Electronic Supplementary Information for:

Expeditious Synthesis of Aromatic-Free Piperidinium-Functionalized Polyethylene as Alkaline Anion Exchange Membranes

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Experimental Methods and Materials

^{1}H and ^{13}C NMR spectra were collected in deuterated solvents on Varian INOVA 400, Bruker 500, or Varian INOVA 600 NMR spectrometers at 22 °C or 50 °C with shifts reported relative to the residual solvent peaks ($CDCl_3$ 7.26 ppm (^{1}H) and 77.16 ppm (^{13}C); or CD_3OD or CD_3OH 3.31 ppm (^{1}H) and 49.00 ppm (^{13}C)). Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm), broad peak (br), apparent (appr.) multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant (Hz) and integration; data for ^{13}C NMR are reported in terms of chemical shift and no special nomenclature is used for equivalent carbons. IR spectra were recorded on a Bruker Vertex V80v Vacuum FT-IR spectrometer using the attenuated total reflectance (ATR) mode of acquisition and are reported in terms of frequency of absorption (4000–800 cm^{-1}). High resolution mass spectrometry analyses were obtained at Princeton University Mass Spectrometry Facility using an Agilent 6210 TOF LC/MS (Electrospray Ionization, ESI).

All reactions and manipulations of air or water sensitive compounds were carried out under dry nitrogen using a Braun UniLab drybox or standard Schlenk techniques unless otherwise specified. Methyl iodide, triphenylphosphine, thiophenol, 2-bromo-5-methylpyridine, XPhos Pd G3, Ir(III) chloride hydrate, 4,4'-di-*tert*-butyl-2,2'-bipyridine, and Grubbs' 2nd generation catalyst ($Cl_2Ru(IMes)(PCy_3)CHPh$) were purchased from Sigma-Aldrich and used as received. Piperidine and *cis*-cyclooctene (95%) were purchased from Sigma-Aldrich and distilled prior to use. 2-(Piperidin-4-yl)ethanol was purchased from J&K Scientific and used as received. Ethyl iodide, n-butyl iodine, n-octyl iodide and 3-(trimethylsilyl)-1-propanesulfonic acid sodium salt (NaDSS) were purchased from TCI and used as received. *N*-Bromosuccinimide and silver hexafluorophosphate were purchased from Oakwood Chemical and used as received. (2,4-Difluorophenyl)boronic acid was purchased from Accela and used as received. Crabtree's catalyst

[(COD)Ir(py)(PCy_3)]PF_6 was purchased from Strem and used as received. Methanol-d_3 (CD_3OH) was purchased from Acros and used as received. Potassium hydroxide, sodium bicarbonate, and sodium chloride were purchased from Mallinckrodt and used as received. All solvents (methylene chloride, diethyl ether, tetrahydrofuran, acetonitrile, toluene, and methanol) were purchased from Sigma-Aldrich or Mallinckrodt. All solvents were purified according to the method of Grubbs.[1] Hydrogen (99.99%) was purchased from Airgas. NMR solvents ($CDCl_3$, CD_3OD, CD_2Cl_2) were purchased from Cambridge Isotope Laboratories (CIL) and used as received. 2,4,6-Triisopropylbenzenethiol (TRIP-thiol) was prepared according to literature procedure.[2] 1-Hexyl-1-methylpiperidin-1-ium bromide (**6**) was prepared according to literature procedures.[3] Chromatographic purification of products was accomplished by flash chromatography on Silicycle F60 silica gel.

The in-plane hydroxide conductivity of the AAEM sample was measured by four-probe electrochemical impedance spectroscopy (EIS) using a Solartron 1280B electrochemical workstation along with ZPlot and ZView software. The conductivity cell was purchased from BekkTeck LLC (Loveland, CO), and a helpful schematic and description of a similar experimental setup has been reported.[4] A strip of the thin film in iodide form (*ca.* 4 cm long × 0.5 cm wide) was converted to the hydroxide form by immersing it in a stirring 30 mL portion of 1 M potassium hydroxide for a minimum of 2 h and the 1 M KOH solution was replaced twice with fresh solution during that time. Residual potassium hydroxide was washed away by immersing the membrane in 3 × 60 mL portions of deionized water for 20 minutes each. The AAEM was then clamped into the cell using a Proto 6104 torque screwdriver set to 1 inch ounce and completely immersed in deionized water at 22 °C during the measurement time. EIS was performed by imposing a small sinusoidal (AC signal) voltage, 10 mV, across the membrane sample at frequencies between

20,000 Hz and 0.1 Hz (scanning from high to low frequencies) and measuring the resultant current response. A Bode plot was used to assess the frequency range over which the impedance approached a constant and the phase angle approached zero. In a Nyquist plot of the data, the high frequency intercept on the real impedance axis was taken to be the resistance of the membrane. This was then used to calculate the hydroxide conductivity by employing the following formula: $\sigma = L / Z' \times A$ where L is the length between sense electrodes (0.425 cm), Z' is the real impedance response at high frequency, and A is the membrane area available for hydroxide conduction (width × thickness). The dimensional measurements were performed using a digital micrometer (± 0.001 mm) purchased from Marathon Watch Company Ltd. (Richmond Hill, ON). The hydroxide conductivity was measured for a minimum of three separate AAEMs (per composition).

Water uptake and percentage dimensional change were measured by the change between the fully hydrated and dried AAEMs. Conversion to the hydroxide form was achieved by immersing it in a stirring 30 mL portion of 1 M potassium hydroxide for a minimum of 2 h and the 1 M KOH solution was replaced twice with fresh solution during that time. Residual potassium hydroxide was washed away by immersing the membrane in 3 × 60 mL portions of deionized water for 20 minutes each. Immediately following hydroxide ion exchange, a sample was dried with a paper towel, measured by length, and weighed on the balance with a piece a weighing paper. The thin film (in the hydroxide form) was dried under full vacuum at 60 °C in order to completely dehydrate it and then weighed and measured. The water uptake percentage value was calculated by: $WU = [(Mass_{wet} - Mass_{dry})/Mass_{dry}] \times 100$. The dimensional change percentage was calculated by: $\Delta L = [(L_{wet} - L_{dry})/L_{dry}] \times 100$.

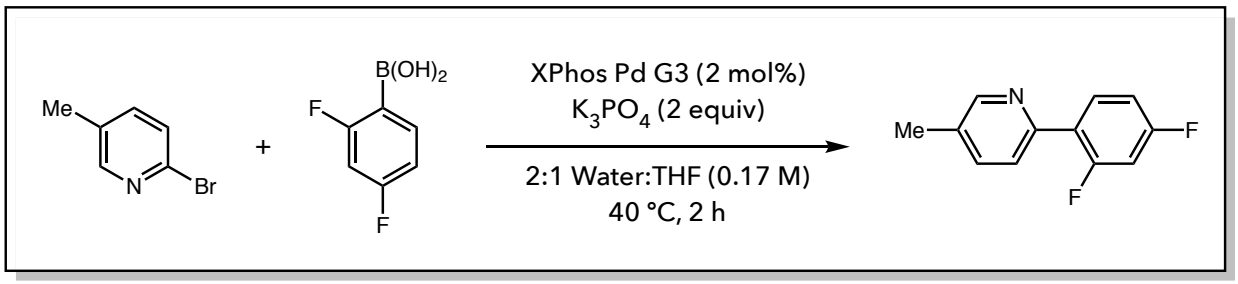
The samples were exchanged to the iodide form in 2 M KI (aq) for 48 hours and washed with water before the mechanical and FT-IR test. Uniaxial tensile elongation was carried out using a Shimadzu Autograph AGS-X tensile tester.

The conductive stability was evaluated according to literature procedures.[5] Strips of the thin film in the iodide form (*ca.* 3 cm long × 0.3 cm wide) were removed from 1 M KOH following the typical exchange procedure and placed in a polypropylene (PP) or a glass vial containing 1 M KOH. The vial was sealed in air and was heated at 80 °C. The KOH solution was periodically replaced with fresh solution to ensure the alkaline concentration remained unchanged. At specified time intervals, membrane strips were re-exchanged with 1 M KOH (typical procedure with a 2 h exchange), washed with water to remove any residual base, and the in-plane hydroxide conductivity was measured at 22 °C.

Synthesis of $[Ir(dF(Me)ppy)_2(dtbbpy)]PF_6$

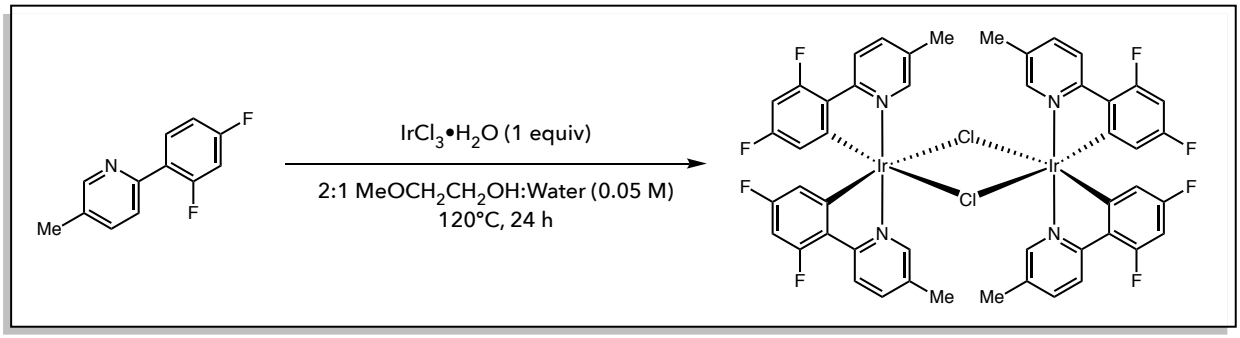
Note: This photocatalyst is commercially available from both Sigma-Aldrich and Strem Chemicals.

2-(2,4-difluorophenyl)-5-methylpyridine



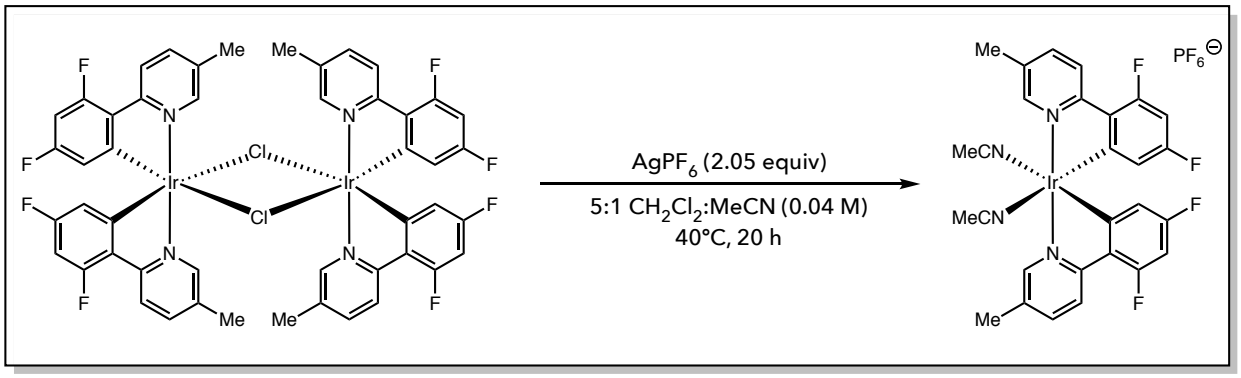
To a 50 mL round-bottom flask was added K_3PO_4 (2.30 g, 10 mmol, 2.0 equiv) and water (20 mL). This solution was degassed by sparging with N_2 for 20 minutes. To a 100 mL round-bottom flask charged with a magnetic stir bar was added 2-bromo-5-methylpyridine (0.86 g, 5.0 mmol, 1.0 equiv), (2,4-difluorophenyl)boronic acid (1.18 g, 7.5 mmol, 1.5 equiv), and XPhos Pd G3 (85 mg, 0.10 mmol, 2 mol%). The flask was evacuated and backfilled with N_2 three times. To this flask was added THF (10 mL) and the aqueous K_3PO_4 solution. The reaction was heated to 40 ºC with vigorous stirring for 2 h. The reaction mixture was then cooled to room temperature and diluted with water (30 mL) and Et_2O (30 mL). The aqueous phase was separated in a separatory funnel and washed with Et_2O (20 mL) three times. The combined organic layers were washed with brine (30 mL), and then dried over Na_2SO_4. Following removal of the solvent *in vacuo*, the crude residue was purified by silica gel chromatography (gradient from 0-5% EtOAc/hexane) to afford 2-(2,4-difluorophenyl)-5-methylpyridine (0.44 g) as a pale yellow solid in 43% yield. Characterization data was consistent with reported literature values.[6]

[Ir(dF(Me)ppy)$_2$Cl]$_2$-dimer



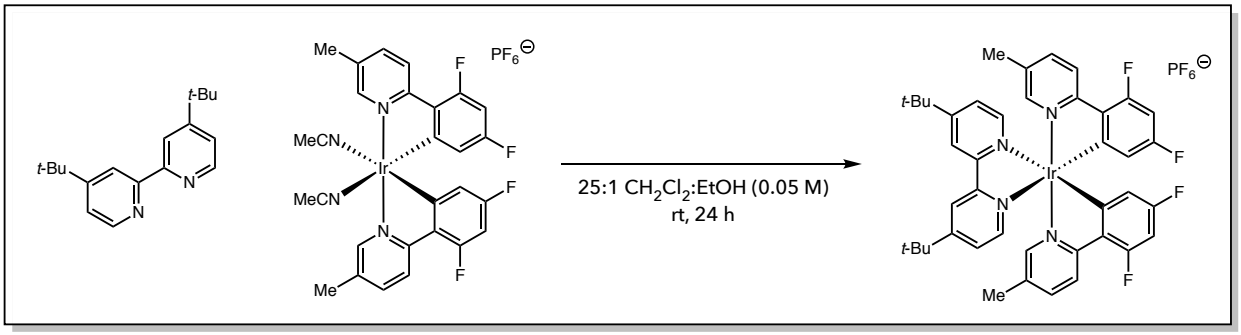
To a flame-dried 250 mL three-necked round-bottom flask with a reflux condenser and stir bar was added $IrCl_3•H_2O$ (0.32 g, 1.0 mmol, 1.0 equiv) and 2-(2,4-difluorophenyl)-5- methylpyridine (0.42 g, 2.1 mmol, 2.1 equiv). The flask was evacuated and backfilled with N_2 three times. 2-Methoxyethanol (13 mL) and water (6.7 mL), each degassed by sparging N_2 for 20 minutes, were added and the reaction was heated to 120 ºC overnight. The reaction mixture was cooled to room temperature, which resulted in the formation of a large amount of yellow precipitate. The solid was filtered and washed with water (20 mL) three times to afford 0.49 g of the crude dimer in 77% yield. The crude dimer was carried on without any further purification.

[Ir(dF(Me)ppy)$_2$(MeCN)$_2$]PF$_6$



To a 50 mL three-necked round-bottom flask charged with a stir bar was added the crude $[Ir(dF(Me)ppy)_2Cl]_2$-dimer (0.48 g, 0.38 mmol, 1.0 equiv) from the previous step. The flask was pumped into a glovebox wherein $AgPF_6$ (0.20 g, 0.78 mmol, 2.1 equiv) was added and the flask capped. After exchanging a cap for a reflux condenser, the flask was evacuated and backfilled with N_2 three times. Dry CH_2Cl_2 (8.0 mL) and MeCN (1.6 mL) were added and the reaction mixture was heated to 40 ºC for 20 h. The reaction mixture was cooled to room temperature and solvent removed *in vacuo*. After taking up the crude residue in acetone, the AgCl salts were filtered off. Pentane was added to the filtrate to afford 0.48 g of $[Ir(dF(CF_3)ppy)_2(MeCN)_2]PF_6$ as a yellow solid in 85% yield. The crude product was carried on without any further purification.

$[Ir(dF(Me)ppy)_2(dtbbpy)]PF_6$



To a 100 mL round-bottom flask with a stir bar was added $[Ir(dF(Me)ppy)_2(MeCN)_2]PF_6$ (0.48 g, 0.65 mmol, 1.0 equiv) and 4,4'-di-*tert*-butyl-2,2'-bipyridine (0.21 g, 0.77 mmol, 1.2 equiv). CH_2Cl_2 (12 mL) and EtOH (0.5 mL) were added and the reaction mixture was stirred at rt overnight. The reaction mixture was filtered through a pad of celite and washed copiously with CH_2Cl_2 to dissolve as much of the crude iridium complex as possible. The resulting filtrate was concentrated *in vacuo* and recrystallized from acetone and pentane to afford 0.54 g of $[Ir(dF(Me)ppy)_2(dtbbpy)]PF_6$ as yellow crystals in 82% yield. Characterization data was consistent with reported literature values.[7]

Synthesis of Piperidinium Monomers

General Procedure:

An oven-dried 16 × 25 mm screw-capped culture tube was equipped with an oven-dried stir bar and charged with $[Ir(dF(Me)ppy)_2(dtbbpy)]PF_6$ (5.1 mg, 0.0050 mmol, 0.25 mol%). The reaction was then pumped into the glovebox, wherein it was sealed with a Teflon cap. Electrical tape was used to seal the sides of the cap, and the reaction vessel was removed from the glovebox. Degassed anhydrous toluene (10 mL, 0.20 M) was then added *via* syringe, followed by 1,5-cyclooctadiene (2.5 mL, 20 mmol, 10 equiv), piperidine (200 μL, 2.0 mmol, 1.0 equiv), and thiophenol (31 μL, 0.30 mmol, 15 mol%). The top of the culture tube was then wrapped in parafilm. This pale yellow solution was irradiated by a single 34W Kessil KSH150B blue LED lamp and magnetically stirred for 24 h. A small rotary fan was placed adjacent to the vial to cool the reaction during irradiation. A typical reaction was measured to run at about 35 ºC. Once completed, the reaction mixture was transferred to a tared 25 mL round-bottom flask and concentrated *via* rotary evaporation. The flask was then evacuated, backfilled with N_2, and quaternized with alkyl iodides.

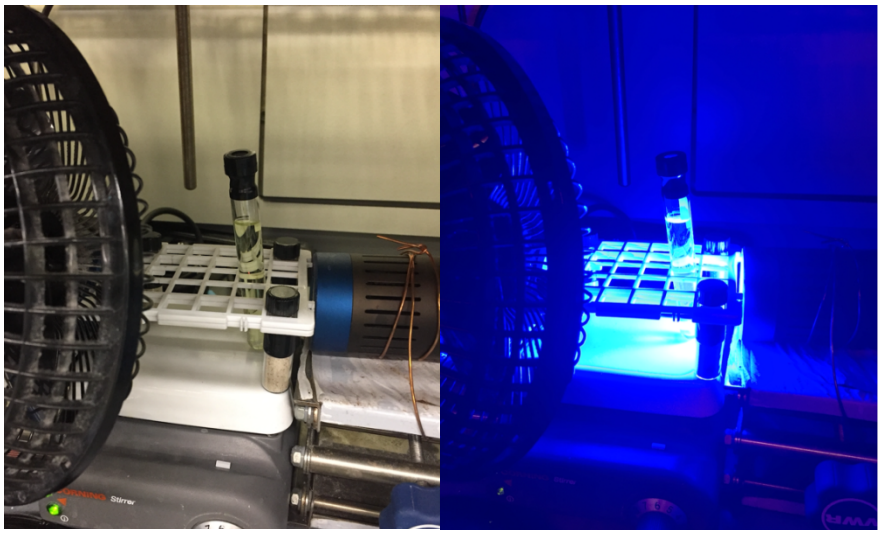


Figure S1. Experimental setup for 2.0 mmol scale hydroamination reaction.

(*Z*)-1-(Cyclooct-4-en-1-yl)-1-methylpiperidinium iodide (1)

Following the general procedure, degassed anhydrous tetrahydrofuran (10 mL, 0.4 M) and iodomethane (0.25 mL, 4.0 mmol, 2.0 equiv) were added into the flask *via* syringe. This mixture was stirred at 65 ºC for 2 h. Over the course of the reaction, white solids crashed out of solution. After cooling the reaction to 22 °C, the solids were triturated. This process was repeated twice more with 5 mL diethyl ether, then the residual solvent was removed under reduced pressure to reveal the title compound as a white solid (0.54 g, 81% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 5.83 (appr. q, *J* = 7.9 Hz, 1H), 5.65 (appr. q, *J* = 9.2 Hz, 1H), 3.98–3.83 (m, 2H), 3.83–3.74 (m, 1H), 3.67–3.74 (m, 2H), 3.16 (s, 3H), 2.58–2.43 (m, 1H), 2.35–2.18 (m, 3H), 2.07 (appr. t, *J* = 10.7 Hz, 1H), 2.02–1.69 (m, 10H), 1.46–1.30 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ 131.8, 128.4, 59.9, 59.4, 44.8, 28.2, 26.6, 26.3, 25.9, 22.6, 20.7, 20.5, 20.3; **HRMS (ESI+):** Calculated for $C_{14}H_{26}N$ ($[M - I]^+$): 208.2065, Found 208.2068.

(*Z*)-1-(Cyclooct-4-en-1-yl)-1-ethylpiperidin-1-ium iodide (2)

Following the general procedure, degassed anhydrous acetonitrile (5.0 mL, 0.4 M) and iodoethane (0.80 mL, 10 mmol, 5.0 equiv) were added into the flask *via* syringe. This mixture was stirred at 80 ºC for 20 h. After this time, the reaction was cooled to 22 °C and most of the solvent (*ca.* 80%) removed *via* rotary evaporation. To this viscous yellow oil was added 5 mL diethyl ether, resulting in the rapid formation of pale yellow precipitates. This was stirred for 5 min, at which time the stirring was terminated and the solids were triturated. This process was repeated twice more, then the residual solvent was removed under reduced pressure to reveal the title compound as a pale yellow solid (0.55 g, 79% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 5.85 (appr. q, *J* = 8.0 Hz, 1H), 5.64 (appr. q, *J* = 9.8 Hz, 1H), 3.74 (dq, *J* = 13.9, 6.5 Hz, 1H), 3.69–3.54 (m, 5H), 3.52–3.44 (m, 1H), 2.57–2.38 (m, 2H), 2.35–2.19 (m, 3H), 2.09–1.75 (m, 11H), 1.37 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ 132.0, 128.1, 55.3, 28.5, 26.7, 26.6, 26.0, 22.7, 20.8, 20.0, 19.9, 8.6; **HRMS (ESI+):** Calculated for $C_{15}H_{28}N$ ($[M - I]^+$): 222.2222, Found 222.2221.

(*Z*)-1-Butyl-1-(cyclooct-4-en-1-yl)piperidin-1-ium iodide (3)

Following the general procedure, degassed anhydrous acetonitrile (5.0 mL, 0.4 M) and iodobutane (1.8 mL, 10 mmol, 5.0 equiv) were added into the flask *via* syringe. This mixture was stirred at 80 ºC for 24 h. After this time, the reaction was cooled to 22 °C and most of the solvent (*ca.* 80%) removed *via* rotary evaporation. To this viscous yellow oil was added 5 mL diethyl ether, resulting in the rapid formation of pale-yellow precipitates. This was stirred for 5 min, at which time the stirring was terminated and the solids triturated. This process was repeated twice more, then the residual solvent was removed under reduced pressure to reveal the title compound as a pale yellow solid (0.60 g, 79% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ **^{1}H NMR (500 MHz, $CDCl_3$):** δ 5.84 (dt, *J* = 10.5, 7.9 Hz, 1H), 5.64 (td, *J* = 10.1, 6.8 Hz, 1H), 3.72–3.57 (m, 4H), 3.52–3.46 (m, 2H), 3.43–3.37 (m, 1H), 2.58–2.43 (m, 2H), 2.36–2.19 (m, 3H), 2.06–1.78 (m, 11H), 1.74–1.66 (m, 1H), 1.46 (q, *J* = 7.4 Hz, 2H), 1.34 (dddd, *J* = 14.0, 10.6, 10.2, 4.7 Hz, 1H), 1.01 (t, *J* = 7.4 Hz, 3H).; **^{13}C NMR (125 MHz, $CDCl_3$):** δ 132.0, 128.1, 66.0, 55.9, 29.4, 28.6, 26.8, 26.7, 25.9, 25.2, 24.6, 22.7, 20.7, 20.3, 20.1, 20.0, 14.0; **HRMS (ESI+):** Calculated for $C_{17}H_{32}N$ ($[M - I]^+$): 250.2535, Found 250.2534.

(*Z*)-1-(Cyclooct-4-en-1-yl)-1-octylpiperidin-1-ium iodide (4)

Following the general procedure, degassed anhydrous acetonitrile (5.0 mL, 0.4 M) and iodooctane (1.8 mL, 10 mmol, 5.0 equiv) were added into the flask *via* syringe. This mixture was stirred at 80 ºC for 24 h. After this time, the reaction was cooled to 22 °C and most of the solvent (*ca.* 80%) removed *via* rotary evaporation. To this viscous yellow oil was added 5 mL diethyl ether, resulting in the rapid formation of pale yellow precipitates. This was stirred for 5 min, at which time the stirring was terminated and the solids triturated. This process was repeated twice more, then the residual solvent was removed under reduced pressure to reveal the title compound as a pale yellow solid (0.66 g, 76% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 5.85 (appr. q, *J* = 7.9 Hz, 1H), 5.64 (appr. q, *J* = 9.7 Hz, 1H), 3.73–3.57 (m, 4H), 3.56–3.43 (m, 2H), 3.43–3.33 (m, 1H), 2.57–2.43 (m, 2H), 2.33–2.20 (m, 3H), 2.04–1.78 (m, 11H), 1.72–1.65 (m, 2H), 1.46–1.22 (m, 12H), 0.88 (t, *J* = 6.3 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ 132.1, 128.1, 55.8, 31.8, 29.3, 29.2, 28.6, 26.9, 26.8, 26.7, 25.9, 22.7, 22.7, 20.7, 20.1, 20.0, 14.2; **HRMS (ESI+):** Calculated for $C_{21}H_{40}N$ ($[M - I]^+$): 306.3161, Found 306.3164.

(*Z*)-1-(Cyclooct-4-en-1-yl)quinuclidin-1-ium bromide (5)

Following the general procedure, 2-(piperidin-4-yl)ethanol (0.26 g, 2.0 mmol, 1 equiv) was used instead of piperidine. Degassed anhydrous CH_2Cl_2 (5.0 mL, 0.4 M) and triphenylphosphine (0.84 g, 3.2 mmol, 1.6 equiv) were added to the residue, then the reaction was cooled to 0 ºC. *N*-Bromosuccinimide (0.57 g, 3.2 mmol, 1.6 equiv) was added portion wise over 5 min. The reaction was allowed to slowly warm to 22 °C and stirred for 2 h. At this time, the crude reaction mixture was directly subjected to silica gel chromatography, eluting with a gradient of 100% CH_2Cl_2 to 5% MeOH in CH_2Cl_2. The clean fractions were combined and the solvent removed via rotary

evaporation. It was found that upon standing for 24 h at 22 °C that the cyclization spontaneously occurred, furnishing the title compound as an off white solid (0.18 g, 30% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 5.76 (appr. q, *J* = 8.2 Hz, 1H), 5.62 (appr. q, *J* = 9.9 Hz, 1H), 3.63 (t, *J* = 7.5 Hz, 6H), 3.46-3.38 (m, 1H), 2.56–2.39 (m, 2H), 2.34–2.16 (m, 5H), 2.14–2.05 (m, 6H), 1.89–1.82 (m, 1H), 1.77–1.69 (m, 2H), 1.45–1.33 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ 131.5, 128.6, 74.7, 52.3, 28.3, 27.6, 26.3, 25.7, 24.2, 22.8, 20.0; **HRMS (ESI+):** Calculated for $C_{15}H_{26}N$ ($[M - Br]^+$): 220.2065, Found 220.2070.

(*Z*)-1-(Cyclooct-4-en-1-yl)piperidin-1-ium chloride (S1)

Following the general hydroamination procedure, the solvent was removed under reduced pressure. The crude residue was then dissolved in diethyl ether, then 1 M HCl in diethyl ether (2 equiv) was added. This was stirred for 30 minutes, over which time brown solids precipitated. These solids were then filtered. The crude brown solid (500 mg) was dissolved in 1 mL MeOH and carefully precipitated in 10 mL Et_2O. The mixture was stirred for 5 min, at which time the stirring was terminated and the solids were triturated. This process was repeated twice more, then the residual solvent was removed under reduced pressure to reveal the title compound as an off white solid (411 mg).

^{1}H NMR (500 MHz, $CDCl_3$): δ 11.64 (br s, 1H), 5.80–5.56 (m, 2H), 3.34–3.26 (m, 2H), 3.21 (ddt, *J* = 12.1, 6.0, 2.5 Hz, 1H), 2.72 (tdt, *J* = 12.8, 9.6, 3.4 Hz, 2H), 2.50–2.34 (m, 3H), 2.29–2.12 (m, 5H), 1.91 (dt, *J* = 13.4, 3.6 Hz, 1H), 1.85–1.73 (m, 3H), 1.65–1.54 (m, 3H), 1.33 (appr. qt, *J* = 13.3, 3.8 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ 131.1, 128.7, 66.5, 49.6, 49.1, 29.1, 28.1, 26.1, 25.3, 22.8, 22.8, 22.7, 22.6.

Scale-up Procedure:

An oven-dried 40 mL scintillation vial was equipped with an oven-dried stir bar and charged with $[Ir(dF(Me)ppy)_2(dtbbpy)]PF_6$ (15 mg, 0.015 mmol, 0.25 mol%). The reaction was then pumped into the glovebox, wherein it was sealed with a Teflon cap. Electrical tape was used to seal the sides of the cap, and the reaction vessel was removed from the glovebox. Degassed anhydrous toluene (30 mL, 0.20 M) was then added *via* syringe, followed by 1,5-cyclooctadiene (7.4 mL, 60 mmol, 10 equiv), piperidine (593 μL, 6.0 mmol, 1.0 equiv), and thiophenol (92 μL, 0.90 mmol, 15 mol%). The top of the culture tube was then wrapped in parafilm. This pale yellow solution was irradiated by four 34W Kessil KSH150B blue LED lamps and magnetically stirred for 36 h. Two small rotary fans were placed adjacent to the vial to cool the reaction during irradiation. Once completed, the reaction mixture was transferred to a tared 100 mL round-bottom flask and concentrated *via* rotary evaporation. The flask was equipped with a reflux condenser, then degassed anhydrous tetrahydrofuran (30 mL, 0.20 M) and iodomethane (0.75 mL, 12 mmol, 2.0 equiv) were added *via* syringe. This mixture was stirred at 65 ºC for 2 h. Over the course of the reaction, white solids crashed out of solution. After cooling the reaction to 22 °C, the solids were triturated. This process was repeated twice more with 15 mL diethyl ether, then the residual solvent was removed under reduced pressure to reveal **(*Z*)-1-(Cyclooct-4-en-1-yl)-1-methylpiperidinium iodide (1)** as a white solid (1.62 g, 80% yield).

