023423963,0.3661125331,-0.3727278153\C,1.6890751165,0.4271161019,0.9665292104\C,0.8448727559,-0.27682745,2.0656491887\C,-1.7543141344,-0.5827011047,2.0713829698\C,-2.9324955668,-0.5416359382,1.3361102374\C,-2.9001661774,-0.179927866,-0.0356394526\C,-1.6903415647,0.1330095258,-0.6429434258\C,0.9025281272,0.4931575115,3.389386799\C,1.3070292526,-1.7231569737,2.3080444595\C,1.0093088399,1.6877287064,-1.1410832974\C,1.3914932596,-0.7781919652,-1.2757851119\H,1.823692767,1.4791369028,1.2470938294\H,2.6890722481,-0.0134105572,0.8739423451\H,-1.7711286738,-0.8578942485,3.1209200152\H,-1.6577057555,0.4109710016,-1.691377579\H,0.5235924805,1.5121988088,3.2642211871\H,1.9343260647,0.5495065669,3.754522504\H,0.303094879,-0.0016276333,4.1618150684\H,1.2968040152,-2.306579609,1.3832455026\H,0.6462231094,-2.2227594231,3.0250381966\H,2.3246527327,-1.7375725318,2.7147257497\H,0.6134181512,2.517072557,-0.5468077884\H,0.4502714108,1.6448634634,-2.0825809117\H,2.0554659082,1.9047132969,-1.3851721987\H,1.3473171325,-1.7414361861,-0.7600831126\H,2.4261419597,-0.6021372229,-1.5914775975\H,0.7687583931,-0.8518571766,-2.1741847127\O,-4.1664723168,-0.8238645466,1.8292775878\O,-4.1078558995,-0.1681371718,-0.6576620373\C,-4.1280419897,0.1844645575,-2.0226348328\H,-5.1719406809,0.134941602,-2.3306127034\H,-3.5360107101,-0.5170525285,-2.6234252597\H,-3.7494111136,1.2026054921,-2.1760809817\C,-4.2507687914,-1.1902658577,3.1881486106\H,-5.3065249199,-1.3734083773,3.3852914519\H,-3.8913617085,-0.3846853974,3.8403657176\H,-3.677401783,-2.103518052,3.3901252526\Version=ES64L-G09RevD.01\State=1-A\HF=-734.9963105\RMSD=7.652e-09\RMSF=7.967e-06\Dipole=0.2833816,0.0183713,0.0115213\Quadrupole=-2.9543449,-3.9314305,6.8857754,0.2867267,-0.1752376,-3.0612033\PG=C01 [X(C15H22O2)]\@

Model 4f.2

1\1\GINC-R38\FOpt\RM062X\6-31+G(d,p)\C15H22O2\ROOT\04-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\13.c.freq\0,1\C,-0.0012251323,0.013947376,2.2518128222\C,2.4619456977,0.005812419,1.5433416655\C,1.0941748681,-0.6809600117,1.3956169656\C,1.2357845773,-2.1607009345,1.767660694\C,0.5574648138,-0.4887272693,-0.0125791806\C,-0.8120485617,0.9698263671,1.3327145073\C,-0.3367129331,2.4270187961,1.4547310347\C,-2.3106929307,0.9063195537,1.6459035996\C,-0.4898477442,0.4217761911,-0.0459788692\C,-1.0885631544,0.7511549752,-1.2633445549\C,-0.6397972844,0.1578179167,-2.4345548232\C,0.418940796,-0.7769498065,-2.3990687713\C,1.0236716772,-1.0932562387,-1.1829373559\O,0.7651176957,-1.319951093,-3.5989545444\C,1.7846940318,-2.2963147706,-3.6018754441\O,-1.2718326665,0.4394903369,-3.6171599546\C,-0.5036145568,1.2293677304,-4.5172751485\H,-0.6790432034,-0.7538047836,2.6450538649\H,0.4265509612,0.5399741911,3.1136463402\H,1.8368712119,-1.8106384343,-1.1387253543\H,-1.9149493554,1.4541385424,-1.3332401373\H,0.2924345403,-2.693617899,1.6136639178\H,1.523725639,-2.2633317536,2.8200065182\H,2.007614585,-2.6496839528,1.1627905139\H,