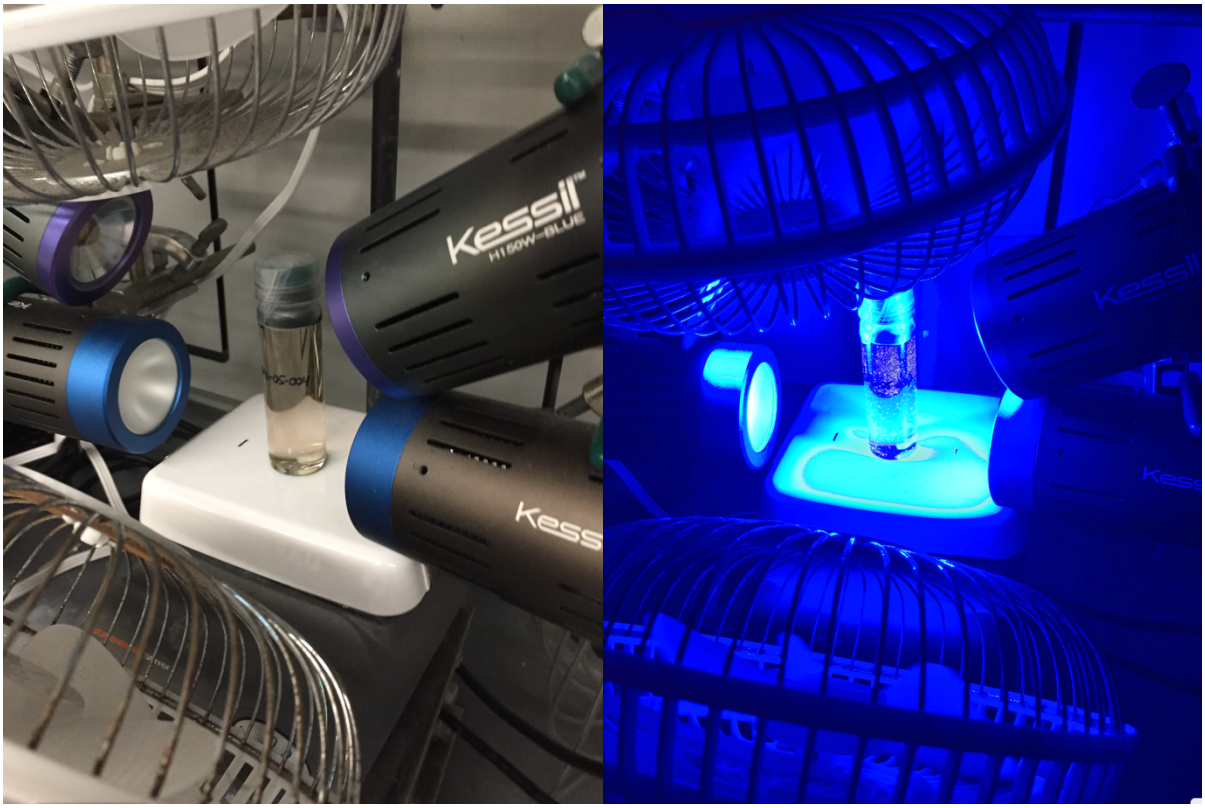


Figure S2. Experimental setup for 6.0 mmol scale hydroamination reaction.

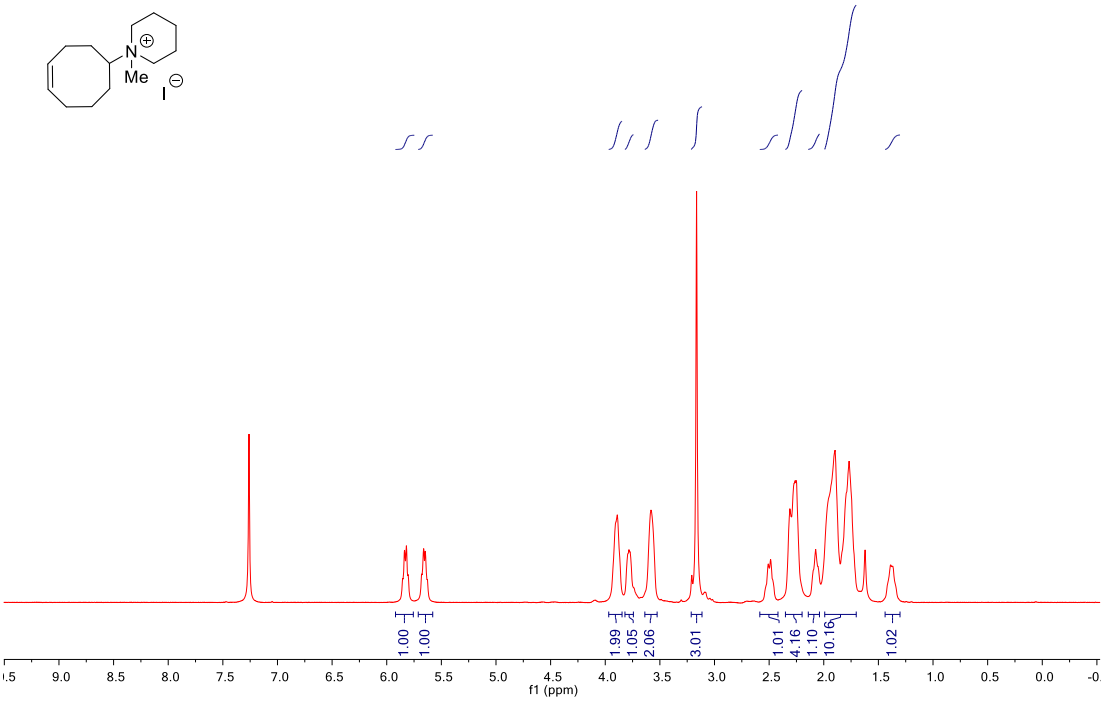


Figure S3. ^{1}H NMR spectrum of **1** in $CDCl_3$.

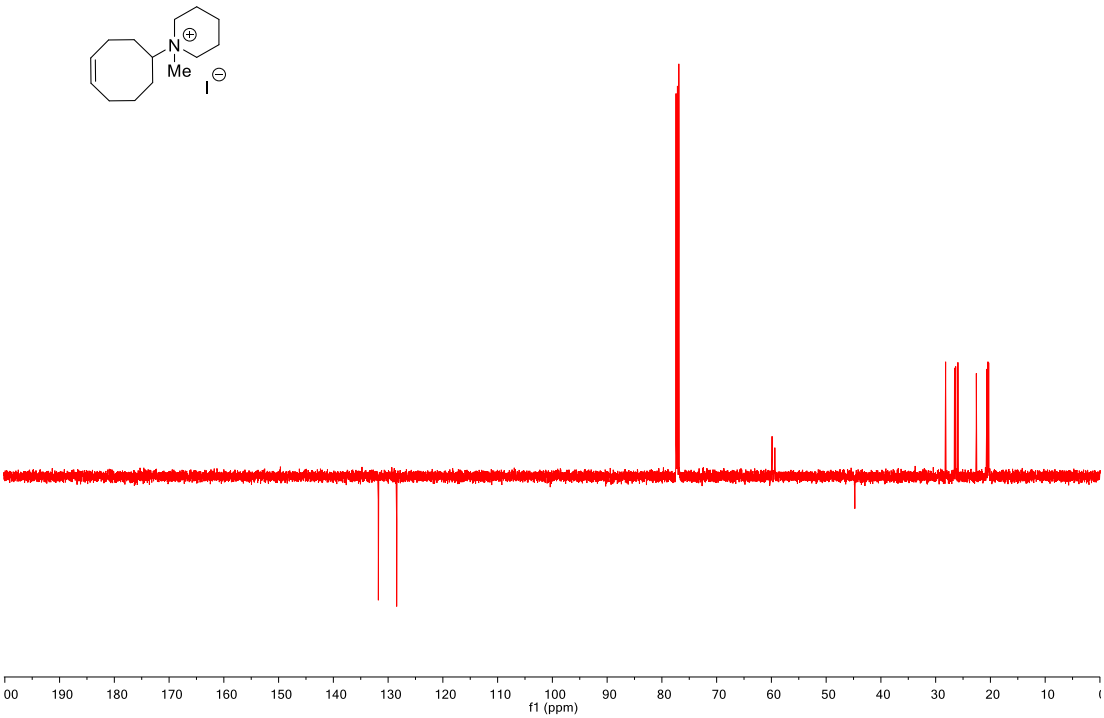


Figure S4. ^{13}C NMR spectrum (APT) of **1** in $CDCl_3$.

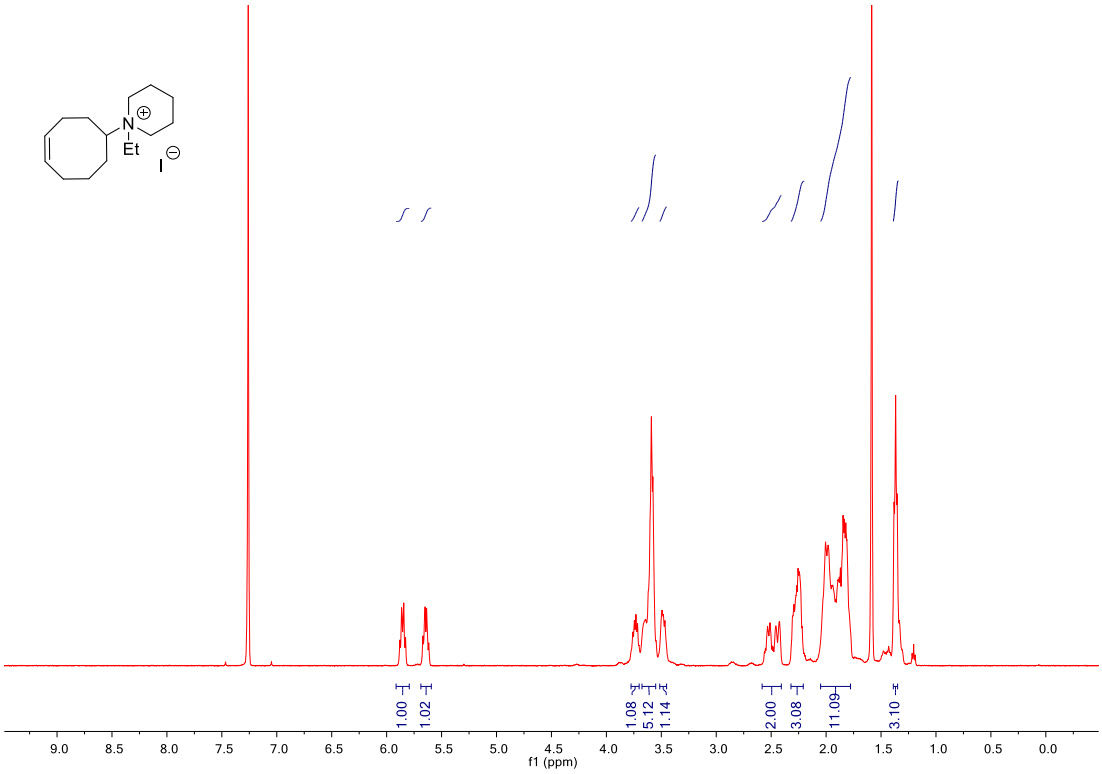


Figure S5. ^{1}H NMR spectrum of **2** in $CDCl_3$.

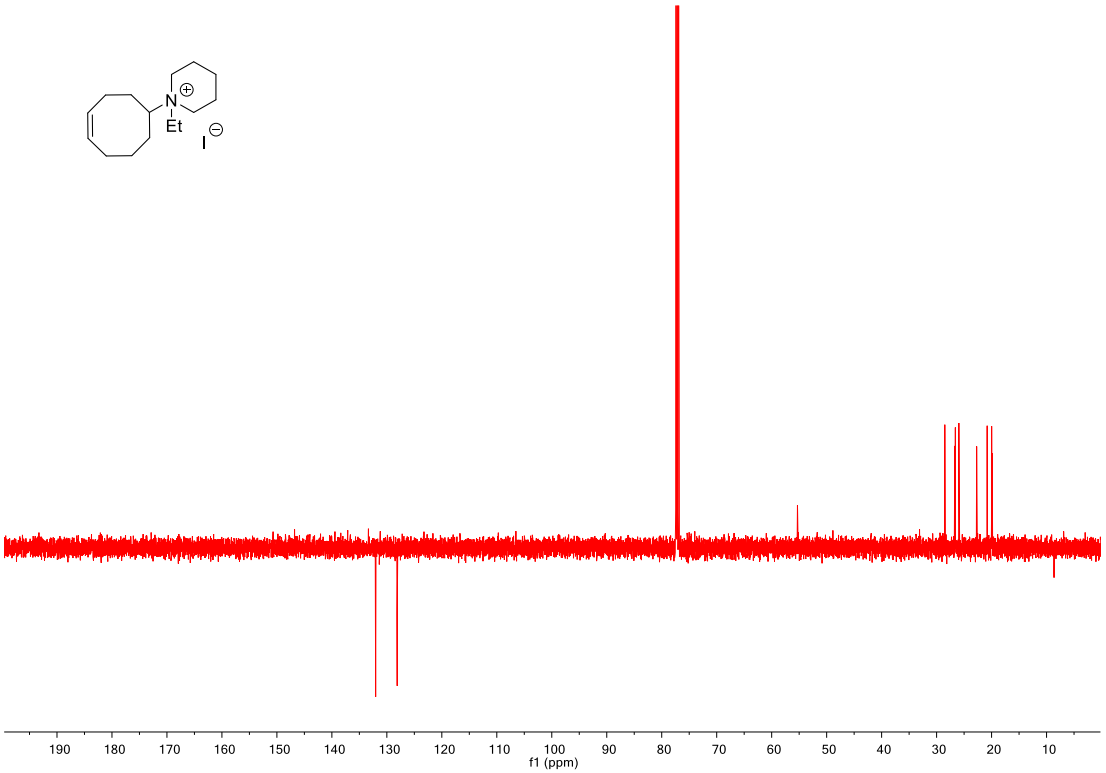


Figure S6. ^{13}C NMR spectrum (APT) of **2** in $CDCl_3$.

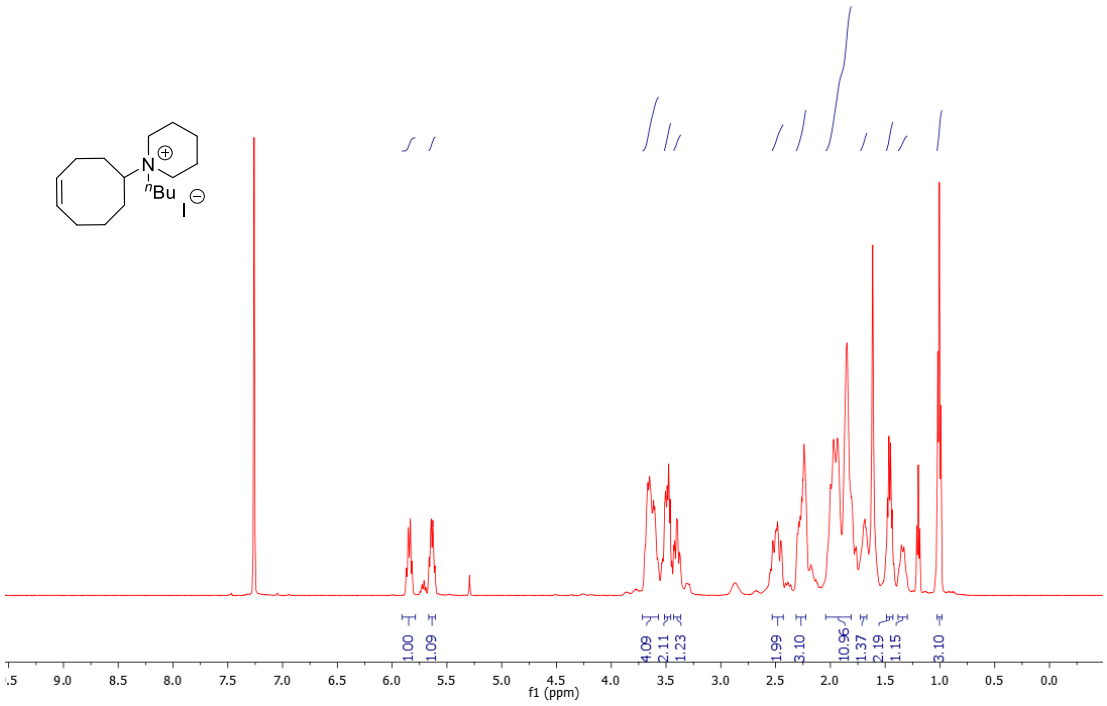


Figure S7. ^{1}H NMR spectrum of **3** in $CDCl_3$.

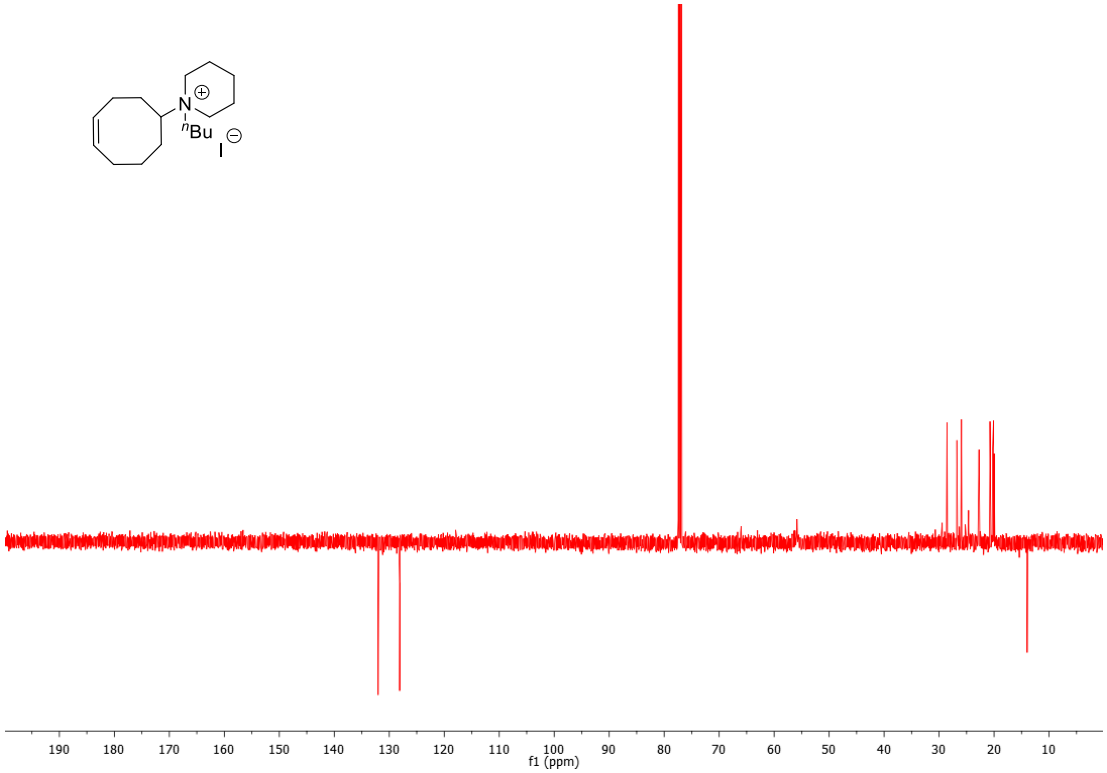


Figure S8. ^{13}C NMR spectrum (APT) of **3** in $CDCl_3$.

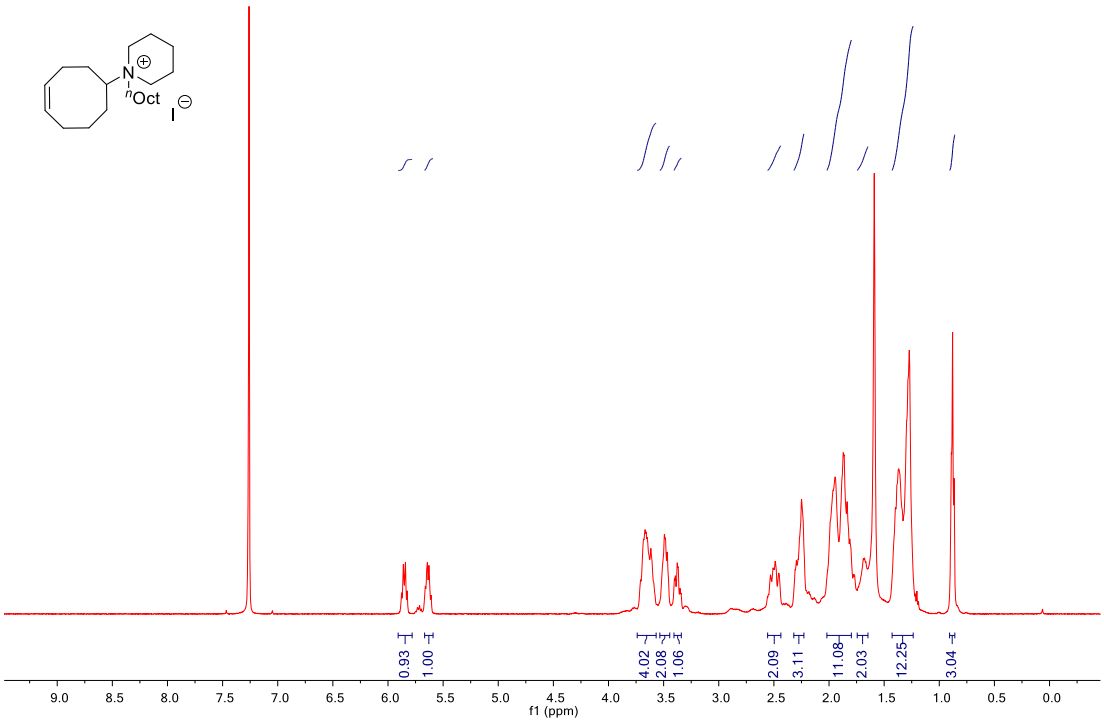


Figure S9. ^{1}H NMR spectrum of **4** in $CDCl_3$.

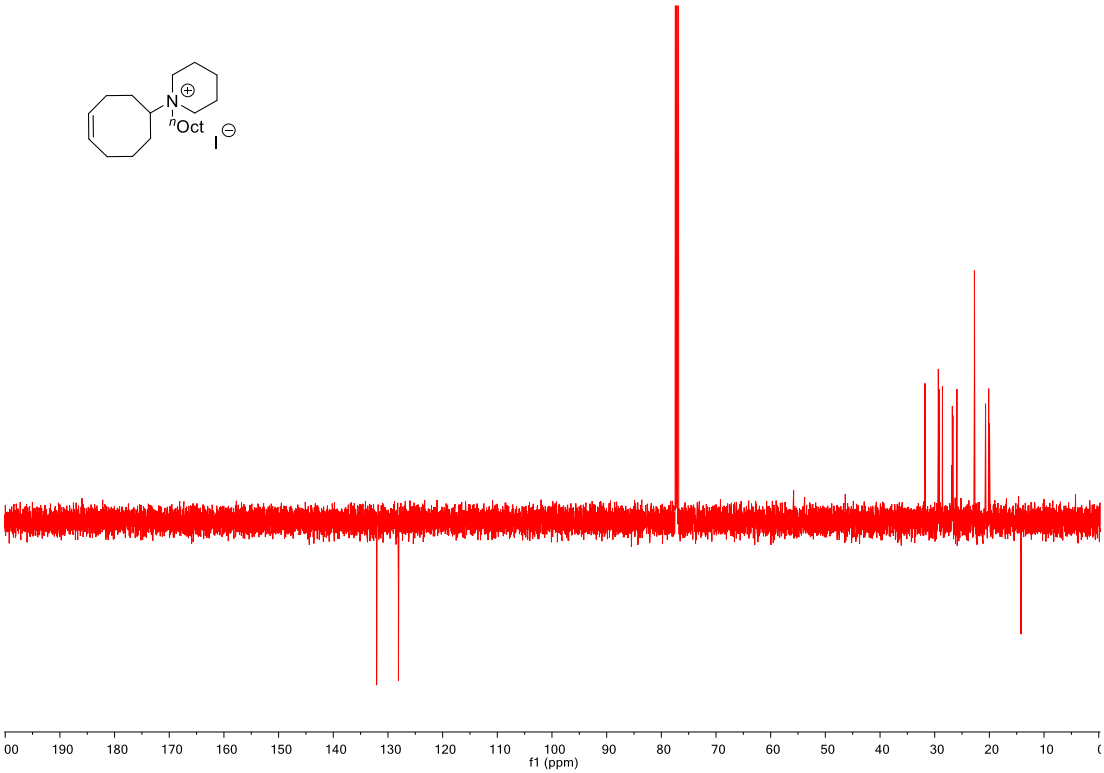


Figure S10. ^{13}C NMR spectrum (APT) of **4** in $CDCl_3$.

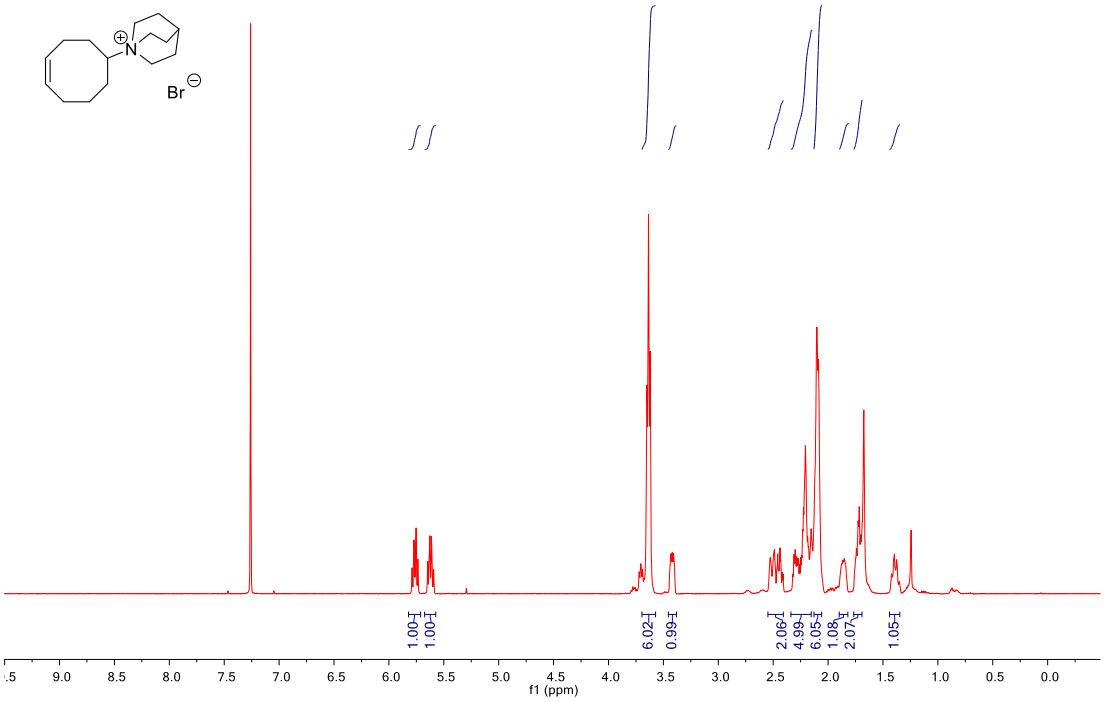


Figure S11. ^{1}H NMR spectrum of **5** in $CDCl_3$.

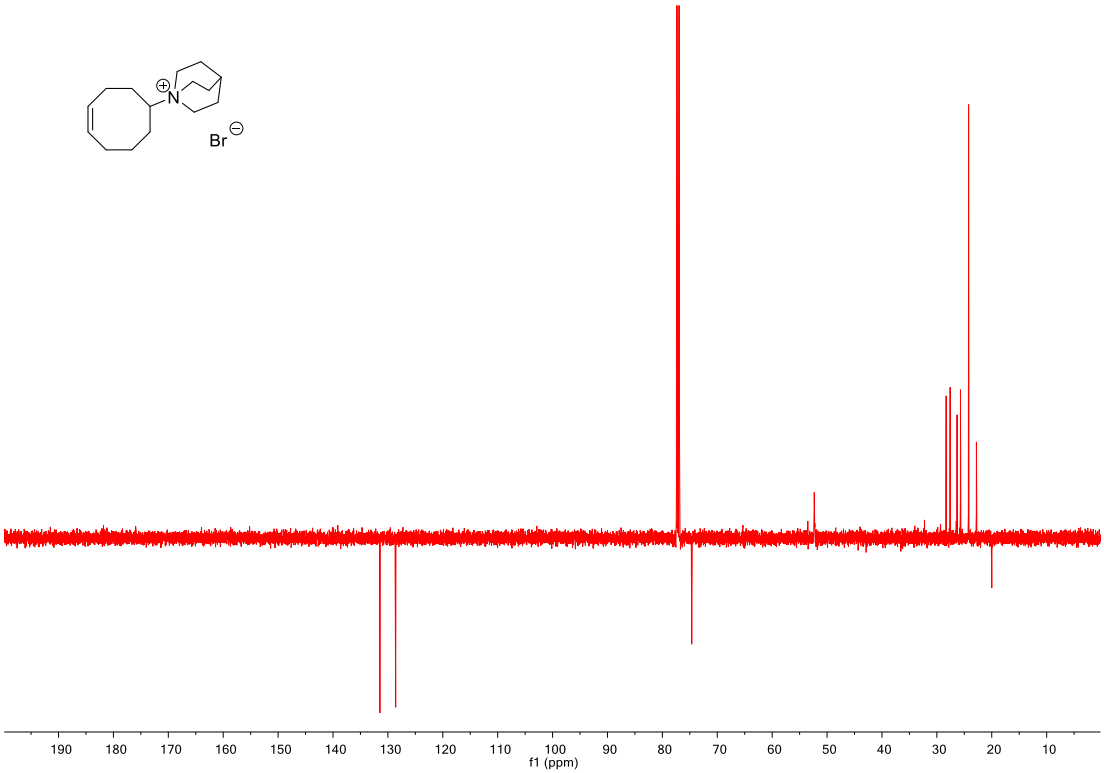


Figure S12. ^{13}C NMR spectrum (APT) of **5** in $CDCl_3$.

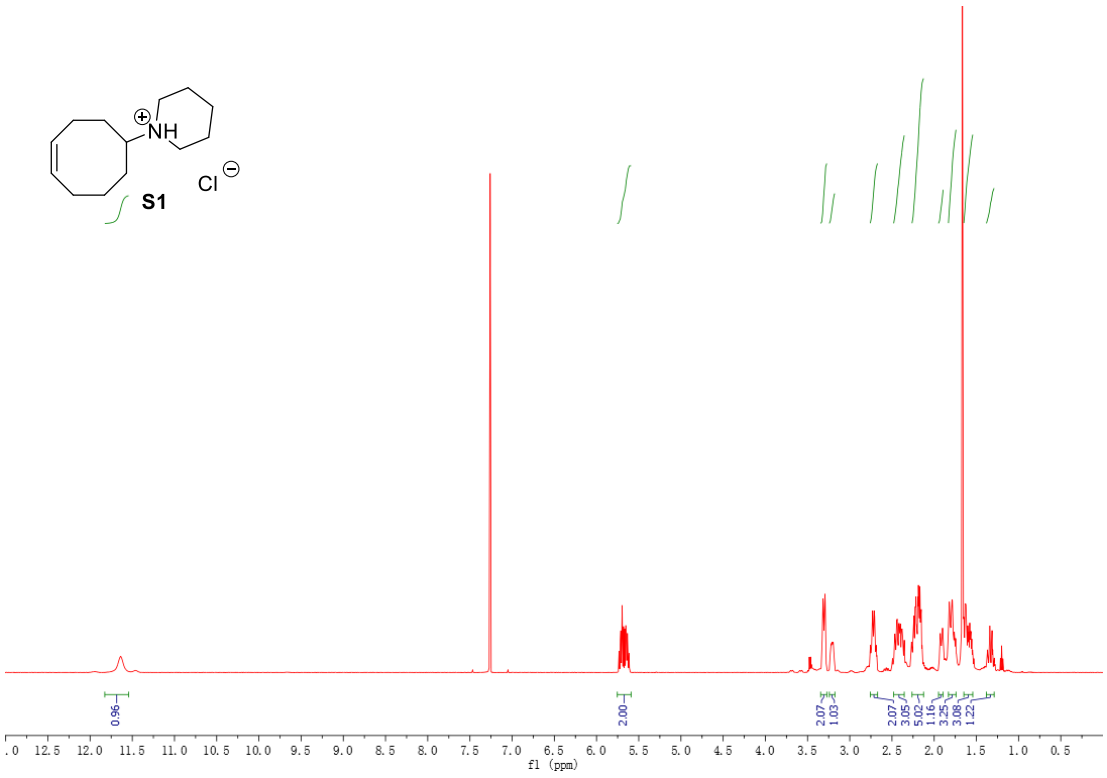


Figure S13. ^{1}H NMR spectrum of **S1** in $CDCl_3$.

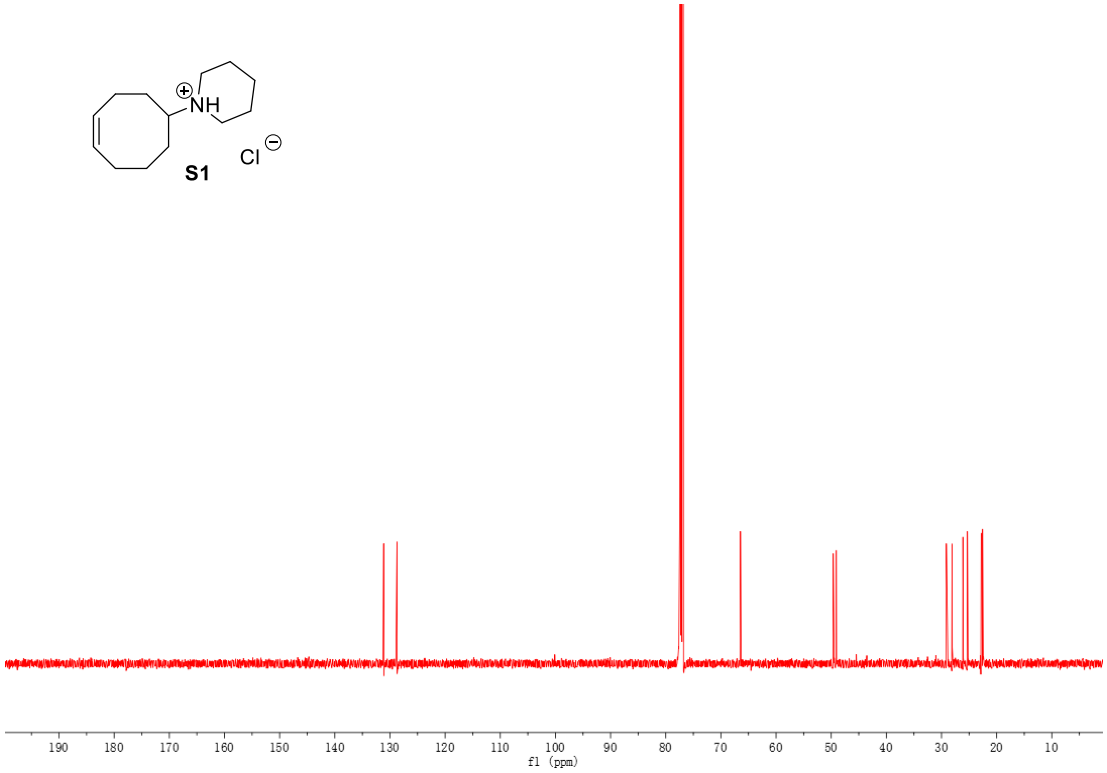
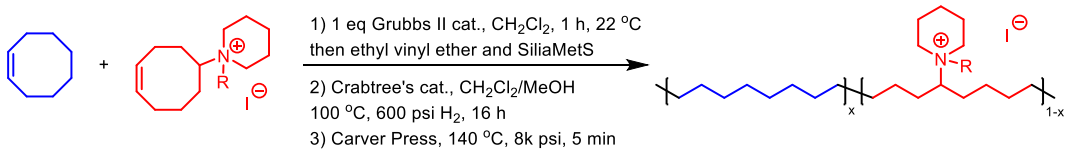


Figure S14. ^{13}C NMR spectrum of **S1** in $CDCl_3$.

Synthesis of Piperidinium-Functionalized AAEMs



Representative Membrane Preparation Procedure:

Under a nitrogen atmosphere piperidinium monomer **1** (0.20 mmol) and COE (0.80 mmol) were combined and dissolved in CH_2Cl_2 (0.80 mL). To the reaction mixture, Grubbs 2nd generation catalyst (0.0010 mmol) dissolved in 0.20 mL of CH_2Cl_2 was added and the solution was stirred vigorously. The reaction was conducted for a minimum of 17 hours. The reaction mixture was then quenched with excess ethyl vinyl ether and silica-bound metal scavenger (SiliaMetS, dimercaptotriazine (DMT)), filtered, and concentrated under reduced pressure. The resultant mixture was washed with acetone three times and dried under high vacuum to afford a pale white polymer. The unsaturated copolymer was then dissolved in a 4:1 CH_2Cl_2/methanol cosolvent (10 mL) forming a yellow solution. The solution and Crabtree's catalyst (0.0020 mmol) were combined in a Parr reactor and sealed. It was pressurized to 40 atm hydrogen and then vented down to 3 atm. This process was repeated twice more to purge the reactor of air, then pressurized to 40 atm and heated to 100 °C with stirring. After 17 hours, it was cooled, vented and the slurry polymer mixture was dried under vacuum furnishing pale yellow solid. The membranes were prepared in a Carver-Press (4120 Hydraulic Unit Carver press and stainless steel die molds, Teflon protective sheets from American Durafilm, 140 °C with 8,000 psig pressure for 5 min).

Representative Ionomer Preparation Procedure:

Under a nitrogen atmosphere piperidinium monomer **1** (0.15 mmol) and COE (0.20 mmol) were combined and dissolved in CH_2Cl_2 (0.80 mL). To the reaction mixture, Grubbs 2nd generation catalyst (0.0010 mmol) dissolved in 0.20 mL of CH_2Cl_2 was added and the solution was stirred

vigorously. The reaction was conducted for a minimum of 17 hours. The reaction mixture was then quenched with excess ethyl vinyl ether and silica-bound metal scavenger (SiliaMetS, dimercaptotriazine (DMT)), filtered, and concentrated under reduced pressure. The resultant mixture was washed with acetone three times and dried under high vacuum to afford a pale brown polymer. The unsaturated copolymer was then dissolved in a 1:1 CH_2Cl_2/methanol cosolvent (10 mL) forming a yellow solution. The solution and Crabtree's catalyst (0.0010 mmol) were combined in a Parr reactor and sealed. It was pressurized to 600 psig hydrogen and then vented down to 50 psig. This process was repeated twice more to purge the reactor of air, then pressurized to 600 psig and heated to 100 °C with stirring. After 17 hours, it was cooled, vented, and directly transferred into a glass solvent evaporation dish. The CH_2Cl_2/methanol cosolvent was removed at 50 °C for 6 hours and 70 °C for 2 hours. The resultant membrane was then soaked in 1 M Na_2CO_3 (aq) for 24 hours and washed with water to exchange the anions to carbonate. The residue polymer was then dried and dissolved in ^{n}PrOH as a 5 wt% solution. The polymer was a gel at 22 °C, and it turned into solution above 50 °C (Figure S15).

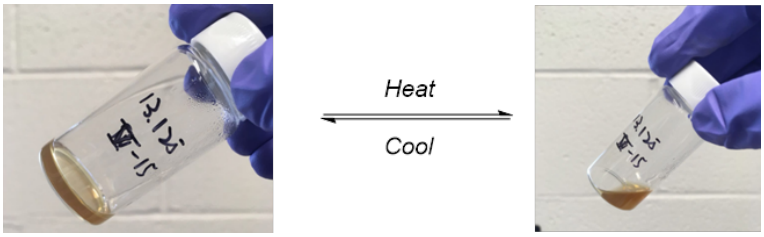


Figure S15. Sol-gel transformation **PEPM$_{43}$** ionomer 5 wt% in ^{n}PrOH.

Representative Oligomer Preparation Procedure:

Under a nitrogen atmosphere piperidinium monomer **1** (0.10 mmol) and COE (0.050 mmol) were combined and dissolved in CH_2Cl_2 (0.20 mL). To the reaction mixture, Grubbs 2nd generation catalyst (0.0020 mmol) dissolved in 0.10 mL of CH_2Cl_2 was added and the solution was stirred vigorously. The reaction was conducted for a minimum of 17 hours. The reaction mixture was then quenched with excess ethyl vinyl ether and silica-bound metal scavenger (SiliaMetS, dimercaptotriazine (DMT)), filtered, and concentrated under reduced pressure. The resultant mixture was washed with acetone:Et_2O (1:1 v/v) three times and dried under high vacuum to afford a pale brown polymer. The unsaturated copolymer was then dissolved in a 1:1 CH_2Cl_2/methanol cosolvent (6 mL) forming a yellow solution. The solution and Crabtree's catalyst (0.0010 mmol) were combined in a Parr reactor and sealed. It was pressurized to 40 atm hydrogen and then vented down to 3 atm. This process was repeated twice more to purge the reactor of air, then pressurized to 40 atm and heated to 100 °C with stirring. After 17 hours, it was cooled, vented, and concentrated to obtain pale brown, viscous oligomers. The oligomers were then subjected to ^{1}H NMR alkaline stability studies in 2 M KOH/CD_3OH at 80 °C for 30 days and the ^{1}H NMR spectra was obtained at 50 °C.

Synthesis of Piperidine-Functionalized Polyethylene (PEP):

Under a nitrogen atmosphere piperidine-HCl monomer **S1** (0.20 mmol) and COE (0.80 mmol) were combined and dissolved in CH_2Cl_2 (0.80 mL) and MeOH (0.10 mL). To the reaction mixture, Grubbs 2nd generation catalyst (0.0010 mmol) dissolved in 0.20 mL of CH_2Cl_2 was added and the solution was stirred vigorously. The reaction was conducted for a minimum of 17 hours. The reaction mixture was then quenched with excess ethyl vinyl ether and silica-bound metal scavenger (SiliaMetS, dimercaptotriazine (DMT)), filtered, and concentrated under reduced

pressure. The resultant mixture was washed with acetone three times and dried under high vacuum to afford a pale white polymer (**pCOEP-HCl**). The polymer was redissolved in 5 mL CH_2Cl_2/methanol cosolvent (4:1 v/v) and was directly transferred into a glass solvent evaporation dish. The solvents were removed at 50 °C for 6 hours and 70 °C for 2 hours. The resultant membrane was then soaked in 1 M KOH (aq) for 24 hours, washed with water, and dried to afford pale white membrane (piperidine-functionalized poly(cyclooctene), **pCOEP)**.

To hydrogenate **pCOEP-HCl**, the unsaturated copolymer was dissolved in a 4:1 CH_2Cl_2/methanol cosolvent (10 mL) forming a yellow solution. The solution and Crabtree's catalyst (0.0020 mmol) were combined in a Parr reactor and sealed. It was pressurized to 40 atm hydrogen and then vented down to 3 atm. This process was repeated twice more to purge the reactor of air, then pressurized to 40 atm and heated to 100 °C with stirring. After 17 hours, it was cooled, vented and the slurry polymer mixture was dried under vacuum furnishing pale yellow solid. The membrane was prepared in a Carver-Press (4120 Hydraulic Unit Carver press and stainless steel die molds, Teflon protective sheets from American Durafilm, 140 °C with 8,000 psig pressure for 5 min). The resultant membrane was then soaked in 1 M KOH (aq) for 24 hours, washed with water, and dried to afford yellow membrane **PEP**.

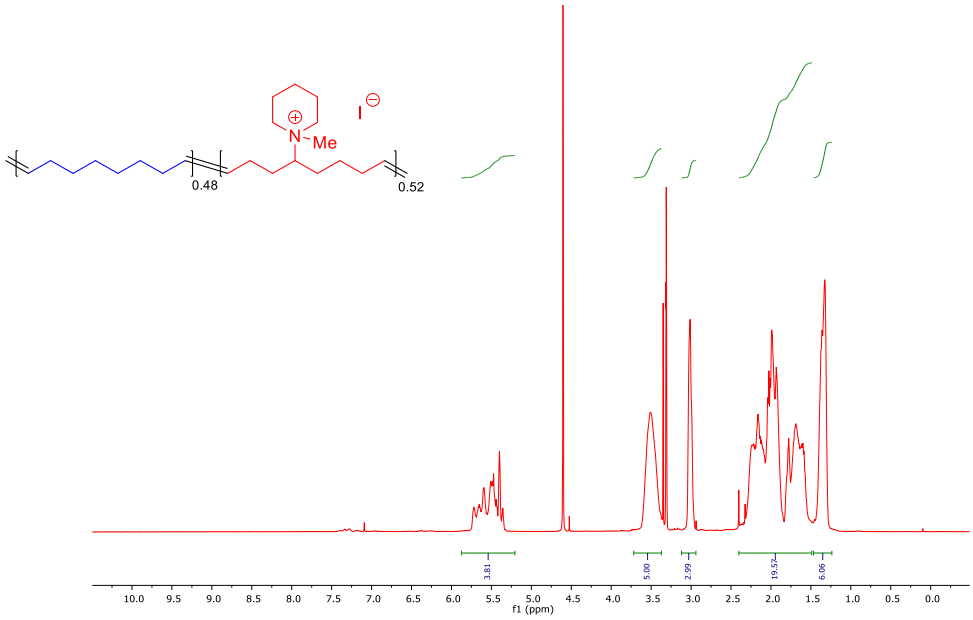


Figure S16. Representative ^{1}H NMR spectrum of oligomer **PEPM$_{52}$** *before hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 5.88–5.21 (br m, 4 H), 3.72–3.37 (br m, 5 H), 3.01 (br s, 3 H), 2.40-1.49 (br m, 20 H), 1.47-1.24 (br m, 6 H).

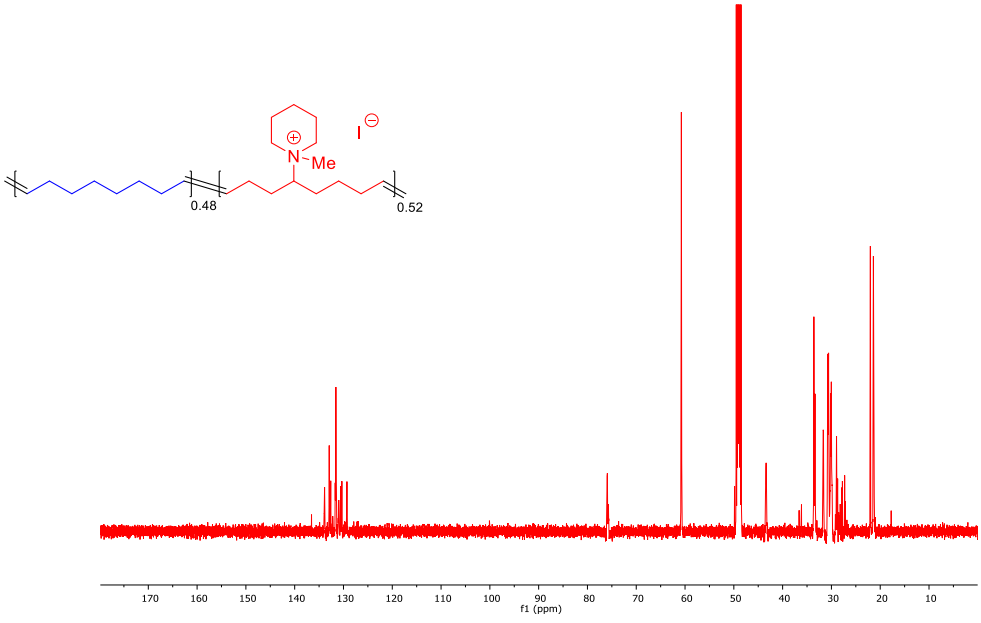


Figure S17. Representative ^{13}C NMR spectrum of oligomer **PEPM$_{52}$** *before hydrogenation* in CD_3OD at 50 °C (500 MHz).

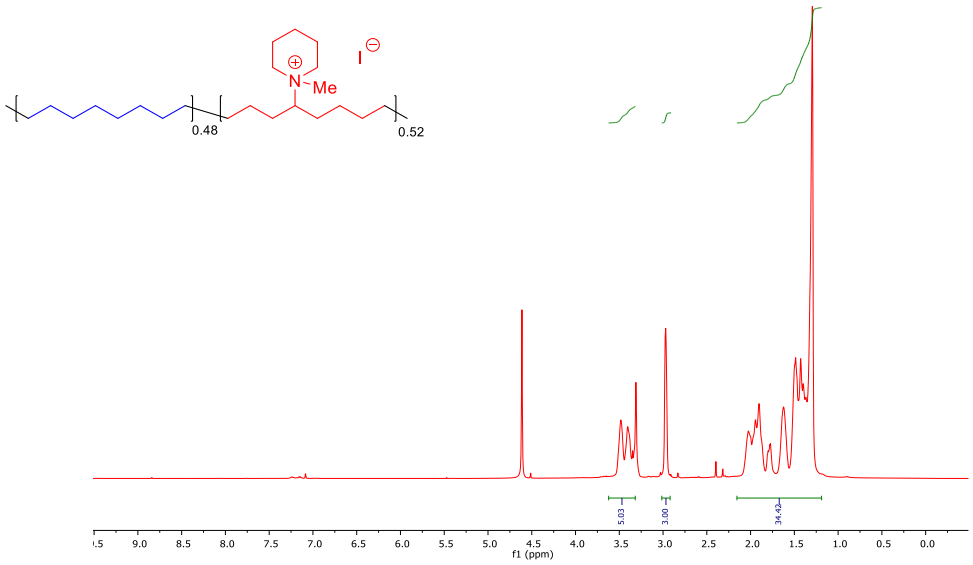


Figure S18. Representative ^{1}H NMR spectrum of oligomer **PEPM$_{52}$** *after hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 3.62–3.32 (br m, 5 H), 2.97 (br s, 3 H), 2.10-1.19 (br m, 34 H).

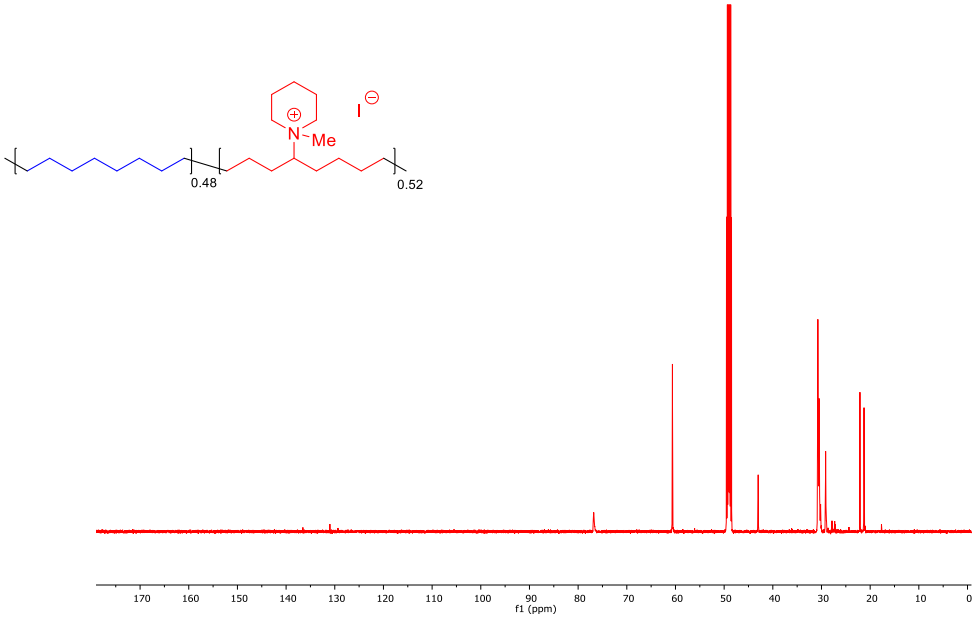


Figure S19. Representative ^{13}C NMR spectrum of oligomer **PEPM$_{52}$** *after hydrogenation* in CD_3OD at 50 °C. **^{13}C NMR (125 MHz, CD_3OD):** δ 76.8, 60.6, 43.0, 30.8, 30.5, 30.2, 29.2, 22.1, 21.3.

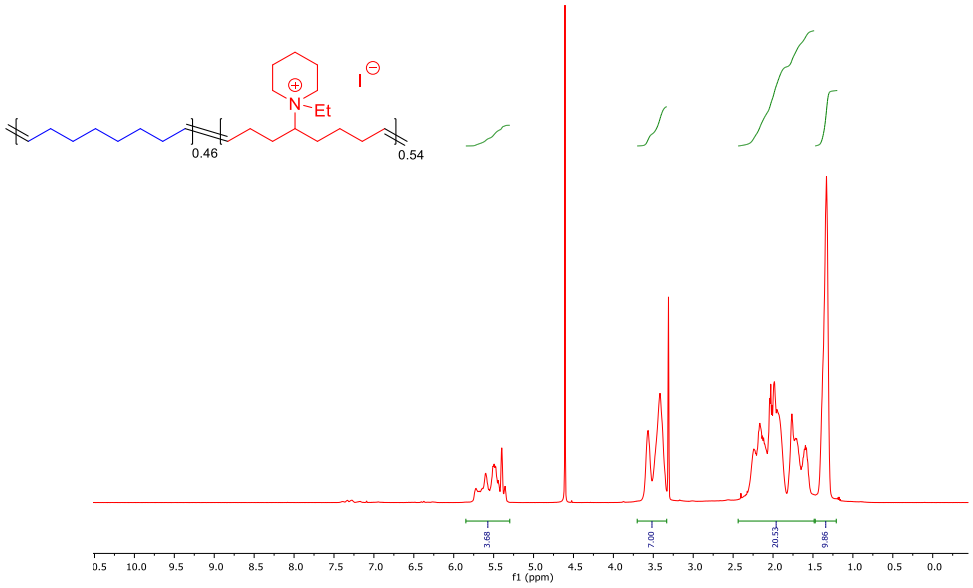


Figure S20. Representative ^{1}H NMR spectrum of oligomer **PEPE$_{54}$** *before hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 5.85–5.30 (br m, 4 H), 3.70–3.33 (br m, 7 H), 2.44–1.49 (br m, 21 H), 1.47-1.21 (br m, 10 H).

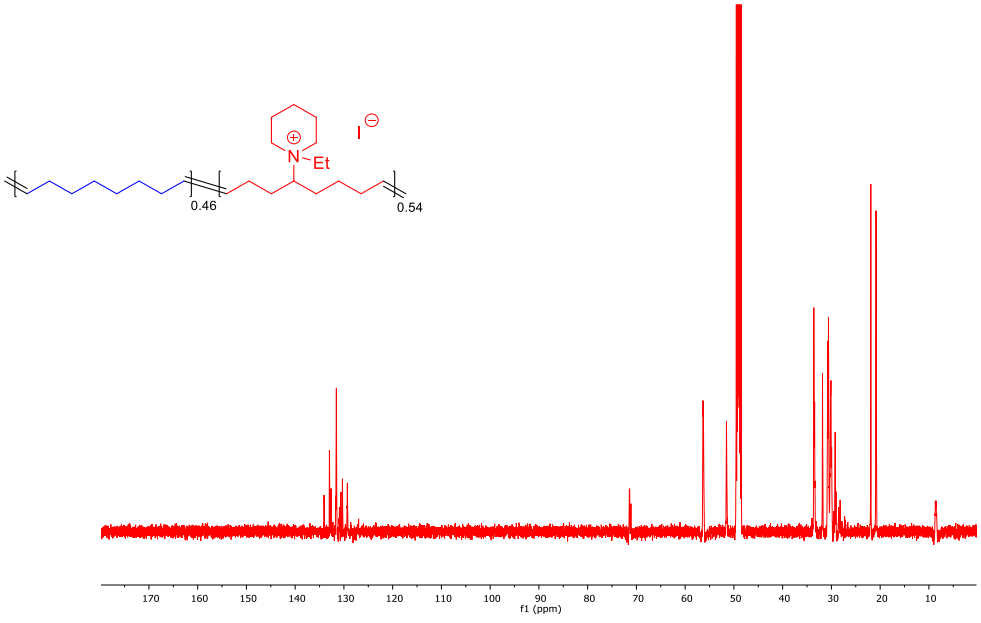


Figure S21. Representative ^{13}C NMR spectrum of oligomer **PEPE$_{54}$** *before hydrogenation* in CD_3OD at 50 °C (500 MHz).

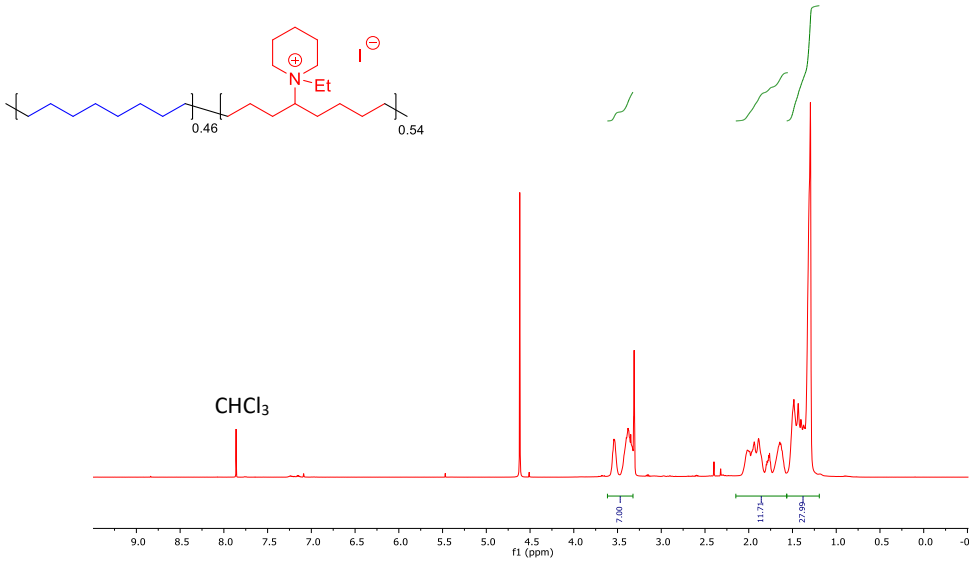


Figure S22. Representative ^{1}H NMR spectrum of oligomer **PEPE$_{54}$** *after hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 3.62–3.32 (br m, 7 H), 2.15–1.57 (br m, 12 H), 1.57–1.19 (br m, 28 H).

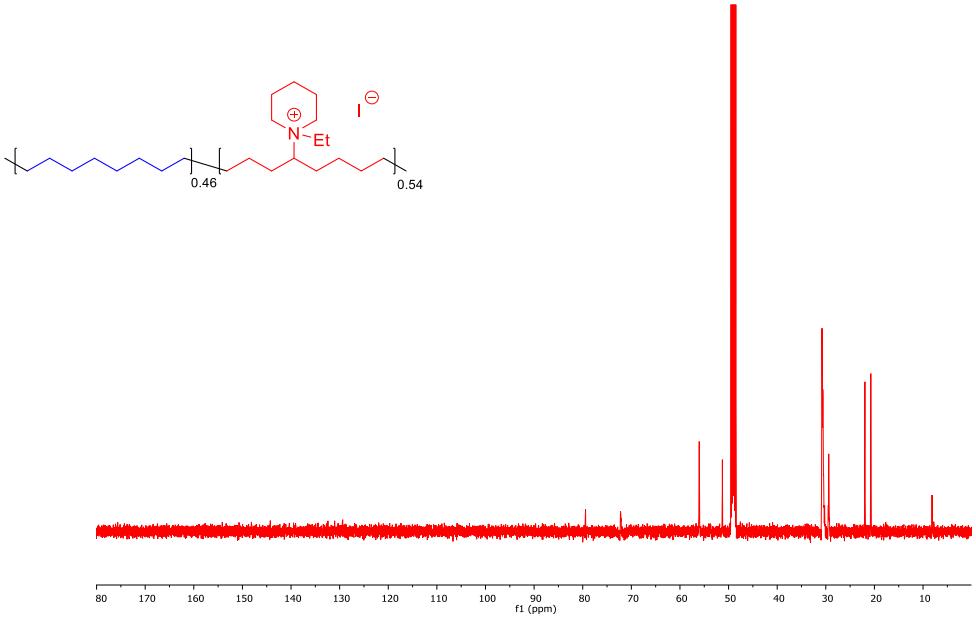


Figure S23. Representative ^{13}C NMR spectrum of oligomer **PEPE$_{54}$** *after hydrogenation* in CD_3OD at 50 °C. **^{13}C NMR (125 MHz, CD_3OD):** δ 72.2, 56.0, 51.3, 30.8, 30.6, 29.4, 22.0, 20.7, 8.2.