2.4041895436,1.0700232553,1.2989223135\H,3.196536319,-0.4518240211,0.8716348864\H,2.8303789047,-0.0931922278,2.5706442258\H,-2.6939487386,-0.1100711933,1.5132139558\H,-2.8799517182,1.5736363654,0.9895828225\H,-2.4982530594,1.2153792261,2.6805063213\H,0.7339595198,2.5178011995,1.2514559786\H,-0.5303658334,2.8098491902,2.4631993335\H,-0.867780711,3.0645985715,0.7395730687\H,-1.1266917681,1.3848535848,-5.3986845462\H,0.4178128971,0.7139170049,-4.8031459371\H,-0.2634162755,2.1981085264,-4.0623426239\H,1.8931192217,-2.6156576864,-4.6378525453\H,1.5088157455,-3.1570521545,-2.9811998829\H,2.7349423806,-1.8801070892,-3.2458556765\Version=ES64L-G09RevD.01\State=1-A\HF=-734.9950203\RMSD=1.970e-09\RMSF=1.564e-05\Dipole=0.8672513,-0.1014567,0.1968625\Quadrupole=-2.2828142,1.2132458,1.0695684,-4.3597369,-4.8609357,0.2375456\PG=C01 [X(C15H22O2)]\@

Model 4g

I\1\GINC-R47\FOpt\RM062X\Gen\C13H17Br1\ROOT\01-Dec-2017\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\14.freq\0,1\C,-0.486794536,-0.2575466296,1.4720629545\C,-0.4600767867,0.0969637925,0.1228998962\C,0.9540618649,0.3684303379,-0.3613791709\C,1.7424444541,0.4361845617,0.9760905681\C,0.9059347448,-0.2729053331,2.0771538472\C,-1.6941863602,-0.5685329123,2.0916607674\C,-2.8798802882,-0.5194934015,1.3581267519\C,-2.8317302567,-0.1634062585,0.011749072\C,-1.6332846346,0.1466011026,-0.6256766139\C,0.9687965026,0.4906158941,3.404241838\C,1.3665878266,-1.7215544793,2.3093263293\C,1.0574461985,1.6852249991,-1.1378536777\C,1.4356513401,-0.7837679695,-1.2585614707\H,1.8703547874,1.4893022453,1.255325456\H,2.7449028329,0.0026810163,0.8813152837\H,-1.7268393975,-0.8450138416,3.1426554103\H,-1.627379585,0.4221197827,-1.6761144181\H,0.5879582214,1.5098472101,3.2875165406\H,2.0030408374,0.5465817488,3.7615363699\H,0.3758576138,-0.0096557613,4.1776121249\H,1.3463860112,-2.3037694044,1.3841355389\H,0.7129355385,-2.220885606,3.0325945561\H,2.3883581383,-1.7367696174,2.7044596767\H,0.6599672614,2.5182799173,-0.5500729573\H,0.5012185182,1.6353059813,-2.0801206618\H,2.1039955273,1.9010274981,-1.3798075999\H,1.3875760185,-1.7451665186,-0.7401543059\H,2.4712183996,-0.6123693346,-1.5724186696\H,0.8137572708,-0.857054893,-2.1571026908\H,-3.8314142141,-0.7513466844,1.8231368435\Br,-4.4521538494,-0.0931574425,-0.9820975883\Version=ES64L-G09RevD.01\State=1-A\HF=-3079.3268506\RMSD=8.603e-09\RMSF=1.137e-05\Dipole=0.9551999,-0.0147977,0.4136474\Quadrupole=-0.5342334,-2.0534621,2.5876955,0.7090276,-1.840668,-1.5445126\PG=C01 [X(C13H17Br1)]\@