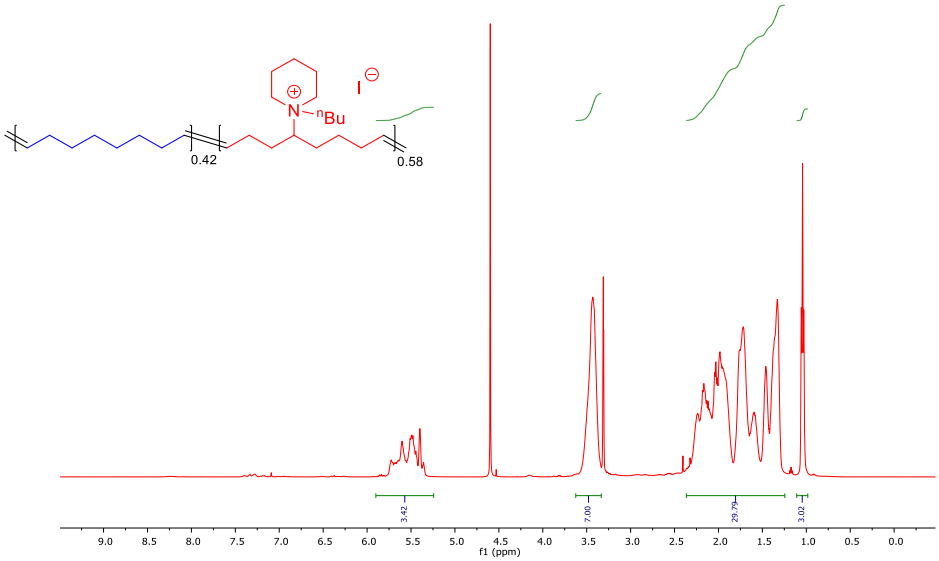


Figure S24. Representative ^{1}H NMR spectrum of oligomer **PEPB$_{58}$** *before hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 5.90–5.24 (br m, 3 H), 3.63–3.34 (br m, 7 H), 2.37–1.25 (br m, 30 H), 1.04 (t, J = 7.3 Hz, 3H).

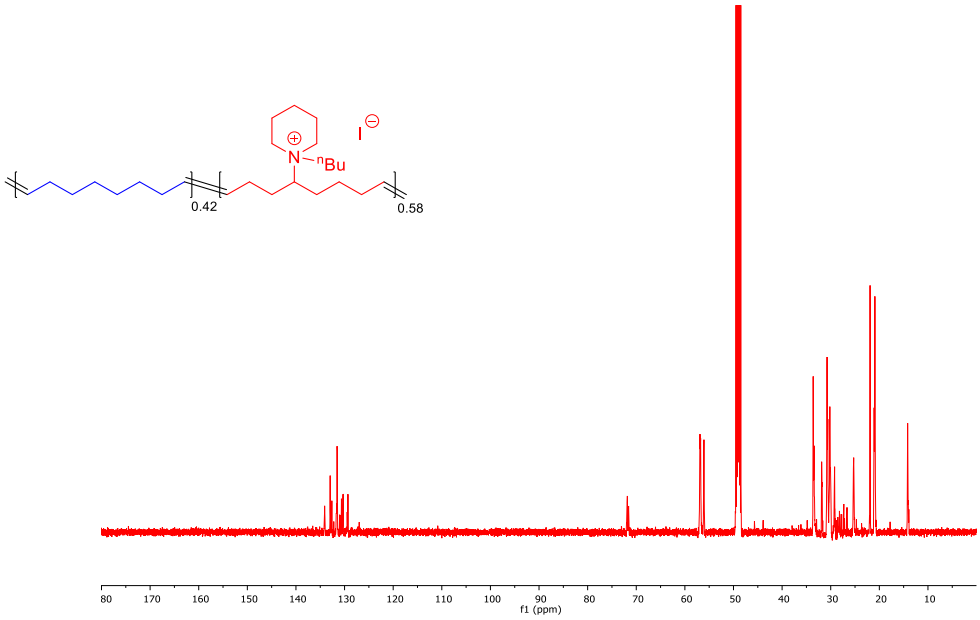


Figure S25. Representative ^{13}C NMR spectrum of oligomer **PEPB$_{58}$** *before hydrogenation* in CD_3OD at 50 °C (125 MHz).

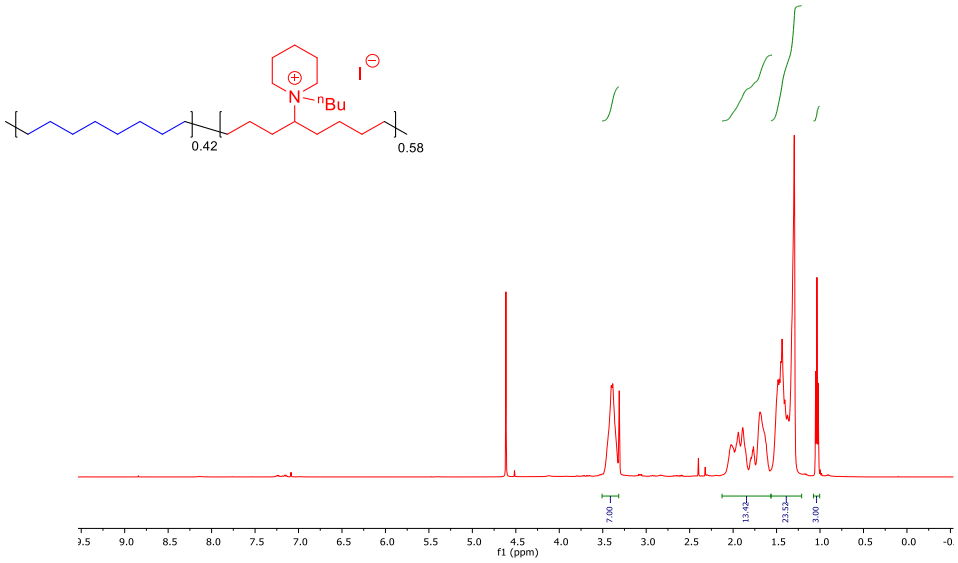


Figure S26. Representative ^{1}H NMR spectrum of oligomer **PEPB$_{58}$** *after hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 3.51–3.32 (br m, 7 H), 2.13–1.57 (br m, 13 H), 1.57–1.21 (br m, 24 H), 1.04 (t, J = 7.4 Hz, 1H).

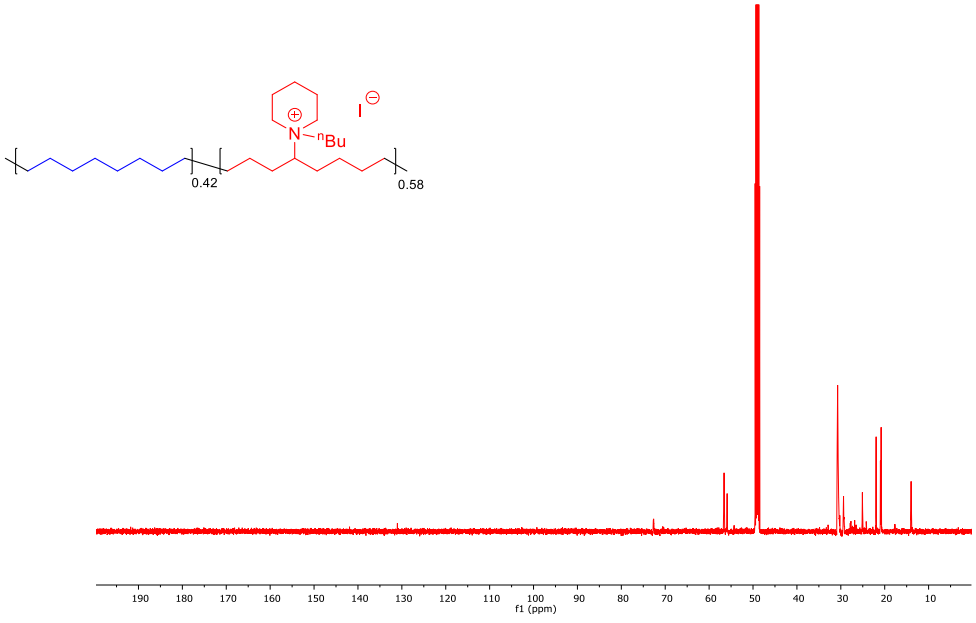


Figure S27. Representative ^{13}C NMR spectrum of oligomer **PEPB$_{58}$** *after hydrogenation* in CD_3OD at 50 °C (125 MHz).

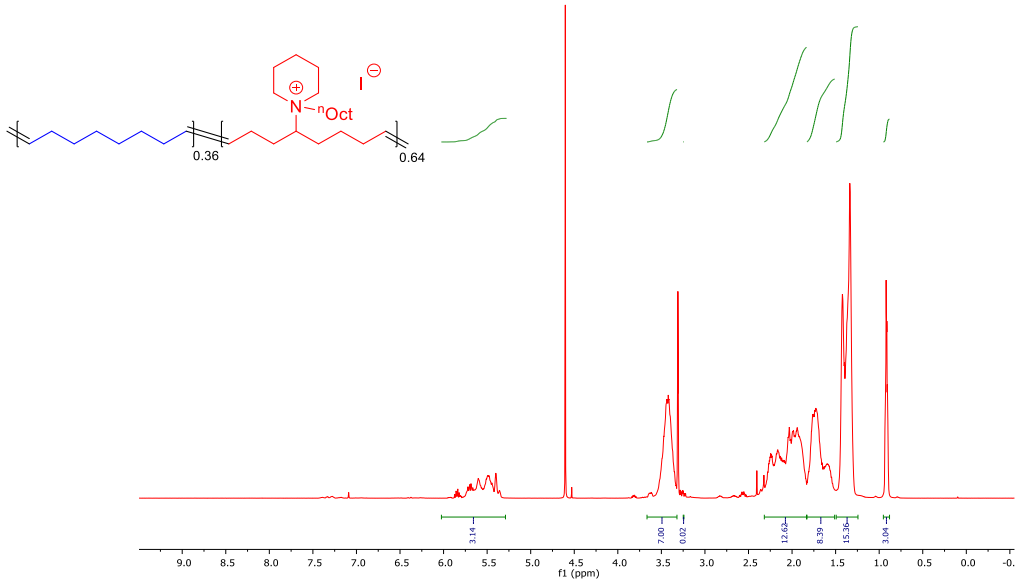


Figure S28. Representative ^{1}H NMR spectrum of oligomer **PEPO$_{64}$** *before hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 6.03–5.29 (br m, 3 H), 3.67–3.32 (br m, 7 H), 2.32–1.83 (br m, 13 H), 1.83–1.51 (br m, 8H), 1.49–1.24 (br m, 15H), 0.95–0.88 (br m, 3H).

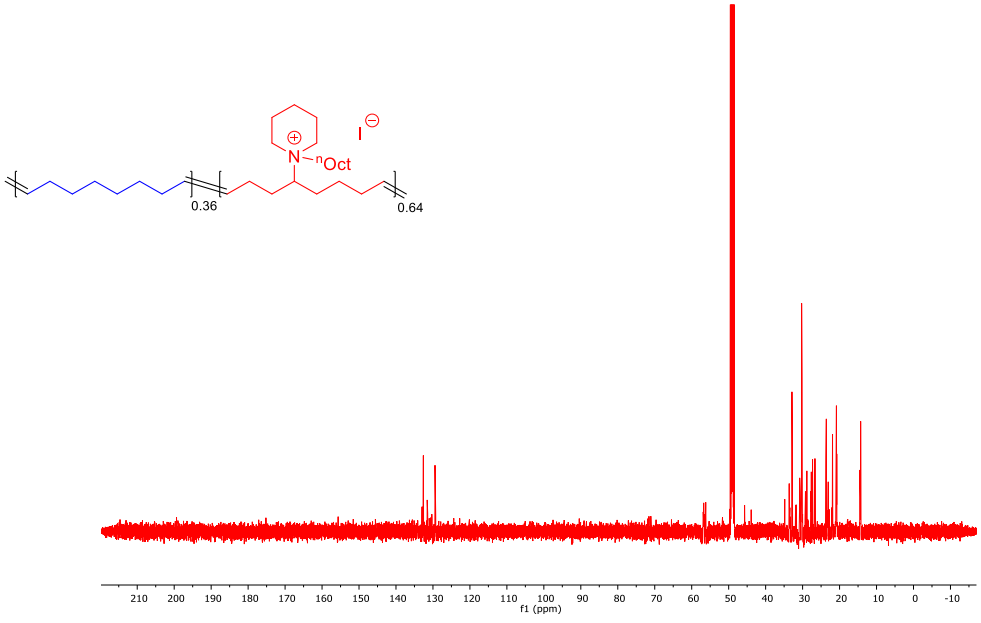


Figure S29. Representative ^{13}C NMR spectrum of oligomer **PEPO$_{64}$** *before hydrogenation* in CD_3OD at 50 °C (125 MHz).

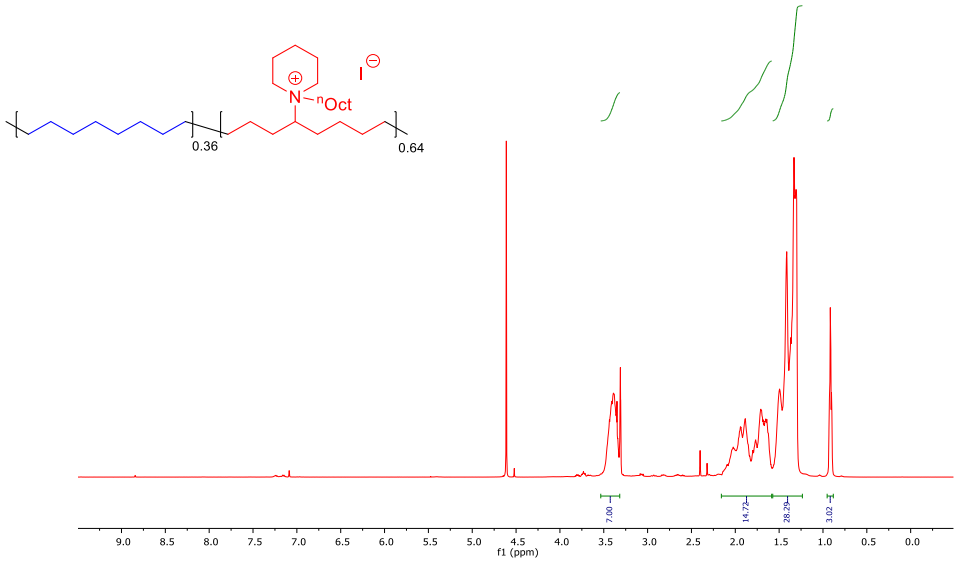


Figure S30. Representative ^{1}H NMR spectrum of oligomer **PEPO$_{64}$** *after hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 3.53–3.32 (br m, 7 H), 2.16–1.59 (br m, 15 H), 1.57–1.24 (br m, 28 H), 0.95–0.88 (br m, 3H).

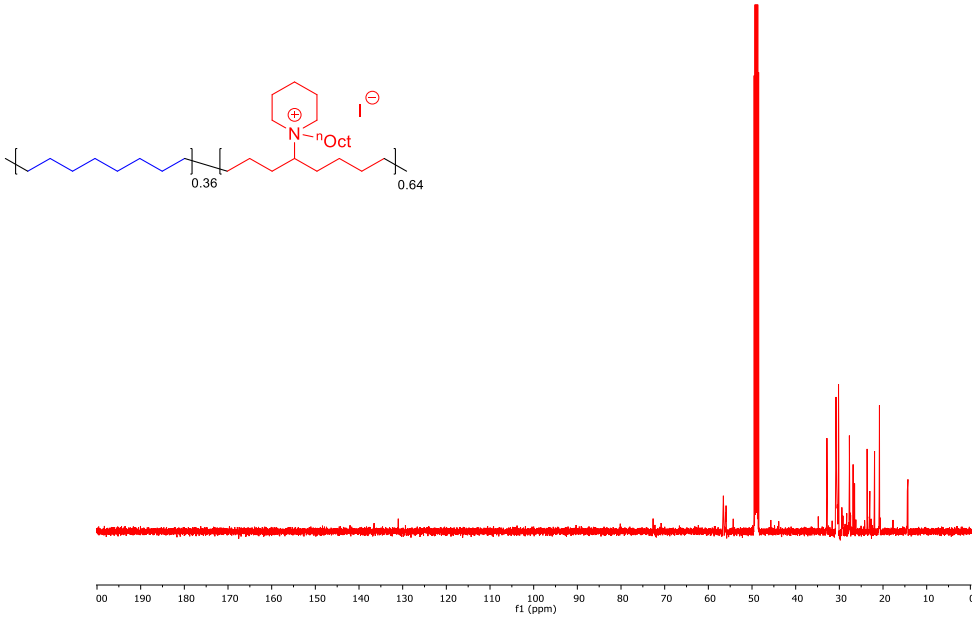


Figure S31. Representative ^{13}C NMR spectrum of oligomer **PEPO$_{64}$** *after hydrogenation* in CD_3OD at 50 °C (125 MHz).

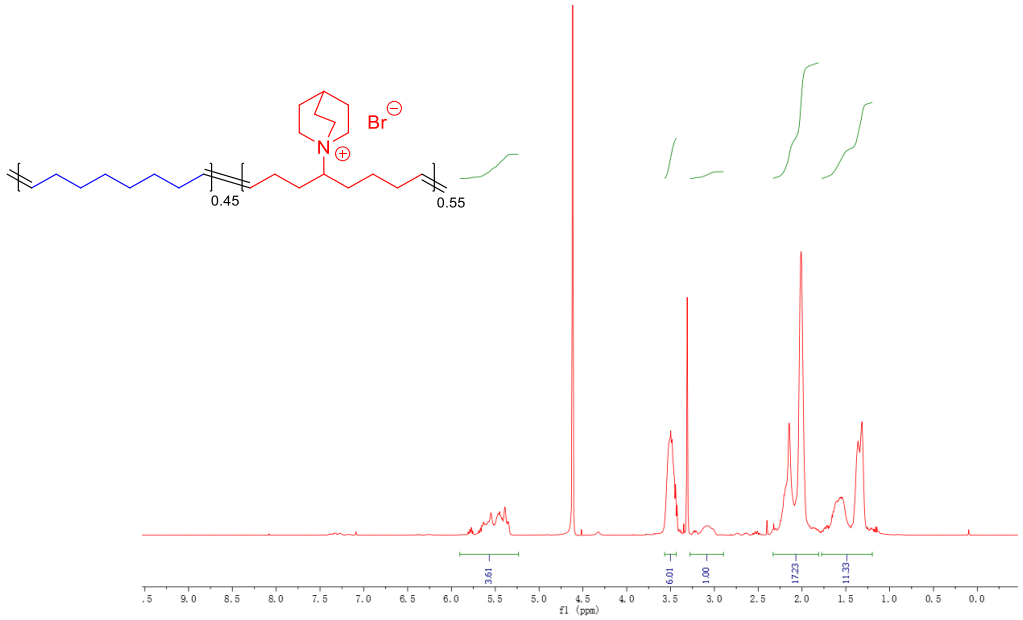


Figure S32. Representative ^{1}H NMR spectrum of oligomer **PEQ$_{55}$** *before hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 5.79–5.27 (br m, 4 H), 3.75–3.35 (br m, 6 H), 3.28–2.90 (br m, 1 H), 2.30–1.84 (br m, 17 H), 1.77–1.24 (br m, 11H).

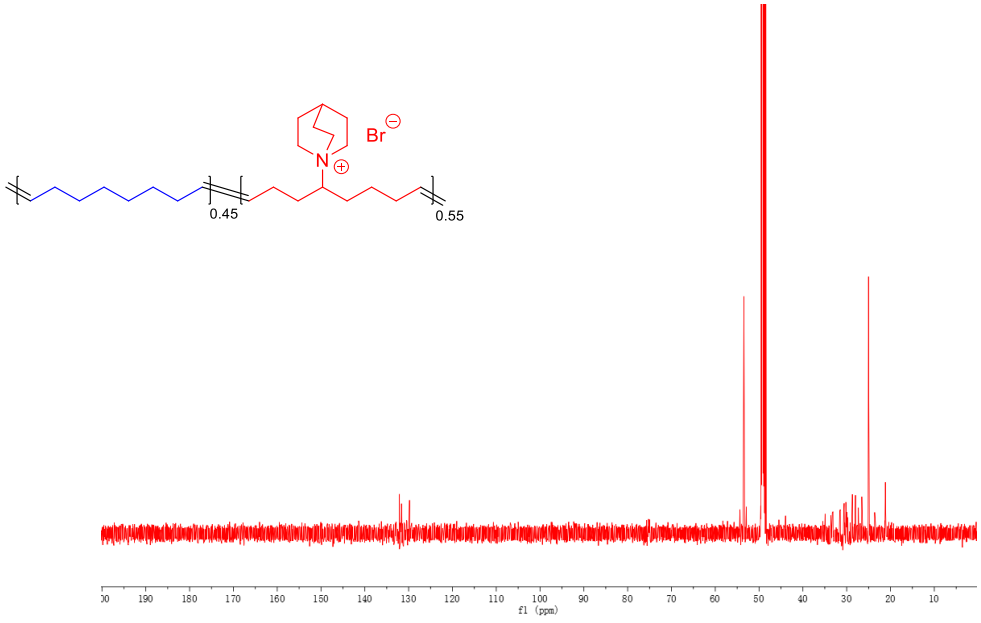


Figure S33. Representative ^{13}C NMR spectrum of oligomer **PEQ$_{55}$** *before hydrogenation* in CD_3OD at 50 °C (125 MHz).

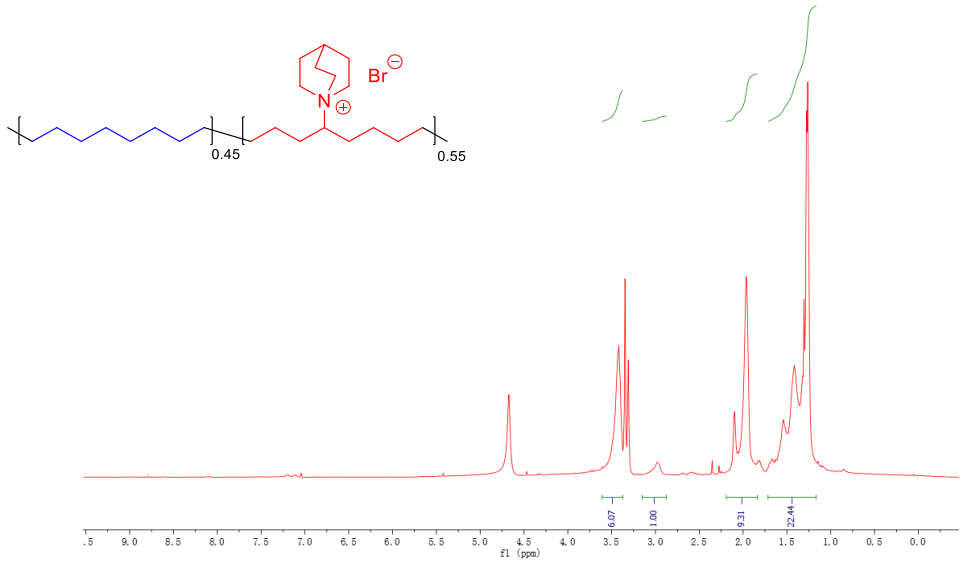


Figure S34. Representative ^{1}H NMR spectrum of oligomer **PEQ$_{55}$** *after hydrogenation* in CD_3OD at 50 °C. **^{1}H NMR (500 MHz, CD_3OD):** δ 3.61–3.37 (br m, 6 H), 3.15–2.88 (br m, 1H), 2.20–2.12 (br m, 9 H), 1.72–1.19 (br m, 22 H).

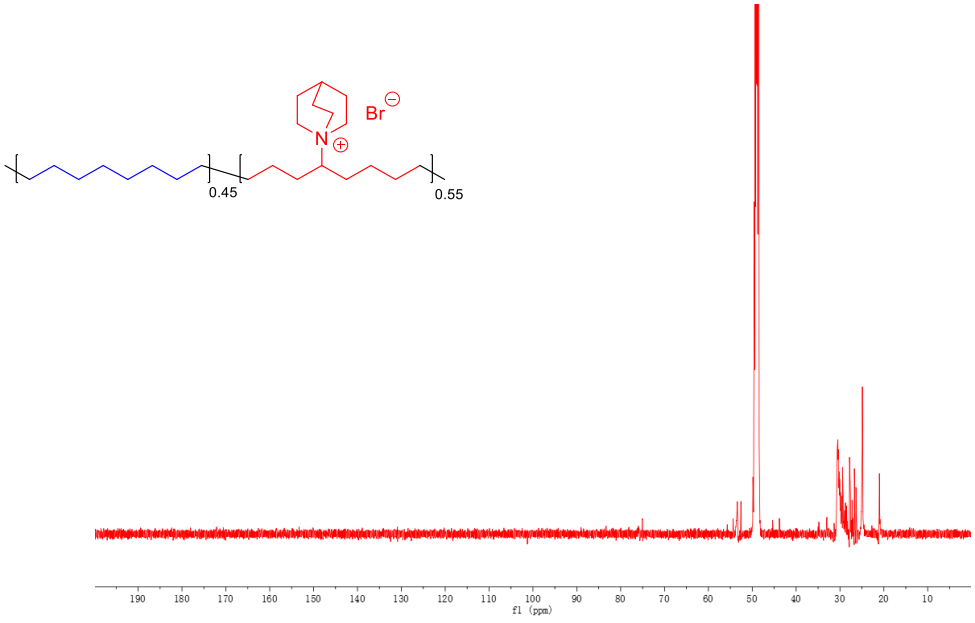


Figure S35. Representative ^{13}C NMR spectrum of oligomer **PEQ$_{55}$** *after hydrogenation* in CD_3OD at 50 °C (125 MHz).

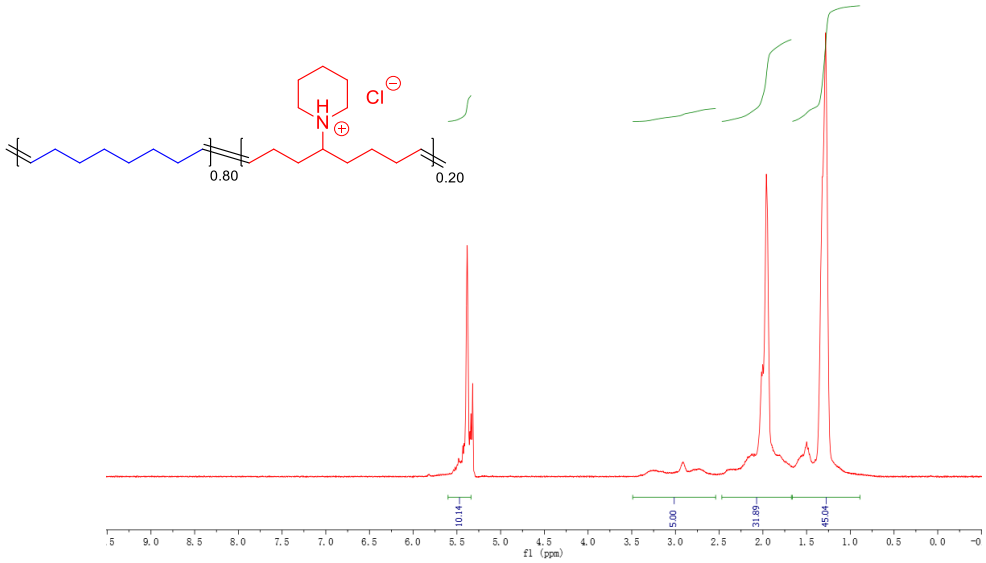


Figure S36. ^{1}H NMR spectrum of **pCOEP-HCl** *before hydrogenation* in CD_2Cl_2 at 22 °C. **^{1}H NMR (400 MHz, CD_2Cl_2):** δ 5.60–5.34 (br m, 10 H), 3.49–2.54 (br m, 5H), 2.47–1.67 (br m, 32 H), 1.66–0.89 (br m, 45 H).

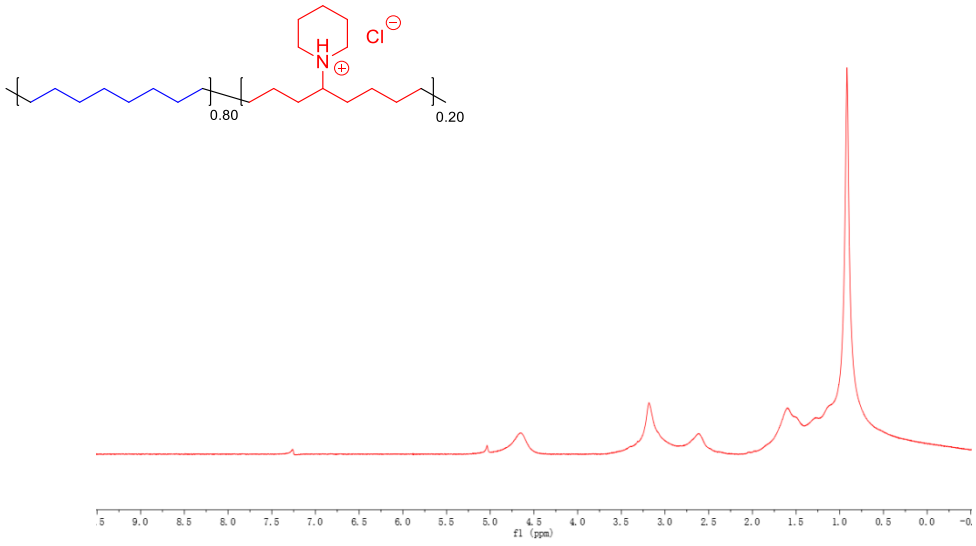


Figure S37. ^{1}H NMR spectrum (400 MHz) of **PEP-HCl** *after hydrogenation* in $CDCl_3$:CD_3OD = 1:1 (v/v) at 22 °C. Solvent residue peaks of dichloromethane and methanol can be observed in this broad spectrum, while all alkene peaks have disappeared after hydrogenation.

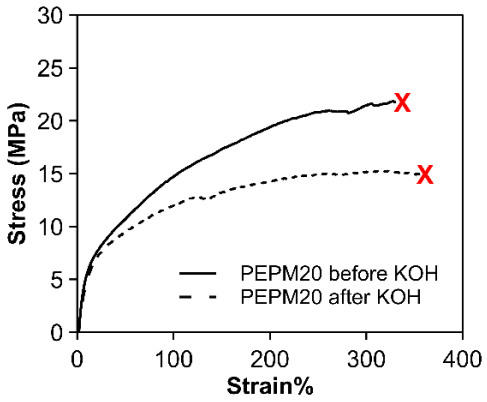


Figure S38. Stress-strain curves of **PEPM$_{20}$** before and after 1 M KOH_{aq} treatment at 80 °C for 30 days.