Model 4h

I\1\GINC-R434\FOpt\RM062X\Gen\C13H16Br2\ROOT\20-Dec-2017\0\#M062X/gen 6D SCF=(Tight,XQC) INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=50GB\15.freq\0,1\C,-0.4652497101,-0.2481246647,1.4620491226\C,-0.4378282963,0.10723802,0.1134142727\C,0.9760122097,0.3767259493,-0.3706276012\C,1.7626617999,0.4439458683,0.968350427\C,0.9263455032,-0.266326435,2.0694590734\C,-1.6682767826,-0.5562718464,2.0841316344\C,-2.8537506566,-0.5035724947,1.348164413\C,-2.8262317729,-0.1476047466,-0.0039683272\C,-1.613260526,0.1572757877,-0.6248134326\C,0.9885441528,0.4954283163,3.3974089306\C,1.3839166064,-1.7164102442,2.2986850788\C,1.0808546613,1.6932862783,-1.1473364418\C,1.4564289075,-0.7766550824,-1.26697854\H,1.8894062422,1.4969074186,1.2484311907\H,2.7651256846,0.0107352329,0.8746173887\H,-1.7084038775,-0.8332435557,3.133485822\H,-1.6109879353,0.4334381812,-1.6750615581\H,0.6082788105,1.5149837377,3.2823954372\H,2.0229860229,0.5504336738,3.7537388161\H,0.3963557542,-0.0058898558,4.1705150903\H,1.3624635935,-2.2975129103,1.3728973952\H,0.7307071895,-2.2157188443,3.0221834048\H,2.405914024,-1.732834627,2.6926930122\H,0.6855816317,2.5273401169,-0.5595601316\H,0.5239781346,1.6437448293,-2.089209263\H,2.1274909856,1.9069296253,-1.3901901898\H,1.4051046148,-1.7382380775,-0.7493684788\H,2.4929184879,-0.6073612565,-1.5784021467\H,0.8365094661,-0.8477833549,-2.1670098581\Br,-4.4704855429,-0.9194298393,2.2389368659\Br,-4.4037493828,-0.0556022005,-1.0450134068\Version=ES64L-G09RevD.01\HF=-5652.6118742\RMSD=6.629e-09\RMSF=9.135e-06\Dipole=1.4254948,0.127557,0.0629308\Quadrupole=-5.3860847,0.5510466,4.8350381,-0.6825385,1.8039196,-0.9790831\PG=C01 [X(C13H16Br2)]\@

Model 4j

I\1\GINC-R49\FOpt\RM062X\6-31+G(d,p)\C13H17N1O2\ROOT\01-Dec-2017\0\#M062X/6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\16.freq\0,1\C,-0.5268378269,-0.2965049113,1.4422978152\C,-0.4965450095,0.0767862507,0.095659685\C,0.9167233654,0.3773241895,-0.3686032737\C,1.693302928,0.4414341106,0.9758895398\C,0.8596268823,-0.2945439695,2.0613543229\C,-1.7267148564,-0.6359245329,2.0555091102\C,-2.8812902679,-0.5842376066,1.28066678\C,-2.8804702237,-0.2159948627,-0.061397779\C,-1.6677746118,0.1164956878,-0.6593760056\C,0.8930240529,0.4549973497,3.3972715908\C,1.3405764334,-1.7384535909,2.2815174442\C,1.0043476564,1.7043376735,-1.1300079267\C,1.4212423504,-0.7582689417,-1.2752499519\H,1.8030855077,1.4926852192,1.2690135356\H,2.7025775326,0.0241918609,0.8839631977\H,-1.7914719824,-0.9295257073,3.0978690349\H,-1.6461117081,0.4080804782,-1.7057912288\H,0.

4966845539,1.4690940709,3.2879371243\H,1.9222287083,0.5244932917,3.7657778992\H,0.3008255186,-0.0639251229,4.1584677179\H,1.341674604,-2.3106596344,1.3498639286\H,0.6881434114,-2.2567754062,2.9921186309\H,2.3577196543,-1.7399673519,2.6879235117\H,0.5899427816,2.5251560522,-0.5367896169\H,0.4576224835,1.6558095881,-2.0777520038\H,2.0494422498,1.9382921661,-1.3599248704\H,1.3829879263,-1.7264727514,-0.769012822\H,2.4568515982,-0.567490729,-1.576545452\H,0.8091490408,-0.8288698318,-2.1806307146\N,-4.1656406889,-0.9327150295,1.9120468918\H,-3.814996576,-0.1929743012,-0.6083027386\O,-5.1693668151,-0.8821064616,1.2225971095\O,-4.1493786731,-1.2523672462,3.0883295137\Version=ES64L-G09RevD.01\State=1-A\HF=-710.4730531\RMSD=8.940e-09\RMSF=1.068e-05\Dipole=2.0880832,0.4848539,-0.810592\Quadrupole=-8.3989791,2.996136,5.4028431,-3.099577,5.5509022,0.1841414\PG=C01 [X(C13H17N1O2)]\@

Model 4k

1\1\GINC-R49\FOpt\RM062X\6-31+G(d,p)\C13H19N1\ROOT\01-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Ti ght INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\17.freq\0,1\C,-0.5425121979,-0.3163222595,1.4322294817\C,-0.503230702,0.0596432626,0.0900480762\C,0.9085640892,0.3774161546,-0.3701690289\C,1.6753843139,0.4457050238,0.9800739736\C,0.8423969431,-0.3033128112,2.0570540852\C,-1.7384522918,-0.6734470525,2.044646588\C,-2.9282352814,-0.6519270474,1.3043775073\C,-2.8864936833,-0.2762859618,-0.0471996392\C,-1.6820222324,0.0759046037,-0.6509879872\C,0.8689472981,0.4392231264,3.3970574438\C,1.3393119778,-1.7425920203,2.2718432773\C,0.9893300582,1.7101275853,-1.1225076777\C,1.4440172427,-0.7410659583,-1.2794769649\H,1.7688330302,1.497549192,1.2779753726\H,2.6916510895,0.0422072889,0.8958198348\H,-1.762317396,-0.9705310593,3.0918426417\H,-1.6755837027,0.3658767065,-1.6994118363\H,0.4598127756,1.4488205655,3.2915356317\H,1.8971709729,0.5195049695,3.7676072094\H,0.2817652394,-0.0901949033,4.1554836531\H,1.3444077425,-2.3088020556,1.3365653814\H,0.6903515345,-2.2714299765,2.9782066439\H,2.3569022275,-1.7376802234,2.6786579663\H,0.5659282517,2.5220634046,-0.5231887356\H,0.4397696836,1.6626503549,-2.0691833436\H,2.0317981623,1.9571024338,-1.3541334024\H,1.4174237137,-1.712502199,-0.7783311869\H,2.4786059173,-0.5331539355,-1.5758686519\H,0.8371017236,-0.8185906242,-2.1881925175\N,-4.1347315293,-1.0554639639,1.8878573729\H,-3.8081361045,-0.2651159437,-0.6233220566\H,-4.9649285019,-0.684275971,1.4475302946\H,-4.1721103641,-0.9623607058,2.893270593\Version=ES64L-G09RevD.01\State=1-A\HF=-561.3763792\RMSD=3.279e-09\RMSF=6.958e-06\Dipole=-0.2900678,0.2864111,0.2939038\Quadrupole=5.1310284,-6.5456635,1.4146351,-1.7263852,-1.7350239,-1.024655\PG=C01 [X(C13H19N1)]\@

Model 7

1\1\GINC-R38\FOpt\RM062X\6-31+G(d,p)\C21H22\ROOT\04-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\19.freq\0,1\C,-0.3254591988,-0.2313531018,1.4306303305\C,-0.3132040872,0.195175175,0.1334196305\C,1.1021868994,0.4803286205,-0.3680409501\C,1.9078266913,0.4362096282,0.9524298059\C,1.0795609643,-0.3073085925,2.0275133258\C,1.2602661863,0.4295431807,3.3669732664\C,1.5412153449,-1.7686919955,2.1729314388\C,1.301556208,1.8672099328,-1.0056681944\C,1.5744209907,-0.6122526992,-1.3443469399\H,0.7633060077,1.4046220536,3.3439947997\H,2.329946589,0.5973629001,3.537143381\H,0.8831958696,-0.125840384,4.2277607839\H,1.5082177967,-2.2913256541,1.2130230886\H,0.9124507806,-2.3253608279,2.8736936038\H,2.5717899548,-1.7982433003,2.544500221\H,0.7988682498,2.6412186508,-0.4170328284\H,0.9422677648,1.9330615171,-2.0343405717\H,2.373027122,2.0972491173,-1.0248644537\H,1.5279901737,-1.6023237544,-0.8825446524\H,2.6113287256,-0.421343356,-1.6433393954\H,0.9608168141,-0.6409756356,-2.2493099925\C,-1.5343186323,0.2923074382,-0.6349290389\C,-2.7725659551,0.0021798127,-0.0021089833\C,-2.7856562975,-0.4533369178,1.3832205246\C,-1.5600270583,-0.6022850118,2.0857470242\C,-3.9619750525,0.1373597334,-0.753446075\C,-3.9428337542,0.5191705031,-2.0782883639\C,-2.7172513656,0.7746394317,-2.7132238792\C,-1.5425715716,0.6625978576,-2.0009100113\C,-3.988446378,-0.7837256588,2.047760982\C,-3.9940461503,-1.262721121,3.3407744471\C,-2.7809229305,-1.4407702739,4.0242130758\C,-1.5936555072,-1.1148281461,3.4045563747\H,-4.9208121163,-0.0669767488,-0.2930558426\H,-4.8738544062,0.6118068378,-2.6283236949\H,-2.6920642213,1.0586863377,-3.7604814545\H,-0.6060599586,0.8550208733,-2.5056111431\H,-4.9381305844,-0.669607644,1.5396681383\H,-4.9348170214,-1.5093478312,3.8224847282\H,-2.7751937772,-1.8337708592,5.0359357453\H,-0.6669844459,-1.2647244413,3.9408515585\H,2.0705401635,1.4660406751,1.2925663968\H,2.8968831736,-0.0170863215,0.8127307938\Version=ES64L-G09RevD.01\State=1-A\HF=-813.2081549\RMSD=4.296e-09\RMSF=2.173e-06\Dipole=0.2063656,-0.0112917,-0.0017686\Quadrupole=4.5111609,-7.1239321,2.6127712,1.0139354,0.3402312,-3.5778937\PG=C01 [X(C21H22)]\@