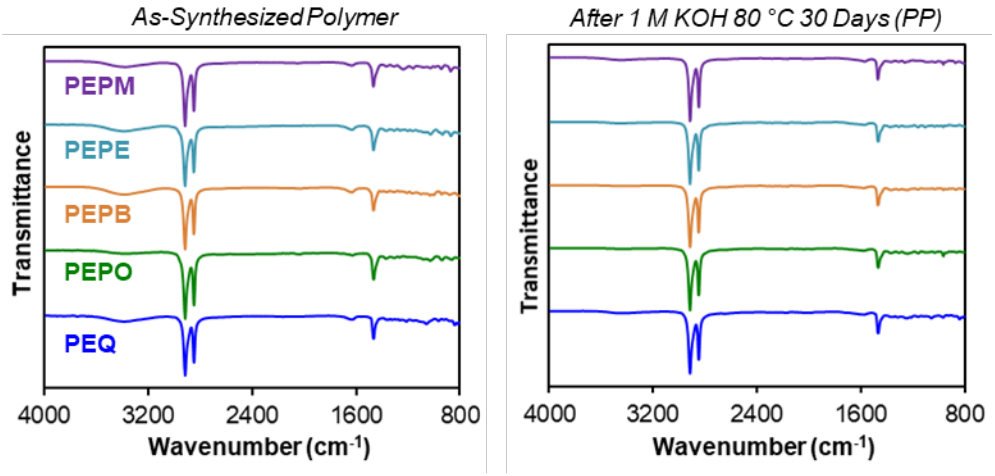


Figure S39. FT-IR spectra of **PEPM$_{20}$**, **PEPE$_{20}$**, **PEPB$_{18}$**, **PEPO$_{23}$**, and **PEQ$_{20}$** before and after 1 M KOH_{aq} at 80 °C for 30 days in PP vials. The IR traces for all samples were almost the same.

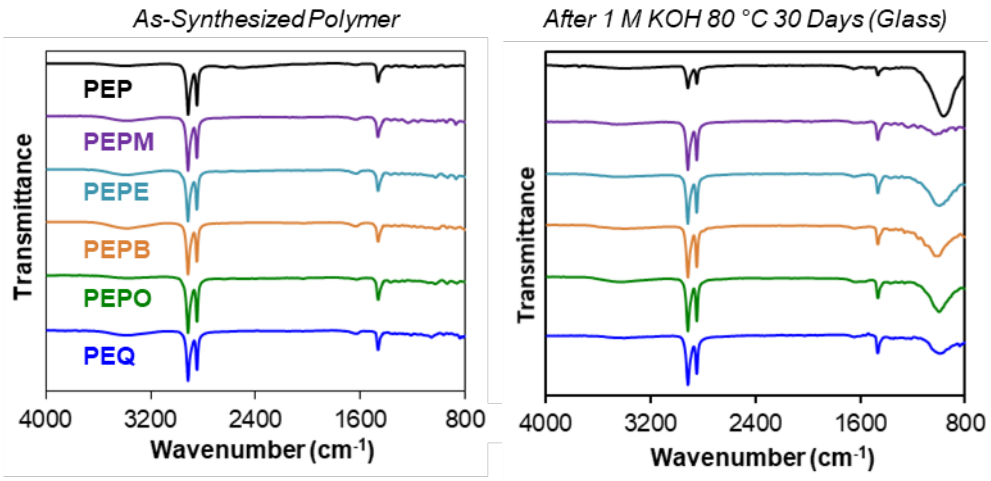


Figure S40. FT-IR spectra of **PEP$_{20}$**, **PEPM$_{20}$**, **PEPE$_{20}$**, **PEPB$_{18}$**, **PEPO$_{23}$**, and **PEQ$_{20}$** before and after 1 M KOH_{aq} at 80 °C for 30 days in soda lime glass vials. Broad peaks near 1050 cm^{-1} appeared in all samples after the stability study, while the neutral sample **PEP$_{20}$** showed the biggest peak. This peak was attributed to Si–O bonds from glass etching.

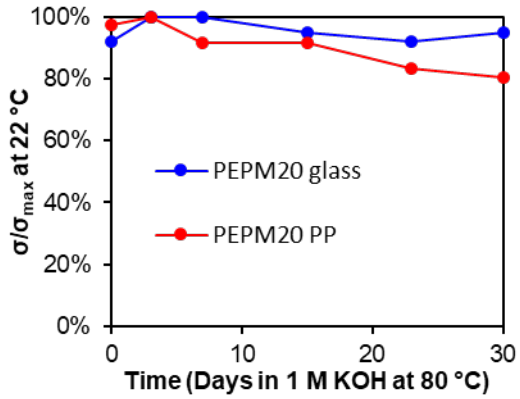


Figure S41. Comparison of conductivity changes of **PEPM$_{20}$** in 1 M KOH_{aq} at 80 °C for 30 days in soda lime glass vials (blue) and in PP vials (red). Relatively slower degradation was observed for the samples in glass vials.

Alkaline Stabilities of Piperidinium Oligomers

General procedure:

Alkaline stability study through ^{1}H NMR analysis was performed according to literature procedure.[8] A solution of the basic methanol were prepared by dissolving KOH (2 M) and 3-(trimethylsilyl)-1-propanesulfonic acid sodium salt (NaDSS, 0.03 M) in CD_3OH. The oligomers (**PEPM$_{52}$**, **PEPE$_{54}$**, **PEPB$_{58}$**, **PEPO$_{64}$**, and **PEQ$_{55}$**, estimated concentration of cationic units in solution was 0.03 M) and model compound **6** were dissolved in the methanol solution (0.5 mL) and passed through a glass wool plug into an NMR tube. The NMR tube was flame sealed and analyzed by ^{1}H NMR spectroscopy for the initial time point. Integration of a selected signal in the model compound relative to a signal related to NaDSS provided the initial quantity of model compound. The tube was heated in an oil bath at 80 °C. At specified time points, every 5 days, the tubes were removed, cooled, and analyzed by ^{1}H NMR spectroscopy at 50 °C in order to determine the quantity of cation remaining in polymer.

Solvent suppression procedure:

Quantitative ^{1}H NMR spectra for imidazolium monomer stability studies were acquired in CD_3OH at 50 °C. The OH signal in CD_3OH was suppressed with a 2 second presaturation delay and continuous wave irradiation with decoupler field strength (γB1) of 138 Hz (equivalent to a presaturation power of 12). Spectra were acquired over a spectral width of –2 to 14 ppm with 20 second relaxation delay and nominal 90° excitation pulse. 32 scans were averaged for each analysis. Residual signals between 5.9–6.2 ppm derive from solvent suppression.

The oligomer ^{1}H NMR stability data was summarized in Table S1 (data plots for Figure 4 in the text).

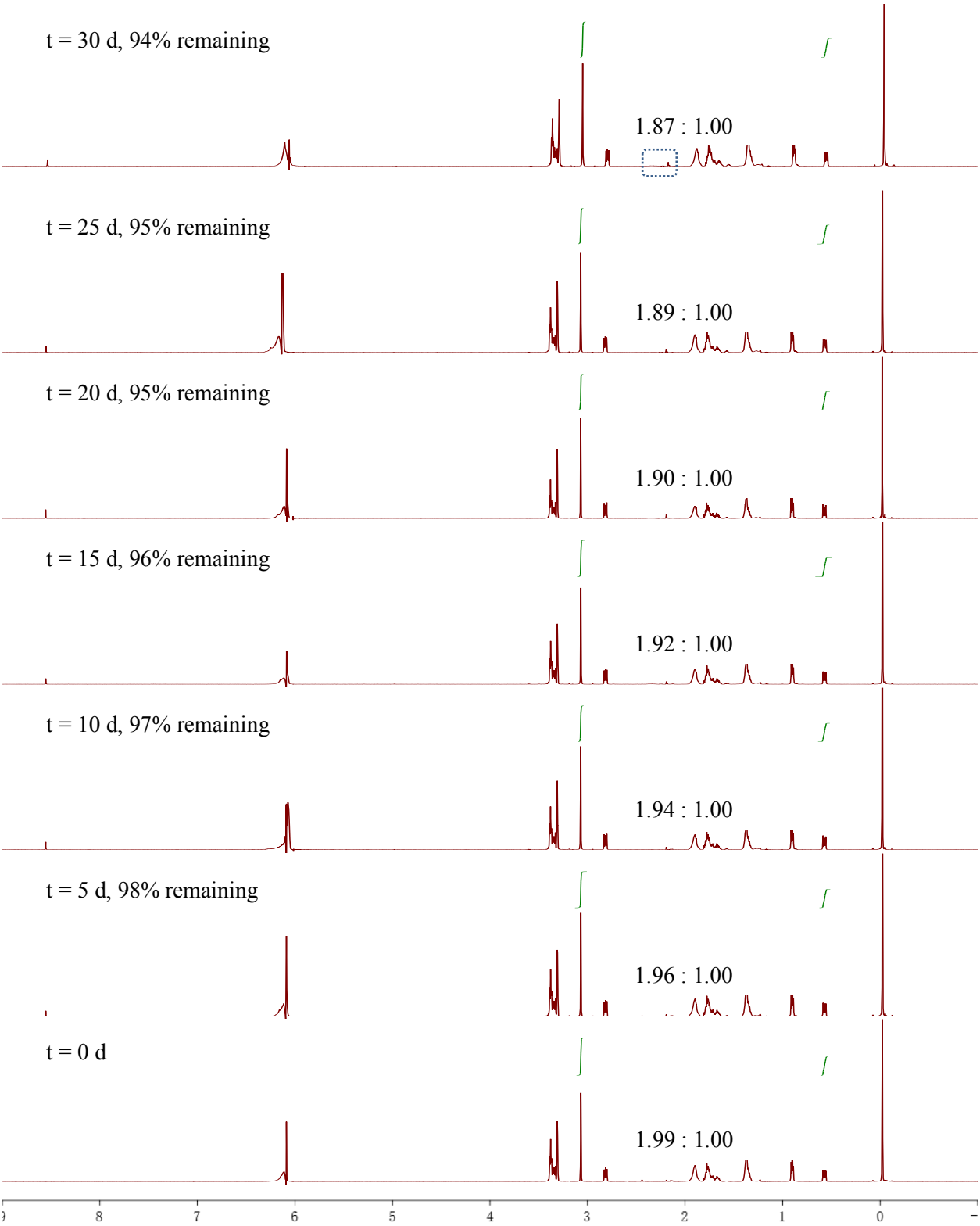


Figure S42. ^{1}H NMR spectra of **6** over 30 days dissolved in a basic CD_3OH solution at 80 °C (2 M KOH) with an internal standard (NaDSS).

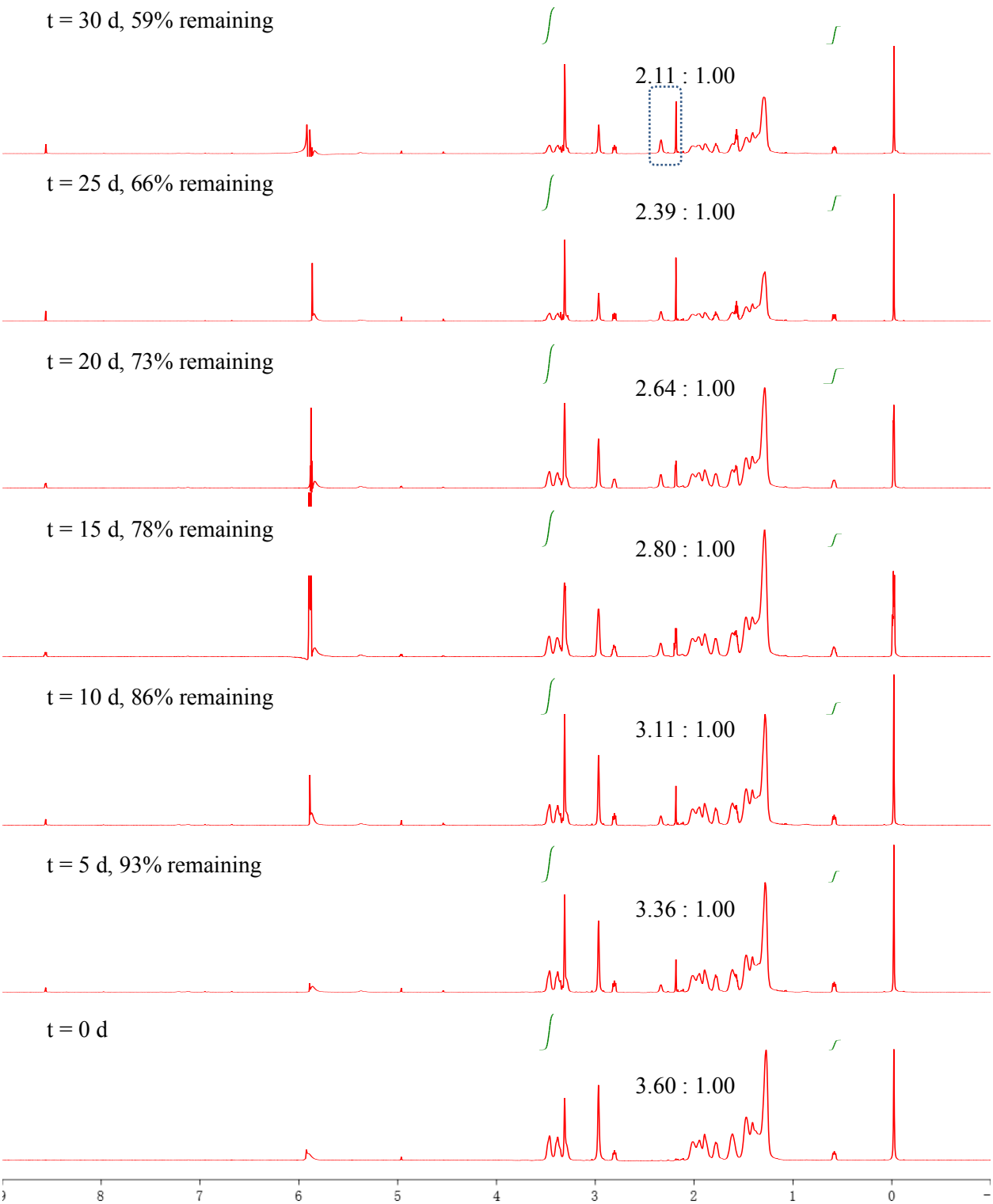


Figure S43. ^{1}H NMR spectra of **PEPM$_{52}$** over 30 days dissolved in a basic CD_3OH solution at 80 °C (2 M KOH) with an internal standard (NaDSS).

Figure S44. ^{1}H NMR spectra of **PEPE$_{54}$** over 30 days dissolved in a basic CD_3OH solution at 80 °C (2 M KOH) with an internal standard (NaDSS).

Figure S45. ^{1}H NMR spectra of **PEPB$_{58}$** over 30 days dissolved in a basic CD_3OH solution at 80 °C (2 M KOH) with an internal standard (NaDSS).

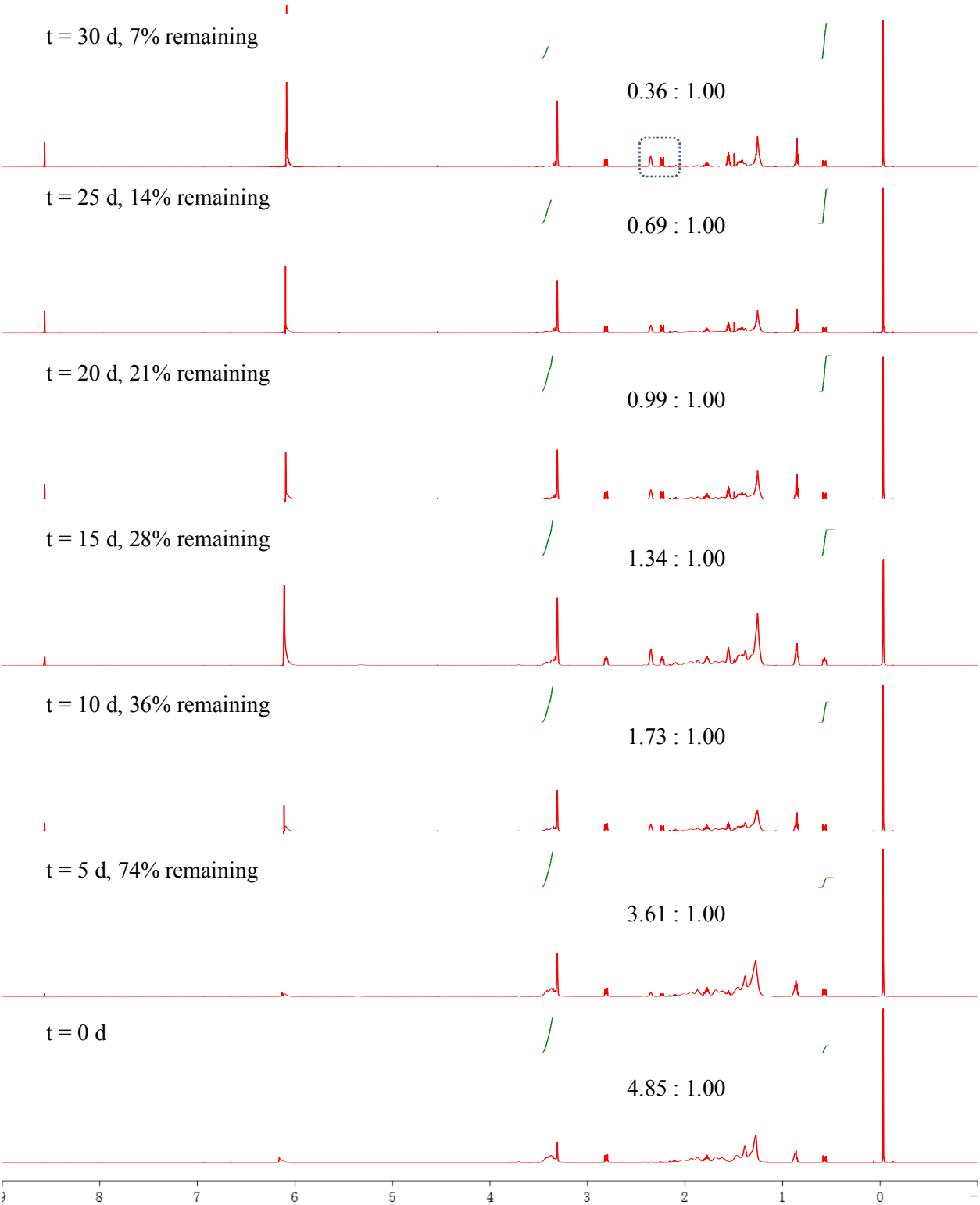


Figure S46. ^{1}H NMR spectra of **PEPO$_{64}$** over 30 days dissolved in a basic CD_3OH solution at 80 °C (2 M KOH) with an internal standard (NaDSS).

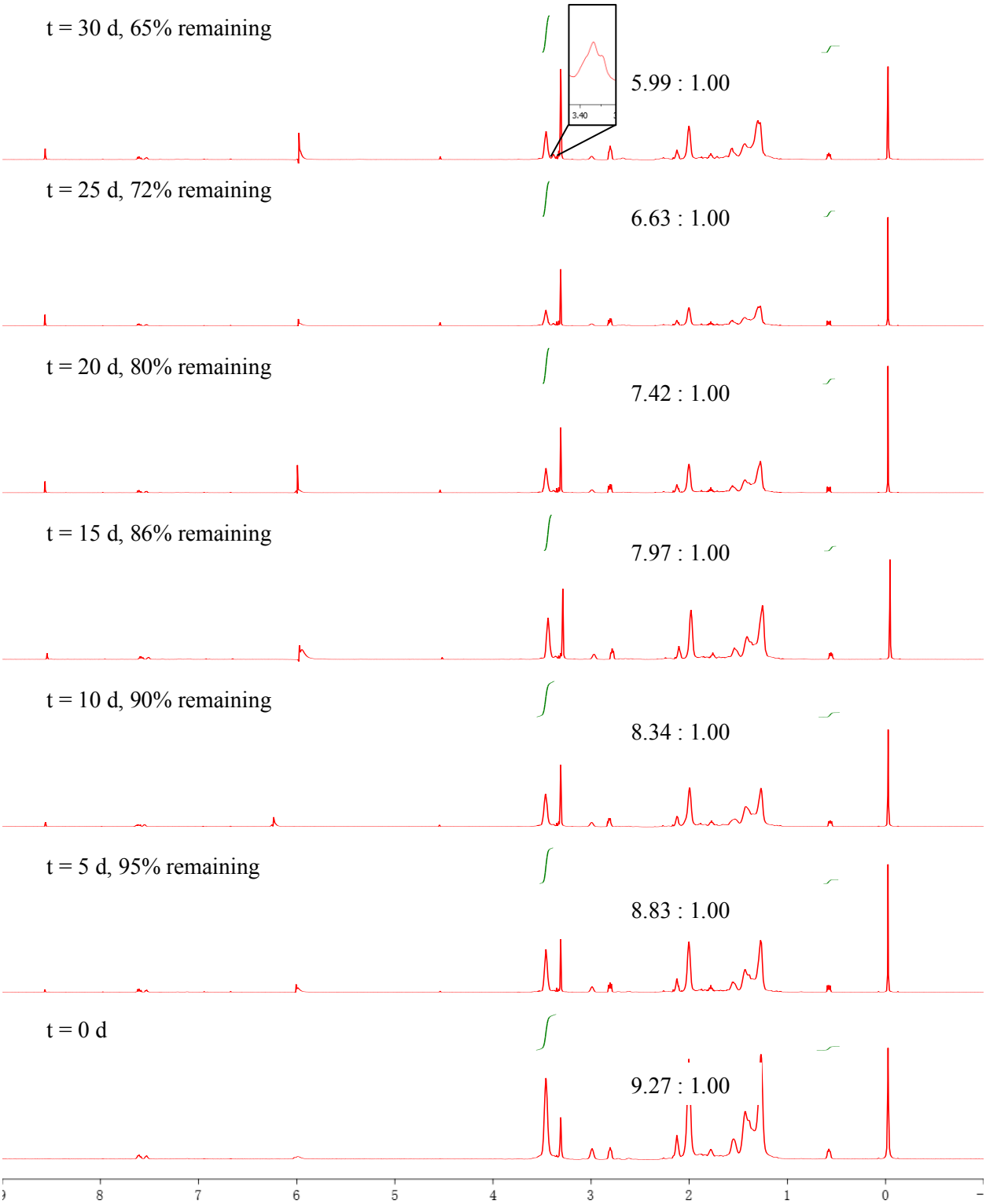


Figure S47. ^{1}H NMR spectra of **PEQ$_{55}$** over 30 days dissolved in a basic CD_3OH solution at 80 °C (2 M KOH) with an internal standard (NaDSS).

Table S1. Summary of piperidinium NMR stability studies (Data for Figure 4).[a]

Piperidinium Oligomers	Cation Remaining (%)[b]					
	5 d	10 d	15 d	20 d	25 d	30 d
Cation 6	98	97	96	95	95	94
PEPM$_{52}$	93	86	78	73	66	59
PEPE$_{54}$	81	72	65	53	43	31
PEPB$_{58}$	87	68	40	25	18	13
PEPO$_{64}$	74	36	28	21	14	7
PEQ$_{55}$	95	90	86	80	72	65

[a] Reaction Conditions: [Cation]:[KOH] = 1:67 in 2 M KOH experiments at 80 °C. [b] Percent of cation remaining, determined by ^{1}H NMR spectroscopy relative to an internal standard (NaDSS).

Table S2. Hydroxide conductivities of **PEPM**s at different temperatures (Data for Figure 1B).

PEPM Membranes	σ (OH^-, 22 °C) (mS/cm)			
	22 °C	40 °C	60 °C	80 °C
PEPM$_{16}$	26	35	54	74
PEPM$_{20}$	35	43	58	79
PEPM$_{23}$	43	51	66	86
PEPM$_{28}$	53	65	81	95

Table S3. Membrane conductivity stability in 1 M KOH_{aq} at 80 °C (Data for Figure 2).

AAEMs	σ (OH^-, 22 °C) (mS/cm)					
	0 d	3 d	7 d	15 d	23 d	30 d
PEPM$_{20}$	35	36	33	33	30	29
PEPE$_{20}$	36	33	29	19	17	15
PEPB$_{18}$	16	19	16	12	6	4
PEPO$_{23}$	15	30	25	22	15	12
PEQ$_{20}$	35	33	32	31	29	25

Table S4. Comparison of IEC determined by ^{1}H NMR analysis and Mohr titration.

Samples	Ionic Monomer	mol% of **1–5**[a]	IEC (mmol I^-/g)[a]	IEC (mmol I^-/g)[b]
$PEPM_{20}$	**1**	20%	1.31	1.49
$PEPE_{20}$	**2**	20%	1.25	1.44
$PEPB_{18}$	**3**	18%	1.12	1.16
$PEPO_{23}$	**4**	23%	1.23	1.28
PEQ_{20}	**5**	20%	1.25	1.45

[a] Determined by integration ratios in ^{1}H NMR spectra. [b] Determined by Mohr titration. The titration was performed by adapting literature procedures.[9] The samples were first exchanged into the chloride form by soaking in 100 mL of 1 M NaCl for 30 min, repeated three times with fresh solution, followed by washing with 100 mL of DI water for 30 min three times. The Cl^-form membranes were then dried for 8 hours under vacuum at 80 °C. The dry, Cl^- form samples were weighed, followed by soaking in a 100 mL sample cup containing 60 mL of 0.1 M $NaNO_3$ solution for a minimum of 6 hours. The solutions were then titrated with a 0.1 M $AgNO_3$ solution using Na_2CrO_4 as the indicator to determine the concentration of Cl^-. The titrated IEC in the Cl^- form was then calculated according to the following equation to convert into the I^- form to compare with the NMR IEC values:

$$IEC(Cl^-) = [Cl^-]/(\text{Weight of membrane in } Cl^- \text{ form})$$

$$IEC(I^-) = IEC(Cl^-)/(1+0.0915\times IEC(Cl^-))$$

Table S5. Weight loss of glass containers after alkaline stability studies.

Containers	Weight before Stability Study (g)	Weight after Stability Study (g)	Weight Loss (g)
Soda Lime Vial[a]	13.1882	12.7048	0.4834
Borosilicate NMR Tube (Norell # S-5-600-7)[b]	2.5098	2.5098	0

[a] The conditions were the same as the membrane alkaline stability study conditions. A dried 20 mL soda lime glass vial was weighed and was then filled with 20 mL 1 M KOH. The vial was then sealed and heated to 80 °C. The vial was kept at 80 °C for 30 days while the KOH solution was refreshed every 5 days. After the study the vial was emptied, washed with DI water, and dried before measuring its final weight. [b] The conditions were the same as the NMR alkaline stability study conditions. A dry NMR tube was weighed and was then filled with a solution of KOH (2 M), NaDSS (0.03 M), and 18-crown-6 (0.03 M as another common internal standard) in 1 mL CD_3OH. The NMR tube was flame sealed. The tube was heated in an oil bath at 80 °C for 30 days. After the stability study, the tube was carefully cut open, emptied, washed, and dried. The tube was then weighed along with the glass pieces removed during flame-seal and cut-open processes.