Model 8

1\1\GINC-R117\FOpt\RM062X\6-31+G(d,p)\C12H23N1O1\ROOT\14-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\Nac.1.freq\0,1\C,-3.2562676335,1.195698900

1,0.2826023658\C,-2.5973503639,2.5563494881,0.0358753178\C,-2.535265726,0.0963576225,-0.4941116484\C,-1.0392816346,-0.0046348129,-0.1447551061\C,-1.1087491741,2.581385578,0.4215948086\C,-0.3942442858,1.3936386266,-0.2584747853\N,-4.664567713,1.2185279394,-0.0917261921\H,-3.2411189288,0.9751964494,1.3550770589\H,-3.1458478142,3.326260817,0.5919807031\H,-2.6961908777,2.7884433859,-1.0359097695\H,-2.6295246269,0.3147863289,-1.5704792831\H,-3.0243232316,-0.8704434546,-0.3154910601\C,-0.3558307002,-0.9259296698,-1.1644830745\C,-0.8526978154,-0.6390766835,1.2430363001\C,-0.9495220445,2.5884081045,1.9512204494\C,-0.4782786019,3.8757059399,-0.1102855797\H,-0.3392672477,1.6303587219,-1.3318924249\H,0.6452042808,1.3409748485,0.0963654504\H,-0.4479832129,-0.5287306742,-2.1811330812\H,-0.8037952286,-1.9258633169,-1.1471510137\H,0.7110702569,-1.0310498098,-0.9373868617\H,-1.43620146,-0.1506629386,2.0245080069\H,0.2007709325,-0.6047553886,1.5420276357\H,-1.1595910918,-1.6906483162,1.2154695877\H,-1.5304908291,1.8124875098,2.451578591\H,-1.2893494636,3.5487044395,2.3533929473\H,0.10191166,2.4572629169,2.2311025048\H,-0.5528520525,3.9332685597,-1.2016750572\H,0.5823387803,3.9312607369,0.1610663159\H,-0.9808550986,4.7527269571,0.311920356\H,-4.9218117419,0.9437069376,-1.0285597751\C,-5.6116460286,1.7482558625,0.7306665361\O,-5.3411952662,2.1767447509,1.8438362412\C,-7.0278289354,1.7705361311,0.1924438238\H,-7.1297313988,1.2943634913,-0.785173074\H,-7.3547598905,2.8103898877,0.1229281372\H,-7.6765157921,1.2655041338,0.9106146488\Version=ES64L-G09RevD.01\State=1-A\HF=-600.9027007\RMSD=9.430e-09\RMSF=3.635e-06\Dipole=0.1421644,-0.5136158,-1.2874715\Quadrupole=3.1819733,-0.3587343,-2.823239,2.0640525,7.4546855,-1.4980434\PG=C01 [X(C12H23N1O1)]\@