Detailed Breakdown of Computed Free Energies

Table S6. Relevant energetic quantities (see *Theoretical and Computational Methods* for more details)

	Electronic (DFT) Energy (B3LYP+D3, Hartree)	Electronic (DFT) Energy (ωB97X-V, Hartree)	Enthalpy (*H*, Hartree)	Entropy (*S*, mHartree/K)	Distance (*D*, Å)	EFEI Potential (V_{EFEI}, Hartree)	Degeneracy (-*RT* ln *g*, mHartree)	Free Energy (*G*, Hartree)
PEPM (F = 0.0 nN)								
Reactant	-682.146432	-682.134514	0.471478	0.247364	3.788	0.000000	0.000000	-681.750392
Path a	-682.112282	-682.091859	0.468504	0.242131	3.859	0.000000	-0.775186	-681.709639
Path b	-682.110723	-682.092497	0.468448	0.246459	3.476	0.000000	0.000000	-681.711086
Path d	-682.110247	-682.096196	0.464709	0.246475	3.786	0.000000	-0.775186	-681.719304
Path e	-682.110686	-682.094664	0.463974	0.243279	4.595	0.000000	-0.775186	-681.717380
PEPM (F = +0.05 nN)								
Reactant	-682.146172	-682.134114	0.471474	0.246562	3.939	-0.004517	0.000000	-681.754230
Path a	-682.112216	-682.091790	0.468386	0.242035	3.978	-0.004562	-0.775186	-681.714217
Path b	-682.110713	-682.092801	0.468310	0.246019	3.935	-0.004513	0.000000	-681.715885
Path d	-682.110189	-682.096145	0.464657	0.245413	3.975	-0.004558	-0.775186	-681.723489
Path e	-682.109950	-682.093314	0.464083	0.245245	4.987	-0.005720	-0.775186	-681.722335
PEPM (F = +0.10 nN)								
Reactant	-682.146051	-682.133989	0.471368	0.246755	4.009	-0.009194	0.000000	-681.758956
Path a	-682.112123	-682.091655	0.468326	0.242258	4.035	-0.009255	-0.775186	-681.718913
Path b	-682.110518	-682.092692	0.468162	0.245265	4.076	-0.009349	0.000000	-681.720495
Path d	-682.110089	-682.096003	0.464628	0.245542	4.033	-0.009249	-0.775186	-681.728112
Path e	-682.109921	-682.093282	0.464076	0.244990	5.002	-0.011472	-0.775186	-681.727972
PEPM (F = +0.15 nN)								
Reactant	-682.1459421	-682.133923	0.471064	0.247862	4.129	-0.014205	0.000000	-681.764597
Path a	-682.111986	-682.091490	0.468245	0.242741	4.084	-0.014052	-0.775186	-681.723797
Path b	-682.109993	-682.092040	0.468138	0.244735	4.258	-0.014650	0.000000	-681.724980
Path d	-682.109929	-682.095825	0.464543	0.246077	4.087	-0.014063	-0.775186	-681.733022
Path e	-682.109890	-682.093230	0.464059	0.245243	5.020	-0.017270	-0.775186	-681.733825
PEPM (F = +0.20 nN)								
Reactant	-682.145485	-682.133459	0.471066	0.247254	4.242	-0.019462	0.000000	-681.769173
Path a	-682.111771	-682.091268	0.468092	0.243695	4.139	-0.018989	-0.775186	-681.729001
Path b	-682.109714	-682.091627	0.468270	0.244506	4.325	-0.019841	0.000000	-681.729545
Path d	-682.109656	-682.095566	0.464393	0.247328	4.154	-0.019055	-0.775186	-681.738346
Path e	-682.109833	-682.093172	0.464026	0.245374	5.035	-0.023099	-0.775186	-681.739674
PEPM (F = +0.25 nN)								
Reactant	-682.145229	-682.133167	0.471127	0.246508	4.291	-0.024608	0.000000	-681.773702
Path a	-682.111156	-682.090676	0.467934	0.245141	4.267	-0.024466	-0.775186	-681.734555
Path b	-682.109441	-682.091254	0.468359	0.244713	4.376	-0.025092	0.000000	-681.734408
Path d	-682.109122	-682.095069	0.464230	0.249461	4.254	-0.024394	-0.775186	-681.744106
Path e	-682.109756	-682.093105	0.463974	0.245362	5.047	-0.028942	-0.775186	-681.745498
PEPM (F = -0.05 nN)								
Reactant	-682.146142	-682.134144	0.471238	0.247140	3.408	0.003909	0.000000	-681.746275
Path a	-682.111775	-682.091048	0.468384	0.242730	3.363	0.003857	-0.775186	-681.705302
Path b	-682.110692	-682.092448	0.468566	0.245218	3.428	0.003932	0.000000	-681.706550
Path d	-682.110175	-682.096124	0.464675	0.247592	3.657	0.004194	-0.775186	-681.715468
Path e	-682.110600	-682.094769	0.463886	0.244645	4.575	0.005247	-0.775186	-681.712808
PEPM (F = -0.10 nN)								
Reactant	-682.146044	-682.133920	0.471439	0.246946	3.378	0.007749	0.000000	-681.741941
Path a	-682.111734	-682.091068	0.468418	0.242814	3.343	0.007669	-0.775186	-681.701506
Path b	-682.110635	-682.092402	0.468630	0.244537	3.397	0.007793	0.000000	-681.702337
Path d	-682.109792	-682.095708	0.464764	0.245916	3.393	0.007782	-0.775186	-681.710783
Path e	-682.110390	-682.094794	0.463877	0.244533	4.541	0.010416	-0.775186	-681.707634
PEPM (F = -0.15 nN)								
Reactant	-682.146007	-682.133991	0.471417	0.246665	3.349	0.011522	0.000000	-681.738162
Path a	-682.111675	-682.091071	0.468447	0.242948	3.324	0.011438	-0.775186	-681.697758
Path b	-682.110558	-682.092346	0.468666	0.244285	3.371	0.011600	0.000000	-681.698349
Path d	-682.109697	-682.095618	0.464843	0.245394	3.360	0.011559	-0.775186	-681.706652
Path e	-682.109993	-682.094676	0.463910	0.244892	4.494	0.015463	-0.775186	-681.702561
PEPM (F = -0.20n N)								
Reactant	-682.145906	-682.133901	0.471482	0.246505	3.324	0.015247	0.000000	-681.734226
Path a	-682.111598	-682.091057	0.468467	0.243112	3.306	0.015166	-0.775186	-681.694055
Path b	-682.110462	-682.092278	0.468687	0.244126	3.348	0.015360	0.000000	-681.694444
Path d	-682.109582	-682.095518	0.464898	0.245124	3.331	0.015281	-0.775186	-681.702680
Path e	-682.109526	-682.094431	0.464076	0.243256	4.443	0.020383	-0.775186	-681.696653
PEPM (F = -0.25 nN)								
Reactant	-682.145787	-682.133802	0.471532	0.246405	3.301	0.018928	0.000000	-681.730361
Path a	-682.111506	-682.091030	0.468489	0.243050	3.288	0.018857	-0.775186	-681.690293
Path b	-682.110350	-682.092197	0.468698	0.244138	3.327	0.019076	0.000000	-681.690640
Path d	-682.109450	-682.095400	0.464954	0.244973	3.305	0.018953	-0.775186	-681.698781
Path e	-682.109296	-682.094350	0.464124	0.243045	4.414	0.025312	-0.775186	-681.691520
PEPE (F = 0.0 nN)								
Reactant	-721.461642	-721.449204	0.501816	0.256414	3.868	0.000000	0.000000	-721.037942

Path a	-721.426312	-721.4060010	0.499083	0.253016	3.666	0.000000	-0.775186	-720.997055
Path b	-721.427625	-721.407404	0.499001	0.255352	3.710	0.000000	0.000000	-720.998580
Path c	-721.429794	-721.417735	0.495885	0.253701	3.626	0.000000	0.000000	-721.011445
Path d	-721.424000	-721.409847	0.495538	0.256877	3.497	0.000000	-0.775186	-721.005799
Path e	-721.423356	-721.406109	0.4946312	0.255824	4.572	0.000000	-0.775186	-721.002597
PEQ (F = 0.0 nN)								
Reactant	-720.251724	-720.245074	0.479181	0.250087	3.494	0.000000	0.000000	-719.854211
Path a	-720.222119	-720.207393	0.475998	0.243065	3.395	0.000000	-0.775186	-719.818008
Path b	-720.220733	-720.206514	0.476243	0.240986	3.418	0.000000	0.000000	-719.815374
Path c	-720.207949	-720.199672	0.473509	0.244426	3.466	0.000000	0.000000	-719.812481
Path d	-720.208792	-720.199329	0.473159	0.245175	3.697	0.000000	-0.775186	-719.813528
Path e	-720.214075	-720.203307	0.471461	0.245705	4.601	0.000000	-0.775186	-719.819392

Optimized Structures

PEPM No Force Reactant
B3LYP+D3 Energy: -682.1464317368

C	-0.5165505430	-0.1341191961	0.2085340147
C	-0.5823204896	0.3855062409	1.6492347321
C	0.4668329236	1.4812666740	1.9047923747
H	-0.4360412154	-0.4525322062	2.3407662388
H	-1.5839165962	0.7878845136	1.8508353441
C	0.3404469097	2.1002620533	3.3046142990
H	0.3299569544	2.2438248402	1.1337828462
H	1.4673846284	1.0523403144	1.7655222887
C	0.5225927857	1.0391823267	4.4165939969
C	-0.8146044601	0.6160583357	5.0440817697
H	1.1663684159	1.3916373208	5.2274763761
H	1.0363342265	0.1618053008	4.0045623210
C	-0.6356947167	-0.4918602307	6.0859819443
H	-1.5058202544	0.2834813143	4.2620248234
H	-1.2803911062	1.4968273679	5.5053129302
N	1.2994899461	3.3223132928	3.4995608121
H	-0.6377346850	2.5859560574	3.3984498687
C	1.0257974719	4.3471007071	2.3962843785
C	0.9351939968	3.9830362046	4.8350715481
C	1.6505352641	5.3080106298	5.0831359390
H	1.1654155548	3.2681641769	5.6234036674
H	-0.1495096994	4.1272120782	4.7718592242
C	1.3713693917	6.3129588255	3.9617098072
H	2.7300633644	5.1561554545	5.2027565400
H	1.2832713389	5.6822864269	6.0460148521
C	1.7301506020	5.6846038206	2.6124984497
H	1.9401380675	7.2361293388	4.1191097450
H	0.3061037523	6.5802348895	3.9695385563
H	-0.0617109534	4.4678354734	2.3953918117
H	1.3486530019	3.9022522647	1.4565836233
H	2.8166942435	5.5652799039	2.5243386335
H	1.4231400444	6.3328402259	1.7832638840
C	2.7361205579	2.8940820594	3.4691368371
H	2.9628900910	2.4917871018	2.4826231298
H	2.8994179151	2.1333491477	4.2305293780
H	3.3812344825	3.7468253774	3.6673357304
H	-0.7087377943	0.6702375693	-0.5122824592
H	-1.2604545620	-0.9209658898	0.0399810701
H	0.4724824190	-0.5530163457	-0.0150295136
H	0.0360751872	-0.1698370391	6.8917777291
H	-0.2019911443	-1.3925442863	5.6331363206
H	-1.5937846763	-0.7717618741	6.5385379138
O	-2.1069053832	4.1983681318	3.6324659705
C	-3.1534964297	3.2912856582	3.7095143781
H	-3.4686779546	3.0545444072	4.7532694254
H	-2.9157052925	2.2983588006	3.2554846147
H	-4.0841200402	3.6250840220	3.1943277149

PEPM No Force Path a
B3LYP+D3 Energy: -682.1122816199

C	-0.3143637102	0.2369192417	-0.2413408119
C	-0.5527184452	0.6592863807	1.2176568007

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C       0.6820429801     1.3366112703     1.8335931430
H      -0.8444092912    -0.2136427119     1.8173726436
H      -1.3971964063     1.3610483680     1.2589028155
C       0.4213208263     1.8925270900     3.2521484201
H       0.9853439321     2.1385889185     1.1554001970
H       1.5151363231     0.6223490128     1.8615436468
C       0.4758620703     0.7650476888     4.3259422282
C      -0.6630827649     0.7836466663     5.3636377009
H       1.4433459703     0.7930887112     4.8425960293
H       0.4545396534    -0.2020761251     3.8097846267
C      -0.4151461618    -0.1715007392     6.5412749568
H      -1.6026254218     0.5201379347     4.8586097512
H      -0.8073357154     1.7959978712     5.7551726983
N       1.3303564139     3.0648788830     3.5708907927
H      -0.5848089573     2.3301124120     3.2600839199
C       0.7646173163     4.5518050701     2.3078627365
C       1.0627514410     3.5721758746     4.9433173656
C       1.7025253571     4.9258239147     5.2527255533
H       1.3854869898     2.8273291462     5.6805926794
H      -0.0241744122     3.6726705123     5.0268223822
C       1.2271023008     6.0374441571     4.3134201919
H       2.7967486780     4.8550600684     5.2278660077
H       1.4370302362     5.1716283837     6.2884025573
C       1.5289320220     5.7301632784     2.8427717858
H       1.7065044290     6.9834115877     4.5904876008
H       0.1436216488     6.1803771206     4.4338048124
H      -0.2577513608     4.3777710258     2.6063217754
H       1.1644503199     3.9932815351     1.4826616861
H       2.6051792640     5.5715634741     2.7000441572
H       1.2578823985     6.5867826757     2.2185499573
C       2.7552943041     2.7428416526     3.3610363578
H       2.9190364522     2.4589030156     2.3209413591
H       3.0801790821     1.9221056876     4.0122994493
H       3.3684900753     3.6167377426     3.5761511658
H      -0.0639539732     1.1062395943    -0.8620388737
H      -1.2058590427    -0.2372106592    -0.6673877924
H       0.5148690721    -0.4776568529    -0.3161996388
H       0.4894825672     0.1152370112     7.0919653053
H      -0.2793480857    -1.2037689330     6.1944970899
H      -1.2554993514    -0.1615686405     7.2448399687
O      -0.2124577355     5.5679467500     0.7230883660
C      -0.8541745281     4.5579240921     0.0069684441
H      -0.1525604411     3.9035239494    -0.5564182192
H      -1.5655577253     4.9604321450    -0.7385544410
H      -1.4448028144     3.8738261162     0.6563847303

PEPM No Force Path b
B3LYP+D3 Energy:   -682.1107231947
C       0.0283858004    -0.6191822955     0.6311338198
C      -0.1860269109     0.0523296455     1.9923112956
C       0.6730822290     1.3196307235     2.1419097739
H       0.0442146430    -0.6641593489     2.7896630262
H      -1.2458811404     0.3179178485     2.1096406797
C       0.4102870705     2.0757416965     3.4579186570
H       0.4549807392     1.9573955681     1.2809936218
H       1.7344464936     1.0462945135     2.0779337615
C       0.7011127879     1.1670759818     4.6844298850
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C	-0.5738233537	0.6815800846	5.3892703389
H	1.3249282949	1.6745125701	5.4242913601
H	1.2889117858	0.3002566111	4.3582497957
C	-0.2742341557	-0.2890785403	6.5356421251
H	-1.2372965972	0.1944395727	4.6630429118
H	-1.1232247284	1.5540779606	5.7693684639
N	1.1539838705	3.4028021293	3.5287657723
H	-0.6563723848	2.3492942796	3.4747538863
C	0.8622653767	4.2310220990	2.3186898545
C	0.7199154346	4.1376012421	4.7633898139
C	1.2557258765	5.5665811317	4.8730442733
H	1.0380613358	3.5618330056	5.6325430890
H	-0.3800576903	4.1604027182	4.7651064867
C	0.9135447339	6.3922685674	3.6321196255
H	2.3417200920	5.5583566298	5.0261621549
H	0.8187989701	6.0082767926	5.7766471236
C	1.4187494985	5.6546550936	2.3909984524
H	1.3561479950	7.3927913874	3.6990136567
H	-0.1759504324	6.5228545702	3.5646764372
H	-0.2292679036	4.2642718162	2.1824601418
H	1.2899653185	3.7256943113	1.4528990743
H	2.5160602538	5.6309193585	2.3918959056
H	1.1163578875	6.1710148039	1.4723972814
C	3.0616480004	3.0484644883	3.5775795963
H	3.1542933642	2.9936010453	2.5052803199
H	2.9442046540	2.1456309030	4.1492051331
H	3.3031194926	3.9645704887	4.0862729779
H	-0.2342119713	0.0594216162	-0.1899733912
H	-0.5863746918	-1.5210752099	0.5311767910
H	1.0773373717	-0.9115365583	0.4976219486
H	0.3557721926	0.1819058387	7.3006702186
H	0.2574754250	-1.1756035869	6.1674027626
H	-1.1959595435	-0.6283615080	7.0220733681
O	5.0590654494	2.6444522657	3.6416934809
C	5.3351107896	2.4637343904	4.9965256709
H	6.4096216943	2.2802981837	5.1810248777
H	4.7909694483	1.6005814093	5.4403157395
H	5.0562516691	3.3443882292	5.6164824036

PEPM No Force Path d
B3LYP+D3 Energy: -682.1102468305

C	-0.6910063059	0.1597884563	0.2290786519
C	-0.6751439066	0.5850982723	1.7018761655
C	0.4101368592	1.6375167419	1.9798429051
H	-0.5176430498	-0.2995384921	2.3304376108
H	-1.6567054911	0.9935154828	1.9794327021
C	0.4047761811	2.1209260300	3.4405076275
H	0.2402672906	2.4778387372	1.3008207899
H	1.3885667712	1.2112006326	1.7243113903
C	0.6569267004	0.9498938708	4.4282513042
C	-0.6134283299	0.4901502284	5.1583807390
H	1.4042949712	1.2162211488	5.1817701370
H	1.0902808820	0.1071851235	3.8751495951
C	-0.3633555855	-0.7343899828	6.0444471112
H	-1.4012102077	0.2640021520	4.4293967876
H	-0.9921057220	1.3203561918	5.7707580594
N	1.3413160926	3.2978211966	3.6729053044

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H    -0.5862627406     2.5439500153     3.6411012808
C     0.9875439943     4.6259550142     2.5376330948
C     1.0695947770     3.8878793678     5.0347289243
C     1.7731301202     5.2199021633     5.3171794559
H     1.3381231308     3.1461122714     5.7925916885
H    -0.0147602214     4.0344243930     5.0841674536
C     1.3701721055     6.3097155694     4.3093255975
H     2.8619017429     5.0847693023     5.3146426294
H     1.4976234221     5.4981938548     6.3443141307
C     1.6352627000     5.8672358355     2.8732882177
H     1.9009303329     7.2423928069     4.5419245422
H     0.2961367438     6.5210720332     4.4459883139
H    -0.1003866708     4.6040635125     2.6527515309
H     1.3006622507     4.1727311256     1.5993859713
H     2.7066382872     5.8665208684     2.6301976207
H     0.9950403645     6.9458699614     1.8965961059
C     2.7693933704     2.9415157298     3.5069126369
H     2.9003494275     2.4016848435     2.5692819587
H     3.1178366260     2.3232980077     4.3384427481
H     3.3557582006     3.8599206911     3.4683569932
H    -0.8798341175     1.0167102719    -0.4295029109
H    -1.4707845495    -0.5870138676     0.0411073288
H     0.2712376059    -0.2787040824    -0.0633972023
H     0.4108163946    -0.5258911105     6.7934142109
H    -0.0248281352    -1.5889717022     5.4452650860
H    -1.2734298291    -1.0354744596     6.5757164408
O     0.5515980300     7.7036904245     1.2227351041
C    -0.2687162007     7.0089060023     0.2994729717
H    -1.3271368119     6.9996399834     0.6076701732
H     0.0522128155     5.9597226263     0.1885624902
H    -0.2110256045     7.4789458607    -0.6916192993

PEPM No Force Path e
B3LYP+D3 Energy:   -682.1106858780
C    -0.0928559678    -0.5439639800     0.2803591909
C    -0.4699730103     0.2247387182     1.5514234306
C     0.7397300100     0.9433377771     2.1733610587
H    -0.9051436566    -0.4584493513     2.2873354003
H    -1.2407941581     0.9725644966     1.3166447633
C     0.3670991418     1.6132534708     3.4970136799
H     1.1107894744     1.6515935840     1.4261248204
H     1.5474458251     0.2237778502     2.3526039161
C     0.6004567706     0.8235400646     4.6834055882
C    -0.1005497065     1.0989487751     6.0190844718
H     1.6494775918     0.5187940533     4.7959007697
H     0.0735743978    -0.4822737789     4.4124935115
C    -1.6277302691     1.2253352511     5.8980002913
H     0.2820996412     1.9747919674     6.5631991209
H     0.1163825102     0.2410407925     6.6719548099
N     1.2706013694     3.2293019345     3.4534832462
H    -0.6253116723     2.0685981080     3.4521839798
C     0.6976633149     4.0825738075     2.3653839662
C     1.0303495483     3.8704158202     4.7845712271
C     1.5194432652     5.3191933928     4.8733228545
H     1.5170959773     3.2426475927     5.5302951294
H    -0.0503255342     3.8274199013     4.9532402043
C     0.9261358009     6.1798347113     3.7514265170
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H     2.6150764373     5.3541344668     4.8321005536
H     1.2315433216     5.7050630131     5.8583589261
C     1.2014946959     5.5287220744     2.3899494502
H     1.3410690286     7.1937560384     3.7859049312
H    -0.1595600271     6.2708388838     3.8970508755
H    -0.3894703065     4.0658299011     2.5052366642
H     0.9223300843     3.6078269338     1.4090877923
H     2.2759704329     5.5567734457     2.1675583352
H     0.6976098613     6.0745179978     1.5836158334
C     2.7091088161     2.9324821706     3.2605835240
H     2.8794864574     2.5882807265     2.2401942308
H     2.9882622860     2.1429873087     3.9628179127
H     3.3283524803     3.8122648472     3.4427654860
H     0.3296545249     0.1252969352    -0.4802269174
H    -0.9660864271    -1.0404946983    -0.1588964411
H     0.6564156031    -1.3146792100     0.4980152904
H    -2.0515398934     0.3490625822     5.3926810074
H    -1.9221767358     2.1111407854     5.3217197248
H    -2.0983264811     1.3086556741     6.8853164510
O    -0.3284707780    -1.6348259860     4.3992765952
C     0.5419417324    -2.4290767175     3.6280993250
H     0.7682814493    -3.3841978234     4.1303614109
H     1.5083210554    -1.9239758967     3.4478735120
H     0.1213453092    -2.6735910634     2.6363827440

PEPM + 0.05nN Force Reactant
B3LYP+D3 Energy:   -682.1461724435
C    -0.4122324035    -0.0805850656     0.0306052558
C    -0.6224649118     0.5435498340     1.4153942594
C     0.5857540625     1.3900498485     1.8524486044
H    -0.8162951110    -0.2487686322     2.1494562453
H    -1.5176902054     1.1787537331     1.4029632857
C     0.3548793661     2.0240713202     3.2343198124
H     0.7465178677     2.1484721092     1.0817092201
H     1.4837900388     0.7594675818     1.8726297262
C     0.4683882174     0.9692448815     4.3627323479
C    -0.7261392121     0.9457352775     5.3290683883
H     1.3982830088     1.0817032431     4.9308831119
H     0.5516340406    -0.0171620844     3.8934493756
C    -0.5661276305    -0.1161651528     6.4215557292
H    -1.6404253167     0.7572489659     4.7517989404
H    -0.8606081294     1.9310295148     5.7909496421
N     1.2868133492     3.2600374254     3.4723802841
H    -0.6334272879     2.4986381313     3.2524506862
C     0.9006524353     4.3519396342     2.4665378063
C     1.0125145265     3.8016277226     4.8747208171
C     1.6919140884     5.1366348200     5.1706615569
H     1.3299000330     3.0373866990     5.5821975065
H    -0.0732271455     3.9107598967     4.9276978371
C     1.2876839073     6.2050701056     4.1510199102
H     2.7818907118     5.0221968115     5.1977997256
H     1.3854460841     5.4228759378     6.1835594085
C     1.5728954225     5.6963571292     2.7354027708
H     1.8255431207     7.1406647362     4.3392798245
H     0.2150617888     6.4175784498     4.2538432066
H    -0.1900005497     4.4216735919     2.5407580997
H     1.1749575403     3.9853659274     1.4790047529
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H     2.6543079169     5.6314801370     2.5652911846
H     1.1832746159     6.3920794732     1.9830191342
C     2.7311728192     2.8877390501     3.3164473406
H     2.9002248830     2.5536811560     2.2938380440
H     2.9746684947     2.0893938546     4.0168315403
H     3.3589601813     3.7516337673     3.5218346270
H    -0.2560269719     0.6941390487    -0.7302042635
H    -1.2816393537    -0.6762268690    -0.2698851010
H     0.4654963396    -0.7385805485     0.0220912915
H     0.3220881043     0.0804875443     7.0355105634
H    -0.4533104201    -1.1171615369     5.9861414661
H    -1.4364560831    -0.1364613140     7.0872349178
O    -2.2356695704     4.0054417542     3.1252588539
C    -3.2100499451     3.0832016088     3.4780633556
H    -3.3625062461     2.9904960737     4.5788920317
H    -2.9848273031     2.0447295853     3.1341659529
H    -4.2196036264     3.3082064023     3.0620868040

PEPM + 0.05nN Force Path a
B3LYP+D3 Energy:   -682.1122163954
C    -0.3454234093     0.0742192388    -0.0892885818
C    -0.5566881310     0.6252793007     1.3257930508
C     0.6776723544     1.3752556040     1.8464836507
H    -0.8161272268    -0.1982368653     2.0051370492
H    -1.4154122964     1.3108557316     1.3299253659
C     0.4557635132     1.9434912440     3.2620517256
H     0.9090486027     2.1721609174     1.1342098108
H     1.5412077734     0.6975918331     1.8500342157
C     0.5221100640     0.8122654165     4.3300148497
C    -0.6805159503     0.7681313701     5.2845519353
H     1.4488952154     0.8906045610     4.9110096189
H     0.5881536424    -0.1520783032     3.8128347161
C    -0.5420764496    -0.3216626233     6.3532098737
H    -1.5923495232     0.5992332758     4.6944910171
H    -0.8103107390     1.7417087192     5.7729184351
N     1.3672832009     3.1129996635     3.5661752995
H    -0.5486859592     2.3842344386     3.2883213790
C     0.7841787530     4.5948237872     2.3063249963
C     1.1098331655     3.6164881968     4.9424589402
C     1.7397103456     4.9758743049     5.2454217577
H     1.4484048836     2.8743122694     5.6750357047
H     0.0224121151     3.7030230326     5.0386035635
C     1.2489778429     6.0830242125     4.3086718040
H     2.8343207559     4.9137109274     5.2109388028
H     1.4812308391     5.2207770497     6.2830821957
C     1.5452688119     5.7774216924     2.8363907599
H     1.7223413599     7.0329025626     4.5827481478
H     0.1650683390     6.2173339828     4.4351912533
H    -0.2345695199     4.4151092300     2.6135550144
H     1.1822292704     4.0366928303     1.4796701310
H     2.6216212619     5.6236214603     2.6890873287
H     1.2668827475     6.6327235624     2.2135954250
C     2.7888076275     2.7913706047     3.3385782086
H     2.9401133590     2.5189099233     2.2931248615
H     3.1184154586     1.9623205771     3.9770064430
H     3.4059755762     3.6618682662     3.5570213126
H    -0.1375064687     0.8842475392    -0.7994151978
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H    -1.2331524174    -0.4626302635    -0.4429483347
H     0.5021188554    -0.6219258728    -0.1199127074
H     0.3402996234    -0.1439331196     6.9810250265
H    -0.4296515252    -1.3129312851     5.8959945209
H    -1.4198530851    -0.3525216535     7.0089651128
O    -0.2132964788     5.6017742783     0.7325983575
C    -0.8675257430     4.5885464474     0.0323782516
H    -0.1762505333     3.9336717985    -0.5428774561
H    -1.5946793127     4.9878077044    -0.6994543177
H    -1.4439648096     3.9053538002     0.6957607613

PEPM + 0.05nN Force Path b
B3LYP+D3 Energy:   -682.1107127191
C     0.1274254728    -0.6183596297     0.5104560001
C    -0.2004306809     0.0998655490     1.8256131655
C     0.7943228691     1.2329002921     2.1233064691
H    -0.2122360853    -0.6311544171     2.6445661692
H    -1.2142297272     0.5208437307     1.7734139370
C     0.4403270802     1.9974628638     3.4153086644
H     0.7919617474     1.8977821037     1.2556866681
H     1.8084179359     0.8203581341     2.2021839968
C     0.6731780161     1.0957227949     4.6615106907
C    -0.5932190424     0.8403305026     5.4902786985
H     1.4449615545     1.5154718788     5.3130746126
H     1.0766951290     0.1326798586     4.3282182094
C    -0.3314352575    -0.0649800850     6.6992474986
H    -1.3578428468     0.3856367628     4.8456938793
H    -1.0092046341     1.7980118829     5.8303471433
N     1.1496633379     3.3383567859     3.5249466602
H    -0.6301970265     2.2503725254     3.3648451763
C     0.8109123021     4.2026641292     2.3527836567
C     0.7203740696     4.0193960660     4.7909934293
C     1.2289154920     5.4544792505     4.9445110549
H     1.0635476412     3.4196886003     5.6346132774
H    -0.3796395928     4.0202453525     4.8086563093
C     0.8501388026     6.3178685254     3.7400329812
H     2.3171560304     5.4630090279     5.0817107198
H     0.7977373584     5.8542066235     5.8702342333
C     1.3427324149     5.6327786741     2.4640037997
H     1.2778899504     7.3226323380     3.8340547559
H    -0.2424658099     6.4323339753     3.6977190941
H    -0.2844126593     4.2179375690     2.2459166695
H     1.2239164210     3.7387977760     1.4571728691
H     2.4399690716     5.6285569591     2.4422932133
H     1.0126871364     6.1756075147     1.5705083744
C     3.0692281808     3.0288128363     3.5255459221
H     3.1359033479     2.9976215357     2.4502450970
H     2.9822447712     2.1126706889     4.0817058926
H     3.2968933441     3.9417505594     4.0460174963
H     0.1039006347     0.0784155379    -0.3366274811
H    -0.5910100087    -1.4203025033     0.3053801260
H     1.1286542261    -1.0652843567     0.5457540346
H     0.4034400588     0.3859772487     7.3776756252
H     0.0610947038    -1.0400375198     6.3843622934
H    -1.2504062720    -0.2425918589     7.2697273253
O     5.0726857099     2.6756025953     3.5452528319
C     5.3836240470     2.5378870593     4.8977441493
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H     6.4668820589     2.3912734755     5.0620567133
H     4.8751941218     1.6709417802     5.3748682936
H     5.0918891401     3.4257035303     5.5011040462

PEPM + 0.05nN Force Path d
B3LYP+D3 Energy:   -682.1101890320
C    -0.4017444564     0.1386528337    -0.0264900619
C    -0.5896294113     0.6961560479     1.3893765076
C     0.6512328104     1.4538247892     1.8850256533
H    -0.8317047504    -0.1257920540     2.0766970991
H    -1.4523607286     1.3763373445     1.4075865675
C     0.4552640663     2.0075785041     3.3090045454
H     0.8608325964     2.2601118363     1.1754840567
H     1.5191296210     0.7824424728     1.8643389273
C     0.5618062634     0.8792010049     4.3724805245
C    -0.6140743733     0.8243391678     5.3593477477
H     1.5056954495     0.9585021857     4.9248785833
H     0.6173659089    -0.0823316808     3.8491016126
C    -0.4473106421    -0.2807876117     6.4079081663
H    -1.5411129631     0.6636552790     4.7912508322
H    -0.7301210518     1.7913301507     5.8638833214
N     1.3648955902     3.1933968229     3.5947879111
H    -0.5490732738     2.4450254366     3.3617953779
C     0.9262583147     4.5643101367     2.5371442817
C     1.1137330745     3.7095857829     4.9871449082
C     1.7847608635     5.0488884236     5.3144512163
H     1.4266459772     2.9405038725     5.6985244649
H     0.0282188684     3.8239392151     5.0719516848
C     1.3223733851     6.1719932606     4.3705714944
H     2.8764810635     4.9491687800     5.2810835618
H     1.5265921030     5.2705040296     6.3596652693
C     1.5500338661     5.8074110942     2.9062439155
H     1.8349400753     7.1073224049     4.6310757587
H     0.2478697766     6.3462367093     4.5494899684
H    -0.1532058080     4.5038027864     2.7041099617
H     1.2018918664     4.1641540748     1.5638822058
H     2.6099308297     5.8555160561     2.6217362760
H     0.8406669132     6.9088172198     2.0234160220
C     2.7975607776     2.8905629328     3.3812106562
H     2.9360924581     2.4589992242     2.3902064557
H     3.1662882741     2.1951684103     4.1405192089
H     3.3640785235     3.8201715625     3.4369184569
H    -0.2037030006     0.9439949252    -0.7445585126
H    -1.2963550080    -0.3980501886    -0.3623044759
H     0.4436158287    -0.5594475217    -0.0669830357
H     0.4532329775    -0.1144998865     7.0126282486
H    -0.3512927475    -1.2656647723     5.9334318380
H    -1.3058719295    -0.3187417113     7.0881770985
O     0.3389497359     7.6931650163     1.4174334138
C    -0.5269883813     7.0285974310     0.5143550510
H    -1.5753492349     7.0471776902     0.8544768462
H    -0.2390530973     5.9711631794     0.3906247025
H    -0.4867222896     7.4999604369    -0.4774821452

PEPM + 0.05nN Force Path e
B3LYP+D3 Energy:   -682.1099502085
C     0.1634666985     0.0007283901    -0.0374267129
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C    -0.2903627896     0.7678182973     1.2090510746
C     0.7877496193     0.8106490021     2.3030617579
H    -1.1944394720     0.3016313966     1.6223297803
H    -0.5726905321     1.7909859259     0.9286974610
C     0.3305912212     1.5152321639     3.5897293672
H     1.6962583132     1.2598173755     1.8881082594
H     1.0710265462    -0.2145721607     2.5604492971
C     0.4868444019     0.7274592491     4.7903399756
C     0.0097202566     1.1934439696     6.1647535933
H     1.4527450121     0.2064561055     4.8380628337
H    -0.4082326849    -0.2990725481     4.4387463306
C    -0.1714294635     0.0313707940     7.1556175757
H    -0.9443865533     1.7318533313     6.0612850358
H     0.7085194789     1.9084230062     6.6266833882
N     1.2169860891     3.1709225098     3.5747186107
H    -0.6515332000     1.9845677272     3.4899382795
C     1.1049319975     3.8063779202     2.2220186678
C     0.5127223951     4.0302927592     4.5813341616
C     0.9709158016     5.4925405341     4.5863006231
H     0.6578338144     3.5820066513     5.5614382150
H    -0.5539407812     3.9761681119     4.3378275758
C     0.8497787016     6.1235976488     3.1954966171
H     2.0075636831     5.5611187420     4.9392934024
H     0.3552129780     6.0291450402     5.3178998584
C     1.5929613182     5.2579562414     2.1729030275
H     1.2466267347     7.1452570515     3.1990848612
H    -0.2107587491     6.1897166808     2.9139199302
H     0.0444252911     3.7637040819     1.9503735783
H     1.6622494920     3.1958450551     1.5109854322
H     2.6739046000     5.2981076123     2.3578456484
H     1.4342402692     5.6261876465     1.1524617308
C     2.6151734229     2.8924495143     3.9633011834
H     3.0900891880     2.2980693481     3.1803420653
H     2.6034839568     2.3159638660     4.8899455919
H     3.1871771720     3.8106381456     4.1095755130
H     1.0535221711     0.4608675812    -0.4856228694
H    -0.6232351863    -0.0185396760    -0.8006541426
H     0.4153336317    -1.0383382885     0.2091501753
H     0.7638359071    -0.5324242180     7.2707640404
H    -0.9368341692    -0.6713246910     6.8100657235
H    -0.4620383356     0.3978906953     8.1479069635
O    -1.2343922104    -1.2110310964     4.1853722738
C    -0.5974640480    -2.2469656296     3.4787784673
H    -1.0923801062    -3.2159938668     3.6581926387
H     0.4595298838    -2.3703832355     3.7812652581
H    -0.5986358594    -2.0832980951     2.3844637311

PEPM + 0.10nN Force Reactant
B3LYP+D3 Energy:   -682.1460505681
C    -0.4122324035    -0.0805850656     0.0306052558
C    -0.6224649118     0.5435498340     1.4153942594
C     0.5857540625     1.3900498485     1.8524486044
H    -0.8162951110    -0.2487686322     2.1494562453
H    -1.5176902054     1.1787537331     1.4029632857
C     0.3548793661     2.0240713202     3.2343198124
H     0.7465178677     2.1484721092     1.0817092201
H     1.4837900388     0.7594675818     1.8726297262
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C     0.4683882174     0.9692448815     4.3627323479
C    -0.7261392121     0.9457352775     5.3290683883
H     1.3982830088     1.0817032431     4.9308831119
H     0.5516340406    -0.0171620844     3.8934493756
C    -0.5661276305    -0.1161651528     6.4215557292
H    -1.6404253167     0.7572489659     4.7517989404
H    -0.8606081294     1.9310295148     5.7909496421
N     1.2868133492     3.2600374254     3.4723802841
H    -0.6334272879     2.4986381313     3.2524506862
C     0.9006524353     4.3519396342     2.4665378063
C     1.0125145265     3.8016277226     4.8747208171
C     1.6919140884     5.1366348200     5.1706615569
H     1.3299000330     3.0373866990     5.5821975065
H    -0.0732271455     3.9107598967     4.9276978371
C     1.2876839073     6.2050701056     4.1510199102
H     2.7818907118     5.0221968115     5.1977997256
H     1.3854460841     5.4228759378     6.1835594085
C     1.5728954225     5.6963571292     2.7354027708
H     1.8255431207     7.1406647362     4.3392798245
H     0.2150617888     6.4175784498     4.2538432066
H    -0.1900005497     4.4216735919     2.5407580997
H     1.1749575403     3.9853659274     1.4790047529
H     2.6543079169     5.6314801370     2.5652911846
H     1.1832746159     6.3920794732     1.9830191342
C     2.7311728192     2.8877390501     3.3164473406
H     2.9002248830     2.5536811560     2.2938380440
H     2.9746684947     2.0893938546     4.0168315403
H     3.3589601813     3.7516337673     3.5218346270
H    -0.2560269719     0.6941390487    -0.7302042635
H    -1.2816393537    -0.6762268690    -0.2698851010
H     0.4654963396    -0.7385805485     0.0220912915
H     0.3220881043     0.0804875443     7.0355105634
H    -0.4533104201    -1.1171615369     5.9861414661
H    -1.4364560831    -0.1364613140     7.0872349178
O    -2.2356695704     4.0054417542     3.1252588539
C    -3.2100499451     3.0832016088     3.4780633556
H    -3.3625062461     2.9904960737     4.5788920317
H    -2.9848273031     2.0447295853     3.1341659529
H    -4.2196036264     3.3082064023     3.0620868040

PEPM + 0.10nN Force Path a
B3LYP+D3 Energy:   -682.1121226899
C    -0.3454234093     0.0742192388    -0.0892885818
C    -0.5566881310     0.6252793007     1.3257930508
C     0.6776723544     1.3752556040     1.8464836507
H    -0.8161272268    -0.1982368653     2.0051370492
H    -1.4154122964     1.3108557316     1.3299253659
C     0.4557635132     1.9434912440     3.2620517256
H     0.9090486027     2.1721609174     1.1342098108
H     1.5412077734     0.6975918331     1.8500342157
C     0.5221100640     0.8122654165     4.3300148497
C    -0.6805159503     0.7681313701     5.2845519353
H     1.4488952154     0.8906045610     4.9110096189
H     0.5881536424    -0.1520783032     3.8128347161
C    -0.5420764496    -0.3216626233     6.3532098737
H    -1.5923495232     0.5992332758     4.6944910171
H    -0.8103107390     1.7417087192     5.7729184351
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N     1.3672832009     3.1129996635     3.5661752995
H    -0.5486859592     2.3842344386     3.2883213790
C     0.7841787530     4.5948237872     2.3063249963
C     1.1098331655     3.6164881968     4.9424589402
C     1.7397103456     4.9758743049     5.2454217577
H     1.4484048836     2.8743122694     5.6750357047
H     0.0224121151     3.7030230326     5.0386035635
C     1.2489778429     6.0830242125     4.3086718040
H     2.8343207559     4.9137109274     5.2109388028
H     1.4812308391     5.2207770497     6.2830821957
C     1.5452688119     5.7774216924     2.8363907599
H     1.7223413599     7.0329025626     4.5827481478
H     0.1650683390     6.2173339828     4.4351912533
H    -0.2345695199     4.4151092300     2.6135550144
H     1.1822292704     4.0366928303     1.4796701310
H     2.6216212619     5.6236214603     2.6890873287
H     1.2668827475     6.6327235624     2.2135954250
C     2.7888076275     2.7913706047     3.3385782086
H     2.9401133590     2.5189099233     2.2931248615
H     3.1184154586     1.9623205771     3.9770064430
H     3.4059755762     3.6618682662     3.5570213126
H    -0.1375064687     0.8842475392    -0.7994151978
H    -1.2331524174    -0.4626302635    -0.4429483347
H     0.5021188554    -0.6219258728    -0.1199127074
H     0.3402996234    -0.1439331196     6.9810250265
H    -0.4296515252    -1.3129312851     5.8959945209
H    -1.4198530851    -0.3525216535     7.0089651128
O    -0.2132964788     5.6017742783     0.7325983575
C    -0.8675257430     4.5885464474     0.0323782516
H    -0.1762505333     3.9336717985    -0.5428774561
H    -1.5946793127     4.9878077044    -0.6994543177
H    -1.4439648096     3.9053538002     0.6957607613

PEPM + 0.10nN Force Path b
B3LYP+D3 Energy:   -682.1105181427
C     0.1274254728    -0.6183596297     0.5104560001
C    -0.2004306809     0.0998655490     1.8256131655
C     0.7943228691     1.2329002921     2.1233064691
H    -0.2122360853    -0.6311544171     2.6445661692
H    -1.2142297272     0.5208437307     1.7734139370
C     0.4403270802     1.9974628638     3.4153086644
H     0.7919617474     1.8977821037     1.2556866681
H     1.8084179359     0.8203581341     2.2021839968
C     0.6731780161     1.0957227949     4.6615106907
C    -0.5932190424     0.8403305026     5.4902786985
H     1.4449615545     1.5154718788     5.3130746126
H     1.0766951290     0.1326798586     4.3282182094
C    -0.3314352575    -0.0649800850     6.6992474986
H    -1.3578428468     0.3856367628     4.8456938793
H    -1.0092046341     1.7980118829     5.8303471433
N     1.1496633379     3.3383567859     3.5249466602
H    -0.6301970265     2.2503725254     3.3648451763
C     0.8109123021     4.2026641292     2.3527836567
C     0.7203740696     4.0193960660     4.7909934293
C     1.2289154920     5.4544792505     4.9445110549
H     1.0635476412     3.4196886003     5.6346132774
H    -0.3796395928     4.0202453525     4.8086563093
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C     0.8501388026     6.3178685254     3.7400329812
H     2.3171560304     5.4630090279     5.0817107198
H     0.7977373584     5.8542066235     5.8702342333
C     1.3427324149     5.6327786741     2.4640037997
H     1.2778899504     7.3226323380     3.8340547559
H    -0.2424658099     6.4323339753     3.6977190941
H    -0.2844126593     4.2179375690     2.2459166695
H     1.2239164210     3.7387977760     1.4571728691
H     2.4399690716     5.6285569591     2.4422932133
H     1.0126871364     6.1756075147     1.5705083744
C     3.0692281808     3.0288128363     3.5255459221
H     3.1359033479     2.9976215357     2.4502450970
H     2.9822447712     2.1126706889     4.0817058926
H     3.2968933441     3.9417505594     4.0460174963
H     0.1039006347     0.0784155379    -0.3366274811
H    -0.5910100087    -1.4203025033     0.3053801260
H     1.1286542261    -1.0652843567     0.5457540346
H     0.4034400588     0.3859772487     7.3776756252
H     0.0610947038    -1.0400375198     6.3843622934
H    -1.2504062720    -0.2425918589     7.2697273253
O     5.0726857099     2.6756025953     3.5452528319
C     5.3836240470     2.5378870593     4.8977441493
H     6.4668820589     2.3912734755     5.0620567133
H     4.8751941218     1.6709417802     5.3748682936
H     5.0918891401     3.4257035303     5.5011040462

PEPM + 0.10nN Force Path d
B3LYP+D3 Energy:   -682.1100892572
C    -0.4017444564     0.1386528337    -0.0264900619
C    -0.5896294113     0.6961560479     1.3893765076
C     0.6512328104     1.4538247892     1.8850256533
H    -0.8317047504    -0.1257920540     2.0766970991
H    -1.4523607286     1.3763373445     1.4075865675
C     0.4552640663     2.0075785041     3.3090045454
H     0.8608325964     2.2601118363     1.1754840567
H     1.5191296210     0.7824424728     1.8643389273
C     0.5618062634     0.8792010049     4.3724805245
C    -0.6140743733     0.8243391678     5.3593477477
H     1.5056954495     0.9585021857     4.9248785833
H     0.6173659089    -0.0823316808     3.8491016126
C    -0.4473106421    -0.2807876117     6.4079081663
H    -1.5411129631     0.6636552790     4.7912508322
H    -0.7301210518     1.7913301507     5.8638833214
N     1.3648955902     3.1933968229     3.5947879111
H    -0.5490732738     2.4450254366     3.3617953779
C     0.9262583147     4.5643101367     2.5371442817
C     1.1137330745     3.7095857829     4.9871449082
C     1.7847608635     5.0488884236     5.3144512163
H     1.4266459772     2.9405038725     5.6985244649
H     0.0282188684     3.8239392151     5.0719516848
C     1.3223733851     6.1719932606     4.3705714944
H     2.8764810635     4.9491687800     5.2810835618
H     1.5265921030     5.2705040296     6.3596652693
C     1.5500338661     5.8074110942     2.9062439155
H     1.8349400753     7.1073224049     4.6310757587
H     0.2478697766     6.3462367093     4.5494899684
H    -0.1532058080     4.5038027864     2.7041099617
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H     1.2018918664     4.1641540748     1.5638822058
H     2.6099308297     5.8555160561     2.6217362760
H     0.8406669132     6.9088172198     2.0234160220
C     2.7975607776     2.8905629328     3.3812106562
H     2.9360924581     2.4589992242     2.3902064557
H     3.1662882741     2.1951684103     4.1405192089
H     3.3640785235     3.8201715625     3.4369184569
H    -0.2037030006     0.9439949252    -0.7445585126
H    -1.2963550080    -0.3980501886    -0.3623044759
H     0.4436158287    -0.5594475217    -0.0669830357
H     0.4532329775    -0.1144998865     7.0126282486
H    -0.3512927475    -1.2656647723     5.9334318380
H    -1.3058719295    -0.3187417113     7.0881770985
O     0.3389497359     7.6931650163     1.4174334138
C    -0.5269883813     7.0285974310     0.5143550510
H    -1.5753492349     7.0471776902     0.8544768462
H    -0.2390530973     5.9711631794     0.3906247025
H    -0.4867222896     7.4999604369    -0.4774821452

PEPM + 0.10nN Force Path e
B3LYP+D3 Energy:   -682.1099211065
C     0.1475025206     0.0989132243    -0.1099570178
C    -0.2999221204     0.8441232143     1.1519189817
C     0.7804468809     0.8614093566     2.2444668123
H    -1.2053026422     0.3746176669     1.5582999370
H    -0.5776504113     1.8737794076     0.8917506001
C     0.3288310804     1.5456427244     3.5440743680
H     1.6904814419     1.3133109908     1.8360673720
H     1.0587954476    -0.1695638347     2.4834409347
C     0.4809454538     0.7361154306     4.7307592827
C     0.0053619832     1.1801711672     6.1130835568
H     1.4432186038     0.2077462476     4.7696351562
H    -0.4216603032    -0.2781679921     4.3593397643
C    -0.1942112185     0.0006708951     7.0798066600
H    -0.9419146147     1.7320920642     6.0181172879
H     0.7114442498     1.8771548510     6.5912803685
N     1.2233641742     3.1963766481     3.5574136692
H    -0.6508743042     2.0220996834     3.4542072735
C     1.1072855821     3.8558303948     2.2168069159
C     0.5286936873     4.0399667898     4.5836763291
C     0.9926690989     5.5003251545     4.6106014462
H     0.6791615842     3.5728976247     5.5542393215
H    -0.5398444568     3.9935412068     4.3467651709
C     0.8660895751     6.1556223048     3.2316993219
H     2.0317470671     5.5587178828     4.9584612101
H     0.3836701330     6.0269042867     5.3549756393
C     1.6012876529     5.3060193150     2.1902463863
H     1.2658612662     7.1759369086     3.2514629064
H    -0.1957089048     6.2295930300     2.9568632719
H     0.0451370356     3.8230654064     1.9502950715
H     1.6580221859     3.2553364270     1.4922357477
H     2.6833200936     5.3388748133     2.3708850997
H     1.4391633611     5.6928911509     1.1772917837
C     2.6219849925     2.9045902311     3.9341373708
H     3.0916528476     2.3251373893     3.1370049202
H     2.6116044114     2.3089204042     4.8486419157
H     3.1980202640     3.8174800861     4.0973335260
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H     1.0382996403     0.5635820394    -0.5520091965
H    -0.6411941315     0.0971054747    -0.8713864127
H     0.3956870202    -0.9457016603     0.1161802408
H     0.7319506118    -0.5800368022     7.1836034031
H    -0.9703572439    -0.6825379472     6.7197132629
H    -0.4797481222     0.3513021891     8.0793102657
O    -1.2540038935    -1.1785724135     4.0862426919
C    -0.6223684602    -2.2069088647     3.3640471055
H    -1.1205163520    -3.1765567811     3.5307548944
H     0.4347551962    -2.3383404437     3.6626535486
H    -0.6248843733    -2.0276699940     2.2722009999

PEPM + 0.15nN Force Reactant
B3LYP+D3 Energy:   -682.1459420700
C      -0.3557198565    -0.1418569467     0.0595085009
C      -0.5951249471     0.5035432704     1.4299373419
C       0.5965574010     1.3732591535     1.8678567809
H      -0.7877199810    -0.2787224641     2.1749737709
H      -1.4989410908     1.1247866565     1.3941007837
C       0.3419025583     2.0356424700     3.2323217899
H       0.7605222063     2.1168578484     1.0834426604
H       1.5000719958     0.7516813828     1.9136500518
C       0.4310737595     1.0028787143     4.3831286601
C      -0.7844311885     0.9929300563     5.3233689698
H       1.3465830619     1.1287468533     4.9713717665
H       0.5288699638     0.0079277219     3.9352826572
C      -0.6467908486    -0.0509181052     6.4361594904
H      -1.6860144014     0.7918902266     4.7297600930
H      -0.9296464535     1.9854148025     5.7664099710
N       1.2796839848     3.2692929331     3.4641482235
H      -0.6433991441     2.5186345647     3.2244648322
C       0.9287388512     4.3432959456     2.4265451446
C       0.9761828829     3.8445069830     4.8469477358
C       1.6646419690     5.1772774097     5.1310026483
H       1.2650402277     3.0921972283     5.5791805421
H      -0.1095831904     3.9670533492     4.8678883988
C       1.2961823587     6.2289140120     4.0804660242
H       2.7524056286     5.0512775414     5.1853046795
H       1.3388159464     5.4881782173     6.1304876243
C       1.6072259812     5.6870246725     2.6828255513
H       1.8407710603     7.1621181585     4.2613559426
H       0.2241125019     6.4560053579     4.1545991062
H      -0.1629534315     4.4236948558     2.4711030419
H       1.2236916046     3.9538393194     1.4537095134
H       2.6914356333     5.6089868334     2.5382040731
H       1.2412524338     6.3702767630     1.9074188274
C       2.7239606203     2.8812741975     3.3498286394
H       2.9133142586     2.5277655716     2.3374304100
H       2.9437844598     2.0934447097     4.0693675165
H       3.3552483081     3.7426652483     3.5548400082
H      -0.2005242714     0.6216354654    -0.7128089130
H      -1.2114364388    -0.7562902194    -0.2424898812
H       0.5321398409    -0.7860196441     0.0749488426
H       0.2277146587     0.1569841437     7.0658208058
H      -0.5235063588    -1.0583933400     6.0190788606
H      -1.5314245791    -0.0614967734     7.0828484874
O      -2.2012205792     4.0038446219     3.0503609903
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C      -3.2432102746     3.0886164181     3.0848729633
H      -2.8979519417     2.0268987242     3.1174835982
H      -3.9202112359     3.1405413657     2.2006114184
H      -3.9112232704     3.1983016325     3.9707749016

PEPM + 0.15nN Force Path a
B3LYP+D3 Energy:   -682.1119861563
C    -0.3454234093     0.0742192388    -0.0892885818
C    -0.5566881310     0.6252793007     1.3257930508
C     0.6776723544     1.3752556040     1.8464836507
H    -0.8161272268    -0.1982368653     2.0051370492
H    -1.4154122964     1.3108557316     1.3299253659
C     0.4557635132     1.9434912440     3.2620517256
H     0.9090486027     2.1721609174     1.1342098108
H     1.5412077734     0.6975918331     1.8500342157
C     0.5221100640     0.8122654165     4.3300148497
C    -0.6805159503     0.7681313701     5.2845519353
H     1.4488952154     0.8906045610     4.9110096189
H     0.5881536424    -0.1520783032     3.8128347161
C    -0.5420764496    -0.3216626233     6.3532098737
H    -1.5923495232     0.5992332758     4.6944910171
H    -0.8103107390     1.7417087192     5.7729184351
N     1.3672832009     3.1129996635     3.5661752995
H    -0.5486859592     2.3842344386     3.2883213790
C     0.7841787530     4.5948237872     2.3063249963
C     1.1098331655     3.6164881968     4.9424589402
C     1.7397103456     4.9758743049     5.2454217577
H     1.4484048836     2.8743122694     5.6750357047
H     0.0224121151     3.7030230326     5.0386035635
C     1.2489778429     6.0830242125     4.3086718040
H     2.8343207559     4.9137109274     5.2109388028
H     1.4812308391     5.2207770497     6.2830821957
C     1.5452688119     5.7774216924     2.8363907599
H     1.7223413599     7.0329025626     4.5827481478
H     0.1650683390     6.2173339828     4.4351912533
H    -0.2345695199     4.4151092300     2.6135550144
H     1.1822292704     4.0366928303     1.4796701310
H     2.6216212619     5.6236214603     2.6890873287
H     1.2668827475     6.6327235624     2.2135954250
C     2.7888076275     2.7913706047     3.3385782086
H     2.9401133590     2.5189099233     2.2931248615
H     3.1184154586     1.9623205771     3.9770064430
H     3.4059755762     3.6618682662     3.5570213126
H    -0.1375064687     0.8842475392    -0.7994151978
H    -1.2331524174    -0.4626302635    -0.4429483347
H     0.5021188554    -0.6219258728    -0.1199127074
H     0.3402996234    -0.1439331196     6.9810250265
H    -0.4296515252    -1.3129312851     5.8959945209
H    -1.4198530851    -0.3525216535     7.0089651128
O    -0.2132964788     5.6017742783     0.7325983575
C    -0.8675257430     4.5885464474     0.0323782516
H    -0.1762505333     3.9336717985    -0.5428774561
H    -1.5946793127     4.9878077044    -0.6994543177
H    -1.4439648096     3.9053538002     0.6957607613

PEPM + 0.15nN Force Path b
B3LYP+D3 Energy:   -682.1099925337
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C     0.1274254728    -0.6183596297     0.5104560001
C    -0.2004306809     0.0998655490     1.8256131655
C     0.7943228691     1.2329002921     2.1233064691
H    -0.2122360853    -0.6311544171     2.6445661692
H    -1.2142297272     0.5208437307     1.7734139370
C     0.4403270802     1.9974628638     3.4153086644
H     0.7919617474     1.8977821037     1.2556866681
H     1.8084179359     0.8203581341     2.2021839968
C     0.6731780161     1.0957227949     4.6615106907
C    -0.5932190424     0.8403305026     5.4902786985
H     1.4449615545     1.5154718788     5.3130746126
H     1.0766951290     0.1326798586     4.3282182094
C    -0.3314352575    -0.0649800850     6.6992474986
H    -1.3578428468     0.3856367628     4.8456938793
H    -1.0092046341     1.7980118829     5.8303471433
N     1.1496633379     3.3383567859     3.5249466602
H    -0.6301970265     2.2503725254     3.3648451763
C     0.8109123021     4.2026641292     2.3527836567
C     0.7203740696     4.0193960660     4.7909934293
C     1.2289154920     5.4544792505     4.9445110549
H     1.0635476412     3.4196886003     5.6346132774
H    -0.3796395928     4.0202453525     4.8086563093
C     0.8501388026     6.3178685254     3.7400329812
H     2.3171560304     5.4630090279     5.0817107198
H     0.7977373584     5.8542066235     5.8702342333
C     1.3427324149     5.6327786741     2.4640037997
H     1.2778899504     7.3226323380     3.8340547559
H    -0.2424658099     6.4323339753     3.6977190941
H    -0.2844126593     4.2179375690     2.2459166695
H     1.2239164210     3.7387977760     1.4571728691
H     2.4399690716     5.6285569591     2.4422932133
H     1.0126871364     6.1756075147     1.5705083744
C     3.0692281808     3.0288128363     3.5255459221
H     3.1359033479     2.9976215357     2.4502450970
H     2.9822447712     2.1126706889     4.0817058926
H     3.2968933441     3.9417505594     4.0460174963
H     0.1039006347     0.0784155379    -0.3366274811
H    -0.5910100087    -1.4203025033     0.3053801260
H     1.1286542261    -1.0652843567     0.5457540346
H     0.4034400588     0.3859772487     7.3776756252
H     0.0610947038    -1.0400375198     6.3843622934
H    -1.2504062720    -0.2425918589     7.2697273253
O     5.0726857099     2.6756025953     3.5452528319
C     5.3836240470     2.5378870593     4.8977441493
H     6.4668820589     2.3912734755     5.0620567133
H     4.8751941218     1.6709417802     5.3748682936
H     5.0918891401     3.4257035303     5.5011040462

PEPM + 0.15nN Force Path d
B3LYP+D3 Energy:   -682.1099290002
C    -0.4017444564     0.1386528337    -0.0264900619
C    -0.5896294113     0.6961560479     1.3893765076
C     0.6512328104     1.4538247892     1.8850256533
H    -0.8317047504    -0.1257920540     2.0766970991
H    -1.4523607286     1.3763373445     1.4075865675
C     0.4552640663     2.0075785041     3.3090045454
H     0.8608325964     2.2601118363     1.1754840567
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H     1.5191296210     0.7824424728     1.8643389273
C     0.5618062634     0.8792010049     4.3724805245
C    -0.6140743733     0.8243391678     5.3593477477
H     1.5056954495     0.9585021857     4.9248785833
H     0.6173659089    -0.0823316808     3.8491016126
C    -0.4473106421    -0.2807876117     6.4079081663
H    -1.5411129631     0.6636552790     4.7912508322
H    -0.7301210518     1.7913301507     5.8638833214
N     1.3648955902     3.1933968229     3.5947879111
H    -0.5490732738     2.4450254366     3.3617953779
C     0.9262583147     4.5643101367     2.5371442817
C     1.1137330745     3.7095857829     4.9871449082
C     1.7847608635     5.0488884236     5.3144512163
H     1.4266459772     2.9405038725     5.6985244649
H     0.0282188684     3.8239392151     5.0719516848
C     1.3223733851     6.1719932606     4.3705714944
H     2.8764810635     4.9491687800     5.2810835618
H     1.5265921030     5.2705040296     6.3596652693
C     1.5500338661     5.8074110942     2.9062439155
H     1.8349400753     7.1073224049     4.6310757587
H     0.2478697766     6.3462367093     4.5494899684
H    -0.1532058080     4.5038027864     2.7041099617
H     1.2018918664     4.1641540748     1.5638822058
H     2.6099308297     5.8555160561     2.6217362760
H     0.8406669132     6.9088172198     2.0234160220
C     2.7975607776     2.8905629328     3.3812106562
H     2.9360924581     2.4589992242     2.3902064557
H     3.1662882741     2.1951684103     4.1405192089
H     3.3640785235     3.8201715625     3.4369184569
H    -0.2037030006     0.9439949252    -0.7445585126
H    -1.2963550080    -0.3980501886    -0.3623044759
H     0.4436158287    -0.5594475217    -0.0669830357
H     0.4532329775    -0.1144998865     7.0126282486
H    -0.3512927475    -1.2656647723     5.9334318380
H    -1.3058719295    -0.3187417113     7.0881770985
O     0.3389497359     7.6931650163     1.4174334138
C    -0.5269883813     7.0285974310     0.5143550510
H    -1.5753492349     7.0471776902     0.8544768462
H    -0.2390530973     5.9711631794     0.3906247025
H    -0.4867222896     7.4999604369    -0.4774821452

PEPM + 0.15nN Force Path e
B3LYP+D3 Energy:   -682.1098903594
C     0.1634666985     0.0007283901    -0.0374267129
C    -0.2903627896     0.7678182973     1.2090510746
C     0.7877496193     0.8106490021     2.3030617579
H    -1.1944394720     0.3016313966     1.6223297803
H    -0.5726905321     1.7909859259     0.9286974610
C     0.3305912212     1.5152321639     3.5897293672
H     1.6962583132     1.2598173755     1.8881082594
H     1.0710265462    -0.2145721607     2.5604492971
C     0.4868444019     0.7274592491     4.7903399756
C     0.0097202566     1.1934439696     6.1647535933
H     1.4527450121     0.2064561055     4.8380628337
H    -0.4082326849    -0.2990725481     4.4387463306
C    -0.1714294635     0.0313707940     7.1556175757
H    -0.9443865533     1.7318533313     6.0612850358
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H     0.7085194789     1.9084230062     6.6266833882
N     1.2169860891     3.1709225098     3.5747186107
H    -0.6515332000     1.9845677272     3.4899382795
C     1.1049319975     3.8063779202     2.2220186678
C     0.5127223951     4.0302927592     4.5813341616
C     0.9709158016     5.4925405341     4.5863006231
H     0.6578338144     3.5820066513     5.5614382150
H    -0.5539407812     3.9761681119     4.3378275758
C     0.8497787016     6.1235976488     3.1954966171
H     2.0075636831     5.5611187420     4.9392934024
H     0.3552129780     6.0291450402     5.3178998584
C     1.5929613182     5.2579562414     2.1729030275
H     1.2466267347     7.1452570515     3.1990848612
H    -0.2107587491     6.1897166808     2.9139199302
H     0.0444252911     3.7637040819     1.9503735783
H     1.6622494920     3.1958450551     1.5109854322
H     2.6739046000     5.2981076123     2.3578456484
H     1.4342402692     5.6261876465     1.1524617308
C     2.6151734229     2.8924495143     3.9633011834
H     3.0900891880     2.2980693481     3.1803420653
H     2.6034839568     2.3159638660     4.8899455919
H     3.1871771720     3.8106381456     4.1095755130
H     1.0535221711     0.4608675812    -0.4856228694
H    -0.6232351863    -0.0185396760    -0.8006541426
H     0.4153336317    -1.0383382885     0.2091501753
H     0.7638359071    -0.5324242180     7.2707640404
H    -0.9368341692    -0.6713246910     6.8100657235
H    -0.4620383356     0.3978906953     8.1479069635
O    -1.2343922104    -1.2110310964     4.1853722738
C    -0.5974640480    -2.2469656296     3.4787784673
H    -1.0923801062    -3.2159938668     3.6581926387
H     0.4595298838    -2.3703832355     3.7812652581
H    -0.5986358594    -2.0832980951     2.3844637311

PEPM + 0.20nN Force Reactant
B3LYP+D3 Energy:   -682.1454849240
C      -0.3557198565    -0.1418569467     0.0595085009
C      -0.5951249471     0.5035432704     1.4299373419
C       0.5965574010     1.3732591535     1.8678567809
H      -0.7877199810    -0.2787224641     2.1749737709
H      -1.4989410908     1.1247866565     1.3941007837
C       0.3419025583     2.0356424700     3.2323217899
H       0.7605222063     2.1168578484     1.0834426604
H       1.5000719958     0.7516813828     1.9136500518
C       0.4310737595     1.0028787143     4.3831286601
C      -0.7844311885     0.9929300563     5.3233689698
H       1.3465830619     1.1287468533     4.9713717665
H       0.5288699638     0.0079277219     3.9352826572
C      -0.6467908486    -0.0509181052     6.4361594904
H      -1.6860144014     0.7918902266     4.7297600930
H      -0.9296464535     1.9854148025     5.7664099710
N       1.2796839848     3.2692929331     3.4641482235
H      -0.6433991441     2.5186345647     3.2244648322
C       0.9287388512     4.3432959456     2.4265451446
C       0.9761828829     3.8445069830     4.8469477358
C       1.6646419690     5.1772774097     5.1310026483
H       1.2650402277     3.0921972283     5.5791805421
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H      -0.1095831904     3.9670533492     4.8678883988
C       1.2961823587     6.2289140120     4.0804660242
H       2.7524056286     5.0512775414     5.1853046795
H       1.3388159464     5.4881782173     6.1304876243
C       1.6072259812     5.6870246725     2.6828255513
H       1.8407710603     7.1621181585     4.2613559426
H       0.2241125019     6.4560053579     4.1545991062
H      -0.1629534315     4.4236948558     2.4711030419
H       1.2236916046     3.9538393194     1.4537095134
H       2.6914356333     5.6089868334     2.5382040731
H       1.2412524338     6.3702767630     1.9074188274
C       2.7239606203     2.8812741975     3.3498286394
H       2.9133142586     2.5277655716     2.3374304100
H       2.9437844598     2.0934447097     4.0693675165
H       3.3552483081     3.7426652483     3.5548400082
H      -0.2005242714     0.6216354654    -0.7128089130
H      -1.2114364388    -0.7562902194    -0.2424898812
H       0.5321398409    -0.7860196441     0.0749488426
H       0.2277146587     0.1569841437     7.0658208058
H      -0.5235063588    -1.0583933400     6.0190788606
H      -1.5314245791    -0.0614967734     7.0828484874
O      -2.2012205792     4.0038446219     3.0503609903
C      -3.2432102746     3.0886164181     3.0848729633
H      -2.8979519417     2.0268987242     3.1174835982
H      -3.9202112359     3.1405413657     2.2006114184
H      -3.9112232704     3.1983016325     3.9707749016