Model 9.1

1\1\GINC-R277\FOpt\RM062X\6-31+G(d,p)\C11H22O1\ROOT\14-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\OMe.1.freq\0,1\C,-3.306121718,1.0717995824,0.3631402973\C,-2.7180999063,2.4684646475,0.1577868038\C,-2.5609225649,0.0488378136,-0.4934635679\C,-1.0569655789,-0.0150633664,-0.1633096662\C,-1.2216192544,2.5402877097,0.5195534254\C,-0.4691121137,1.4121326966,-0.2196692356\O,-4.7164277956,1.0407877321,0.1740289679\H,-3.2015089557,0.7959180534,1.4180890466\H,-3.2867153394,3.1940316705,0.753456867\H,-2.8286805318,2.7545779987,-0.8978322359\H,-2.6651981038,0.3253195078,-1.5526435356\H,-3.017893426,-0.9418777416,-0.3680976213\C,-0.3505175145,-0.8575089119,-1.2346417656\C,-0.8206828987,-0.7099732315,1.1877992977\C,-1.0251001932,2.4937606476,2.0438879883\C,-0.6567178976,3.8814559301,0.0312872152\H,-0.4375231015,1.697721131,-1.2819605801\H,0.5760538785,1.3882696669,0.1213454382\C,-5.1846060297,1.222236846,-1.1430045351\H,-0.4751975617,-0.4171752645,-2.2297453644\H,-0.7575939835,-1.8744471386,-1.2593653718\H,0.7234445497,-0.9289768648,-1.0273580323\H,-1.4023612596,-0.2828321633,2.0056427216\H,0.2375075716,-0.6558991248,1.4672680986\H,-1.0942259967,-1.7683072127,1.1129623131\H,-1.5266495945,1.6515290686,2.5223338921\H,-1.4234688359,3.4084630645,2.4967558563\H,0.0404244547,2.4327177882,2.292469533\H,-0.7599721111,3.9821816512,-1.0544728313\H,0.4070455002,3.9696121971,0.2806919413\H,-1.1840512967,4.7186221558,0.5019394875\H,-6.2721734191,1.2819381215,-1.0755223837\H,-4.9218003107,0.3790735601,-1.7944144794\H,-4.8133886614,2.1508149405,-1.5954579847\Version=ES64L-G09RevD.01\State=1-A\HF=-507.4320837\RMSD=2.303e-09\RMSF=1.348e-06\Dipole=0.4337232,0.0763653,-0.3825332\Quadrupole=-1.862599,0.6327836,1.2298153,-0.7101832,3.169458,0.1187208\PG=C01 [X(C11H22O1)]\@

Model 9.2

1\1\GINC-R449\FOpt\RM062X\6-31+G(d,p)\C11H22O1\ROOT\14-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5GB\OMe.2.freq\0,1\C,-3.3016082991,1.0217413052,0.502192333\C,-2.7364898559,2.4142144671,0.2543332613\C,-2.5683742046,-0.0141776215,-0.3513276431\C,-1.0465158412,-0.0344755921,-0.1137436918\C,-1.2270774253,2.5247624681,0.5273921404\C,-0.4928410596,1.4009999063,-0.234558851\O,-4.6833512497,1.0901213204,0.1855417315\H,-3.2081884993,0.7606724829,1.5707053819\H,-3.2879052499,3.1401570838,0.8645301537\H,-2.9372786973,2.6618058575,-0.7976954394\H,-2.7725366627,0.2322568225,-1.4035224008\H,-2.9680231635,-1.0206330805,-0.1718219409\C,-0.387116831,-0.887706889,-1.2061472819\C,-0.7184086039,-0.6925474237,1.2372625068\C,-0.944549156,2.5092733479,2.0389168229\C,-0.7237927408,3.8694307299,-0.0153543076\H,-0.531392155,1.6656294628,-1.3017830043\H,0.5710654264,1.4055341745,0.0440226407\C,-5.4306210091,-0.034441685,0.583393361\H,-0.5791202934,-0.4725341542,-2.2011811641\H,-0.7739026109,-1.9127289642,-1.1849760154\H,0.6983926339,-0.9338714615,-1.0607112214\H,-1.2730075174,-0.2652340615,2.0739967838\H,0.3500529509,-0.5998169895,1.4622828014\H,-0.961171337,-1.7605057638,1.1979190807\H,-1.4095444002,1.6696366422,2.557777736\H,-1.3301220105,3.4269626887,2.4968901118\H,0.1336124179,2.4657005174,2.2305090933\H,-0.8912036026,3.9469772568,-1.094859011\H,0.3498628751,3.9870087429,0.1719641212\H,-1.2444255259,4.7026448246,0.4695267998\H,-6.483883168,0.2200218995,0.4536366402\H,-5.2489690159,-0.2764660024,1.6410868506\H,-5.2059861184,-0.9199523118,-0.0247883793\Version=ES64L-G09RevD.01\State=1-A\HF=-507.4353266\RMSD=7.845e-09\RMSF=4.466e-06\Dipole=0.258927,-0.3911374,0.2187021\Quadrupole=-0.5105208,0.6697922,-0.1592714,2.7867406,-1.2971623,0.0140903\PG=C01 [X(C11H22O1)]\@

Model 10

I1\GINC-R52\FOpt\RM062X\6-31+G(d,p)\C27H26\ROOT\15-Dec-2017\0\#M062X\6-31+G(d,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=12GB\7m.retry.freq\0,1\C,0.2128375068,2.3279274898,1.2872955849\C,1.1633827599,1.1827012882,0.9194715227\C,-0.724137976,-0.0585789612,-0.1825334234\C,-1.3908236328,0.9111659127,-0.9189842024\C,-0.7059792013,2.2338789461,-1.2820554678\C,-0.3269321721,3.0274076895,0.004028054\C,0.9257044017,3.4331032658,2.0859785227\C,-0.9347131457,1.8355320316,2.1987049745\C,2.5380616673,1.2397419196,1.2816103687\C,-1.4269408052,-1.2150743478,0.3000529081\C,-2.7462433892,0.6755700702,-1.2815569585\C,-1.6380442723,3.1650317533,-2.0768133436\C,0.5197915898,2.0004879482,-2.1947791483\H,-1.2112749355,3.5970653256,0.323043702\H,0.4158288768,3.7733547354,-0.3125565465\C,-2.7840022468,-1.4211421552,-0.0742591733\C,-3.4154492841,-0.4557944203,-0.8943327858\C,0.718076398,0.0960348703,0.1791546264\C,1.6507280543,-0.8826026342,-0.3074292726\C,3.0207224373,-0.7964089484,0.0665620833\C,3.4325909381,0.2782281478,0.8903724944\C,-0.8320991519,-2.1573253739,1.1898515049\C,-1.5338744016,-3.2477213414,1.639735691\C,-2.871629302,-3.468185822,1.2280120102\C,-3.4814017668,-2.5687492816,0.392980953\C,3.9462541482,-1.767519054,-0.4046061062\C,3.5415703415,-2.7731469281,-1.2430849282\C,2.1873595331,-2.8410224307,-1.654436218\C,1.2697356952,-1.9266418139,-1.2008407965\H,1.7795012301,3.8500644241,1.5434289956\H,1.2703554261,3.0694799148,3.0597678681\H,0.2200631252,4.2499254982,2.2679155478\H,-1.6257201457,1.150292643,1.7099038424\H,-1.5121807076,2.6988535504,2.5479481512\H,-0.5190938304,1.3294427531,3.0764323553\H,2.8985806482,2.0608770174,1.8883435441\H,-3.2735436025,1.4033732865,-1.8853911773\H,-2.5608143096,3.3886997852,-1.5330778389\H,-1.897780928,2.7400869927,-3.0521288537\H,-1.1224816055,4.1140066051,-2.2553804689\H,1.3411791188,1.4766570024,-1.7080522257\H,0.8998331485,2.9682610605,-2.5408315298\H,0.2212790499,1.4204531116,-3.0743863952\H,-4.4477861232,-0.6130312531,-1.1958975755\H,4.4748984873,0.3432543583,1.191630068\H,0.1884757924,-2.0030555148,1.5224305256\H,-1.0597924827,-3.9474699289,2.3208311543\H,-3.4110083955,-4.3398656605,1.5848566939\H,-4.5130833843,-2.7104255601,0.0816189299\H,4.9845872187,-1.6874160316,-0.0934227264\H,4.2539904001,-3.5087304694,-1.6028999254\H,1.8727817327,-3.6231781689,-2.3382250199\H,0.2395874722,-1.9919902972,-1.5332585692\Version=ES64L-G09RevD.01\State=1-A\HF=-1044.1696475\RMSD=5.279e-09\RMSF=4.203e-06\Dipole=-0.0208125,0.1934992,0.0003672\Quadrupole=3.5254506,1.7867136,-5.3121642,0.1832577,3.2668268,0.3649654\PG=C01 [X(C27H26)]\@

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