PEPM + 0.20nN Force Path a
B3LYP+D3 Energy:   -682.1117707283
C     -0.3454234093     0.0742192388    -0.0892885818
C     -0.5566881310     0.6252793007     1.3257930508
C      0.6776723544     1.3752556040     1.8464836507
H     -0.8161272268    -0.1982368653     2.0051370492
H     -1.4154122964     1.3108557316     1.3299253659
C      0.4557635132     1.9434912440     3.2620517256
H      0.9090486027     2.1721609174     1.1342098108
H      1.5412077734     0.6975918331     1.8500342157
C      0.5221100640     0.8122654165     4.3300148497
C     -0.6805159503     0.7681313701     5.2845519353
H      1.4488952154     0.8906045610     4.9110096189
H      0.5881536424    -0.1520783032     3.8128347161
C     -0.5420764496    -0.3216626233     6.3532098737
H     -1.5923495232     0.5992332758     4.6944910171
H     -0.8103107390     1.7417087192     5.7729184351
N      1.3672832009     3.1129996635     3.5661752995
H     -0.5486859592     2.3842344386     3.2883213790
C      0.7841787530     4.5948237872     2.3063249963
C      1.1098331655     3.6164881968     4.9424589402
C      1.7397103456     4.9758743049     5.2454217577
H      1.4484048836     2.8743122694     5.6750357047
H      0.0224121151     3.7030230326     5.0386035635
C      1.2489778429     6.0830242125     4.3086718040
H      2.8343207559     4.9137109274     5.2109388028
H      1.4812308391     5.2207770497     6.2830821957
C      1.5452688119     5.7774216924     2.8363907599
H      1.7223413599     7.0329025626     4.5827481478
H      0.1650683390     6.2173339828     4.4351912533
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H    -0.2345695199     4.4151092300     2.6135550144
H     1.1822292704     4.0366928303     1.4796701310
H     2.6216212619     5.6236214603     2.6890873287
H     1.2668827475     6.6327235624     2.2135954250
C     2.7888076275     2.7913706047     3.3385782086
H     2.9401133590     2.5189099233     2.2931248615
H     3.1184154586     1.9623205771     3.9770064430
H     3.4059755762     3.6618682662     3.5570213126
H    -0.1375064687     0.8842475392    -0.7994151978
H    -1.2331524174    -0.4626302635    -0.4429483347
H     0.5021188554    -0.6219258728    -0.1199127074
H     0.3402996234    -0.1439331196     6.9810250265
H    -0.4296515252    -1.3129312851     5.8959945209
H    -1.4198530851    -0.3525216535     7.0089651128
O    -0.2132964788     5.6017742783     0.7325983575
C    -0.8675257430     4.5885464474     0.0323782516
H    -0.1762505333     3.9336717985    -0.5428774561
H    -1.5946793127     4.9878077044    -0.6994543177
H    -1.4439648096     3.9053538002     0.6957607613

PEPM + 0.20nN Force Path b
B3LYP+D3 Energy:   -682.1097140992
C     0.1274254728    -0.6183596297     0.5104560001
C    -0.2004306809     0.0998655490     1.8256131655
C     0.7943228691     1.2329002921     2.1233064691
H    -0.2122360853    -0.6311544171     2.6445661692
H    -1.2142297272     0.5208437307     1.7734139370
C     0.4403270802     1.9974628638     3.4153086644
H     0.7919617474     1.8977821037     1.2556866681
H     1.8084179359     0.8203581341     2.2021839968
C     0.6731780161     1.0957227949     4.6615106907
C    -0.5932190424     0.8403305026     5.4902786985
H     1.4449615545     1.5154718788     5.3130746126
H     1.0766951290     0.1326798586     4.3282182094
C    -0.3314352575    -0.0649800850     6.6992474986
H    -1.3578428468     0.3856367628     4.8456938793
H    -1.0092046341     1.7980118829     5.8303471433
N     1.1496633379     3.3383567859     3.5249466602
H    -0.6301970265     2.2503725254     3.3648451763
C     0.8109123021     4.2026641292     2.3527836567
C     0.7203740696     4.0193960660     4.7909934293
C     1.2289154920     5.4544792505     4.9445110549
H     1.0635476412     3.4196886003     5.6346132774
H    -0.3796395928     4.0202453525     4.8086563093
C     0.8501388026     6.3178685254     3.7400329812
H     2.3171560304     5.4630090279     5.0817107198
H     0.7977373584     5.8542066235     5.8702342333
C     1.3427324149     5.6327786741     2.4640037997
H     1.2778899504     7.3226323380     3.8340547559
H    -0.2424658099     6.4323339753     3.6977190941
H    -0.2844126593     4.2179375690     2.2459166695
H     1.2239164210     3.7387977760     1.4571728691
H     2.4399690716     5.6285569591     2.4422932133
H     1.0126871364     6.1756075147     1.5705083744
C     3.0692281808     3.0288128363     3.5255459221
H     3.1359033479     2.9976215357     2.4502450970
H     2.9822447712     2.1126706889     4.0817058926
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H     3.2968933441     3.9417505594     4.0460174963
H     0.1039006347     0.0784155379    -0.3366274811
H    -0.5910100087    -1.4203025033     0.3053801260
H     1.1286542261    -1.0652843567     0.5457540346
H     0.4034400588     0.3859772487     7.3776756252
H     0.0610947038    -1.0400375198     6.3843622934
H    -1.2504062720    -0.2425918589     7.2697273253
O     5.0726857099     2.6756025953     3.5452528319
C     5.3836240470     2.5378870593     4.8977441493
H     6.4668820589     2.3912734755     5.0620567133
H     4.8751941218     1.6709417802     5.3748682936
H     5.0918891401     3.4257035303     5.5011040462

PEPM + 0.20nN Force Path d
B3LYP+D3 Energy:   -682.1096558187
C    -0.4017444564     0.1386528337    -0.0264900619
C    -0.5896294113     0.6961560479     1.3893765076
C     0.6512328104     1.4538247892     1.8850256533
H    -0.8317047504    -0.1257920540     2.0766970991
H    -1.4523607286     1.3763373445     1.4075865675
C     0.4552640663     2.0075785041     3.3090045454
H     0.8608325964     2.2601118363     1.1754840567
H     1.5191296210     0.7824424728     1.8643389273
C     0.5618062634     0.8792010049     4.3724805245
C    -0.6140743733     0.8243391678     5.3593477477
H     1.5056954495     0.9585021857     4.9248785833
H     0.6173659089    -0.0823316808     3.8491016126
C    -0.4473106421    -0.2807876117     6.4079081663
H    -1.5411129631     0.6636552790     4.7912508322
H    -0.7301210518     1.7913301507     5.8638833214
N     1.3648955902     3.1933968229     3.5947879111
H    -0.5490732738     2.4450254366     3.3617953779
C     0.9262583147     4.5643101367     2.5371442817
C     1.1137330745     3.7095857829     4.9871449082
C     1.7847608635     5.0488884236     5.3144512163
H     1.4266459772     2.9405038725     5.6985244649
H     0.0282188684     3.8239392151     5.0719516848
C     1.3223733851     6.1719932606     4.3705714944
H     2.8764810635     4.9491687800     5.2810835618
H     1.5265921030     5.2705040296     6.3596652693
C     1.5500338661     5.8074110942     2.9062439155
H     1.8349400753     7.1073224049     4.6310757587
H     0.2478697766     6.3462367093     4.5494899684
H    -0.1532058080     4.5038027864     2.7041099617
H     1.2018918664     4.1641540748     1.5638822058
H     2.6099308297     5.8555160561     2.6217362760
H     0.8406669132     6.9088172198     2.0234160220
C     2.7975607776     2.8905629328     3.3812106562
H     2.9360924581     2.4589992242     2.3902064557
H     3.1662882741     2.1951684103     4.1405192089
H     3.3640785235     3.8201715625     3.4369184569
H    -0.2037030006     0.9439949252    -0.7445585126
H    -1.2963550080    -0.3980501886    -0.3623044759
H     0.4436158287    -0.5594475217    -0.0669830357
H     0.4532329775    -0.1144998865     7.0126282486
H    -0.3512927475    -1.2656647723     5.9334318380
H    -1.3058719295    -0.3187417113     7.0881770985
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O     0.3389497359     7.6931650163     1.4174334138
C    -0.5269883813     7.0285974310     0.5143550510
H    -1.5753492349     7.0471776902     0.8544768462
H    -0.2390530973     5.9711631794     0.3906247025
H    -0.4867222896     7.4999604369    -0.4774821452

PEPM + 0.20nN Force Path e
B3LYP+D3 Energy:   -682.1098328408
C     0.1634666985     0.0007283901    -0.0374267129
C    -0.2903627896     0.7678182973     1.2090510746
C     0.7877496193     0.8106490021     2.3030617579
H    -1.1944394720     0.3016313966     1.6223297803
H    -0.5726905321     1.7909859259     0.9286974610
C     0.3305912212     1.5152321639     3.5897293672
H     1.6962583132     1.2598173755     1.8881082594
H     1.0710265462    -0.2145721607     2.5604492971
C     0.4868444019     0.7274592491     4.7903399756
C     0.0097202566     1.1934439696     6.1647535933
H     1.4527450121     0.2064561055     4.8380628337
H    -0.4082326849    -0.2990725481     4.4387463306
C    -0.1714294635     0.0313707940     7.1556175757
H    -0.9443865533     1.7318533313     6.0612850358
H     0.7085194789     1.9084230062     6.6266833882
N     1.2169860891     3.1709225098     3.5747186107
H    -0.6515332000     1.9845677272     3.4899382795
C     1.1049319975     3.8063779202     2.2220186678
C     0.5127223951     4.0302927592     4.5813341616
C     0.9709158016     5.4925405341     4.5863006231
H     0.6578338144     3.5820066513     5.5614382150
H    -0.5539407812     3.9761681119     4.3378275758
C     0.8497787016     6.1235976488     3.1954966171
H     2.0075636831     5.5611187420     4.9392934024
H     0.3552129780     6.0291450402     5.3178998584
C     1.5929613182     5.2579562414     2.1729030275
H     1.2466267347     7.1452570515     3.1990848612
H    -0.2107587491     6.1897166808     2.9139199302
H     0.0444252911     3.7637040819     1.9503735783
H     1.6622494920     3.1958450551     1.5109854322
H     2.6739046000     5.2981076123     2.3578456484
H     1.4342402692     5.6261876465     1.1524617308
C     2.6151734229     2.8924495143     3.9633011834
H     3.0900891880     2.2980693481     3.1803420653
H     2.6034839568     2.3159638660     4.8899455919
H     3.1871771720     3.8106381456     4.1095755130
H     1.0535221711     0.4608675812    -0.4856228694
H    -0.6232351863    -0.0185396760    -0.8006541426
H     0.4153336317    -1.0383382885     0.2091501753
H     0.7638359071    -0.5324242180     7.2707640404
H    -0.9368341692    -0.6713246910     6.8100657235
H    -0.4620383356     0.3978906953     8.1479069635
O    -1.2343922104    -1.2110310964     4.1853722738
C    -0.5974640480    -2.2469656296     3.4787784673
H    -1.0923801062    -3.2159938668     3.6581926387
H     0.4595298838    -2.3703832355     3.7812652581
H    -0.5986358594    -2.0832980951     2.3844637311

PEPM + 0.25nN Force Reactant
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B3LYP+D3 Energy: -682.1452294806

C	-0.3557198565	-0.1418569467	0.0595085009
C	-0.5951249471	0.5035432704	1.4299373419
C	0.5965574010	1.3732591535	1.8678567809
H	-0.7877199810	-0.2787224641	2.1749737709
H	-1.4989410908	1.1247866565	1.3941007837
C	0.3419025583	2.0356424700	3.2323217899
H	0.7605222063	2.1168578484	1.0834426604
H	1.5000719958	0.7516813828	1.9136500518
C	0.4310737595	1.0028787143	4.3831286601
C	-0.7844311885	0.9929300563	5.3233689698
H	1.3465830619	1.1287468533	4.9713717665
H	0.5288699638	0.0079277219	3.9352826572
C	-0.6467908486	-0.0509181052	6.4361594904
H	-1.6860144014	0.7918902266	4.7297600930
H	-0.9296464535	1.9854148025	5.7664099710
N	1.2796839848	3.2692929331	3.4641482235
H	-0.6433991441	2.5186345647	3.2244648322
C	0.9287388512	4.3432959456	2.4265451446
C	0.9761828829	3.8445069830	4.8469477358
C	1.6646419690	5.1772774097	5.1310026483
H	1.2650402277	3.0921972283	5.5791805421
H	-0.1095831904	3.9670533492	4.8678883988
C	1.2961823587	6.2289140120	4.0804660242
H	2.7524056286	5.0512775414	5.1853046795
H	1.3388159464	5.4881782173	6.1304876243
C	1.6072259812	5.6870246725	2.6828255513
H	1.8407710603	7.1621181585	4.2613559426
H	0.2241125019	6.4560053579	4.1545991062
H	-0.1629534315	4.4236948558	2.4711030419
H	1.2236916046	3.9538393194	1.4537095134
H	2.6914356333	5.6089868334	2.5382040731
H	1.2412524338	6.3702767630	1.9074188274
C	2.7239606203	2.8812741975	3.3498286394
H	2.9133142586	2.5277655716	2.3374304100
H	2.9437844598	2.0934447097	4.0693675165
H	3.3552483081	3.7426652483	3.5548400082
H	-0.2005242714	0.6216354654	-0.7128089130
H	-1.2114364388	-0.7562902194	-0.2424898812
H	0.5321398409	-0.7860196441	0.0749488426
H	0.2277146587	0.1569841437	7.0658208058
H	-0.5235063588	-1.0583933400	6.0190788606
H	-1.5314245791	-0.0614967734	7.0828484874
O	-2.2012205792	4.0038446219	3.0503609903
C	-3.2432102746	3.0886164181	3.0848729633
H	-2.8979519417	2.0268987242	3.1174835982
H	-3.9202112359	3.1405413657	2.2006114184
H	-3.9112232704	3.1983016325	3.9707749016

PEPM + 0.25nN Force Path a

B3LYP+D3 Energy: -682.1111558135

C	-0.3454234093	0.0742192388	-0.0892885818
C	-0.5566881310	0.6252793007	1.3257930508
C	0.6776723544	1.3752556040	1.8464836507
H	-0.8161272268	-0.1982368653	2.0051370492
H	-1.4154122964	1.3108557316	1.3299253659
C	0.4557635132	1.9434912440	3.2620517256

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H     0.9090486027     2.1721609174     1.1342098108
H     1.5412077734     0.6975918331     1.8500342157
C     0.5221100640     0.8122654165     4.3300148497
C    -0.6805159503     0.7681313701     5.2845519353
H     1.4488952154     0.8906045610     4.9110096189
H     0.5881536424    -0.1520783032     3.8128347161
C    -0.5420764496    -0.3216626233     6.3532098737
H    -1.5923495232     0.5992332758     4.6944910171
H    -0.8103107390     1.7417087192     5.7729184351
N     1.3672832009     3.1129996635     3.5661752995
H    -0.5486859592     2.3842344386     3.2883213790
C     0.7841787530     4.5948237872     2.3063249963
C     1.1098331655     3.6164881968     4.9424589402
C     1.7397103456     4.9758743049     5.2454217577
H     1.4484048836     2.8743122694     5.6750357047
H     0.0224121151     3.7030230326     5.0386035635
C     1.2489778429     6.0830242125     4.3086718040
H     2.8343207559     4.9137109274     5.2109388028
H     1.4812308391     5.2207770497     6.2830821957
C     1.5452688119     5.7774216924     2.8363907599
H     1.7223413599     7.0329025626     4.5827481478
H     0.1650683390     6.2173339828     4.4351912533
H    -0.2345695199     4.4151092300     2.6135550144
H     1.1822292704     4.0366928303     1.4796701310
H     2.6216212619     5.6236214603     2.6890873287
H     1.2668827475     6.6327235624     2.2135954250
C     2.7888076275     2.7913706047     3.3385782086
H     2.9401133590     2.5189099233     2.2931248615
H     3.1184154586     1.9623205771     3.9770064430
H     3.4059755762     3.6618682662     3.5570213126
H    -0.1375064687     0.8842475392    -0.7994151978
H    -1.2331524174    -0.4626302635    -0.4429483347
H     0.5021188554    -0.6219258728    -0.1199127074
H     0.3402996234    -0.1439331196     6.9810250265
H    -0.4296515252    -1.3129312851     5.8959945209
H    -1.4198530851    -0.3525216535     7.0089651128
O    -0.2132964788     5.6017742783     0.7325983575
C    -0.8675257430     4.5885464474     0.0323782516
H    -0.1762505333     3.9336717985    -0.5428774561
H    -1.5946793127     4.9878077044    -0.6994543177
H    -1.4439648096     3.9053538002     0.6957607613

PEPM + 0.25nN Force Path b
B3LYP+D3 Energy:   -682.1094413185
C     0.1274254728    -0.6183596297     0.5104560001
C    -0.2004306809     0.0998655490     1.8256131655
C     0.7943228691     1.2329002921     2.1233064691
H    -0.2122360853    -0.6311544171     2.6445661692
H    -1.2142297272     0.5208437307     1.7734139370
C     0.4403270802     1.9974628638     3.4153086644
H     0.7919617474     1.8977821037     1.2556866681
H     1.8084179359     0.8203581341     2.2021839968
C     0.6731780161     1.0957227949     4.6615106907
C    -0.5932190424     0.8403305026     5.4902786985
H     1.4449615545     1.5154718788     5.3130746126
H     1.0766951290     0.1326798586     4.3282182094
C    -0.3314352575    -0.0649800850     6.6992474986
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H    -1.3578428468     0.3856367628     4.8456938793
H    -1.0092046341     1.7980118829     5.8303471433
N     1.1496633379     3.3383567859     3.5249466602
H    -0.6301970265     2.2503725254     3.3648451763
C     0.8109123021     4.2026641292     2.3527836567
C     0.7203740696     4.0193960660     4.7909934293
C     1.2289154920     5.4544792505     4.9445110549
H     1.0635476412     3.4196886003     5.6346132774
H    -0.3796395928     4.0202453525     4.8086563093
C     0.8501388026     6.3178685254     3.7400329812
H     2.3171560304     5.4630090279     5.0817107198
H     0.7977373584     5.8542066235     5.8702342333
C     1.3427324149     5.6327786741     2.4640037997
H     1.2778899504     7.3226323380     3.8340547559
H    -0.2424658099     6.4323339753     3.6977190941
H    -0.2844126593     4.2179375690     2.2459166695
H     1.2239164210     3.7387977760     1.4571728691
H     2.4399690716     5.6285569591     2.4422932133
H     1.0126871364     6.1756075147     1.5705083744
C     3.0692281808     3.0288128363     3.5255459221
H     3.1359033479     2.9976215357     2.4502450970
H     2.9822447712     2.1126706889     4.0817058926
H     3.2968933441     3.9417505594     4.0460174963
H     0.1039006347     0.0784155379    -0.3366274811
H    -0.5910100087    -1.4203025033     0.3053801260
H     1.1286542261    -1.0652843567     0.5457540346
H     0.4034400588     0.3859772487     7.3776756252
H     0.0610947038    -1.0400375198     6.3843622934
H    -1.2504062720    -0.2425918589     7.2697273253
O     5.0726857099     2.6756025953     3.5452528319
C     5.3836240470     2.5378870593     4.8977441493
H     6.4668820589     2.3912734755     5.0620567133
H     4.8751941218     1.6709417802     5.3748682936
H     5.0918891401     3.4257035303     5.5011040462

PEPM + 0.25nN Force Path d
B3LYP+D3 Energy:   -682.1091222401
C    -0.4017444564     0.1386528337    -0.0264900619
C    -0.5896294113     0.6961560479     1.3893765076
C     0.6512328104     1.4538247892     1.8850256533
H    -0.8317047504    -0.1257920540     2.0766970991
H    -1.4523607286     1.3763373445     1.4075865675
C     0.4552640663     2.0075785041     3.3090045454
H     0.8608325964     2.2601118363     1.1754840567
H     1.5191296210     0.7824424728     1.8643389273
C     0.5618062634     0.8792010049     4.3724805245
C    -0.6140743733     0.8243391678     5.3593477477
H     1.5056954495     0.9585021857     4.9248785833
H     0.6173659089    -0.0823316808     3.8491016126
C    -0.4473106421    -0.2807876117     6.4079081663
H    -1.5411129631     0.6636552790     4.7912508322
H    -0.7301210518     1.7913301507     5.8638833214
N     1.3648955902     3.1933968229     3.5947879111
H    -0.5490732738     2.4450254366     3.3617953779
C     0.9262583147     4.5643101367     2.5371442817
C     1.1137330745     3.7095857829     4.9871449082
C     1.7847608635     5.0488884236     5.3144512163
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H     1.4266459772     2.9405038725     5.6985244649
H     0.0282188684     3.8239392151     5.0719516848
C     1.3223733851     6.1719932606     4.3705714944
H     2.8764810635     4.9491687800     5.2810835618
H     1.5265921030     5.2705040296     6.3596652693
C     1.5500338661     5.8074110942     2.9062439155
H     1.8349400753     7.1073224049     4.6310757587
H     0.2478697766     6.3462367093     4.5494899684
H    -0.1532058080     4.5038027864     2.7041099617
H     1.2018918664     4.1641540748     1.5638822058
H     2.6099308297     5.8555160561     2.6217362760
H     0.8406669132     6.9088172198     2.0234160220
C     2.7975607776     2.8905629328     3.3812106562
H     2.9360924581     2.4589992242     2.3902064557
H     3.1662882741     2.1951684103     4.1405192089
H     3.3640785235     3.8201715625     3.4369184569
H    -0.2037030006     0.9439949252    -0.7445585126
H    -1.2963550080    -0.3980501886    -0.3623044759
H     0.4436158287    -0.5594475217    -0.0669830357
H     0.4532329775    -0.1144998865     7.0126282486
H    -0.3512927475    -1.2656647723     5.9334318380
H    -1.3058719295    -0.3187417113     7.0881770985
O     0.3389497359     7.6931650163     1.4174334138
C    -0.5269883813     7.0285974310     0.5143550510
H    -1.5753492349     7.0471776902     0.8544768462
H    -0.2390530973     5.9711631794     0.3906247025
H    -0.4867222896     7.4999604369    -0.4774821452

PEPM + 0.25nN Force Path e
B3LYP+D3 Energy:   -682.1097564439
C     0.1475025206     0.0989132243    -0.1099570178
C    -0.2999221204     0.8441232143     1.1519189817
C     0.7804468809     0.8614093566     2.2444668123
H    -1.2053026422     0.3746176669     1.5582999370
H    -0.5776504113     1.8737794076     0.8917506001
C     0.3288310804     1.5456427244     3.5440743680
H     1.6904814419     1.3133109908     1.8360673720
H     1.0587954476    -0.1695638347     2.4834409347
C     0.4809454538     0.7361154306     4.7307592827
C     0.0053619832     1.1801711672     6.1130835568
H     1.4432186038     0.2077462476     4.7696351562
H    -0.4216603032    -0.2781679921     4.3593397643
C    -0.1942112185     0.0006708951     7.0798066600
H    -0.9419146147     1.7320920642     6.0181172879
H     0.7114442498     1.8771548510     6.5912803685
N     1.2233641742     3.1963766481     3.5574136692
H    -0.6508743042     2.0220996834     3.4542072735
C     1.1072855821     3.8558303948     2.2168069159
C     0.5286936873     4.0399667898     4.5836763291
C     0.9926690989     5.5003251545     4.6106014462
H     0.6791615842     3.5728976247     5.5542393215
H    -0.5398444568     3.9935412068     4.3467651709
C     0.8660895751     6.1556223048     3.2316993219
H     2.0317470671     5.5587178828     4.9584612101
H     0.3836701330     6.0269042867     5.3549756393
C     1.6012876529     5.3060193150     2.1902463863
H     1.2658612662     7.1759369086     3.2514629064
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H    -0.1957089048     6.2295930300     2.9568632719
H     0.0451370356     3.8230654064     1.9502950715
H     1.6580221859     3.2553364270     1.4922357477
H     2.6833200936     5.3388748133     2.3708850997
H     1.4391633611     5.6928911509     1.1772917837
C     2.6219849925     2.9045902311     3.9341373708
H     3.0916528476     2.3251373893     3.1370049202
H     2.6116044114     2.3089204042     4.8486419157
H     3.1980202640     3.8174800861     4.0973335260
H     1.0382996403     0.5635820394    -0.5520091965
H    -0.6411941315     0.0971054747    -0.8713864127
H     0.3956870202    -0.9457016603     0.1161802408
H     0.7319506118    -0.5800368022     7.1836034031
H    -0.9703572439    -0.6825379472     6.7197132629
H    -0.4797481222     0.3513021891     8.0793102657
O    -1.2540038935    -1.1785724135     4.0862426919
C    -0.6223684602    -2.2069088647     3.3640471055
H    -1.1205163520    -3.1765567811     3.5307548944
H     0.4347551962    -2.3383404437     3.6626535486
H    -0.6248843733    -2.0276699940     2.2722009999

PEPM - 0.05nN Force Reactant
B3LYP+D3 Energy:   -682.1461422740
C    -0.5905330179    -0.1270578463     0.2758039383
C    -0.5972865763     0.3711111213     1.7261168411
C     0.4143463155     1.5105320708     1.9356392546
H    -0.3721918448    -0.4692005085     2.3917223176
H    -1.6027775913     0.7253040383     1.9876780580
C     0.3348007463     2.1151768375     3.3444406995
H     0.2037918703     2.2726503926     1.1809308325
H     1.4231015959     1.1256452717     1.7386692855
C     0.5500985976     1.0439320067     4.4362492304
C    -0.7800535743     0.5393034713     5.0172446585
H     1.1467525685     1.4161725408     5.2738999772
H     1.1234237315     0.2044297805     4.0231253572
C    -0.5695197487    -0.5863470870     6.0346722326
H    -1.4415314156     0.1960571363     4.2172050161
H    -1.2941980999     1.3844607914     5.4944233104
N     1.3041907751     3.3329076589     3.5196988891
H    -0.6390684052     2.6029829687     3.4748162652
C     1.0212569431     4.3504973112     2.4128157656
C     0.9651692760     4.0029309566     4.8570914992
C     1.6856654268     5.3290600273     5.0829773625
H     1.2113363223     3.2935616097     5.6457976046
H    -0.1202243149     4.1443811429     4.8176131912
C     1.3904259190     6.3261574331     3.9588777344
H     2.7667969416     5.1763015219     5.1856994999
H     1.3346394173     5.7106602452     6.0489604253
C     1.7314420352     5.6877514659     2.6097352604
H     1.9608729659     7.2505671853     4.1022097155
H     0.3251923584     6.5930789078     3.9791580563
H    -0.0658492960     4.4751613695     2.4251004264
H     1.3307776194     3.8962349328     1.4730611330
H     2.8166105572     5.5655333738     2.5093450038
H     1.4153504126     6.3305070967     1.7796265079
C     2.7377690555     2.8960973576     3.4739639075
H     2.9494282012     2.4818955887     2.4889476847
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H     2.9063023494     2.1429025965     4.2416379579
H     3.3899786667     3.7475154443     3.6540572947
H    -0.8550817082     0.6771444270    -0.4218427030
H    -1.3097024865    -0.9422649774     0.1370273658
H     0.4009225733    -0.5017799205    -0.0077491170
H     0.0659955908    -0.2532947377     6.8650268893
H    -0.0798580391    -1.4511794203     5.5691739949
H    -1.5223039127    -0.9265776837     6.4559916284
O    -2.0901265352     4.1823961795     3.7147738946
C    -3.1922815194     3.3496965114     3.5869581048
H    -3.8377853981     3.3095943637     4.4954883703
H    -2.9209883989     2.2844884748     3.3845854205
H    -3.8790914088     3.6326521519     2.7554498375

PEPM - 0.05nN Force Path a
B3LYP+D3 Energy:   -682.1117748685
N       -0.1258721961      0.7037670939      0.4631223911
C       -1.0341873236     -2.1637173830     -1.8322262535
C       -1.6294526049      1.5558041849     -0.6189920320
C       -1.8206848984      2.8570044239      0.1094151281
H       -0.9909359848      1.5050372433     -1.4876268583
H       -2.2602786927      0.7150105742     -0.3941810550
C       -0.5623827798      3.7290571890      0.1268010923
H       -2.1666521256      2.6665616249      1.1327985272
H       -2.6343272551      3.3847795601     -0.3957615604
C        2.1011282513     -2.3473949172     -0.6290423724
C        0.5569775458      3.1016331958      0.9593028470
H       -0.8098289700      4.7180823724      0.5306759366
H       -0.2185253201      3.8847595534     -0.9059504461
C        0.9740019822      1.7080914232      0.4804642038
H        0.2551652593      3.0655132725      2.0135390168
H        1.4562614432      3.7284193526      0.9200415474
H        1.7945904533      1.3488459318      1.1121667984
H        1.3484018242      1.7736684667     -0.5476032437
C        0.2745272119     -0.5271915434     -0.3294745738
C       -0.8651801838     -1.5697797652     -0.4244242882
C        1.5826346764     -1.1576823492      0.1937229776
H        0.4671558877     -0.1384965782     -1.3378168816
C       -0.5991987578      0.3784522243      1.8219586802
H       -0.6820503907     -2.3771629656      0.2965603233
H       -1.8264273656     -1.1342231727     -0.1395186781
H        1.4387667025     -1.4850749716      1.2320636729
H        2.3731211227     -0.4006807255      0.2101998385
H       -0.0859820242     -2.5787519707     -2.1904939885
H       -1.2994094547     -1.3553257696     -2.5251464603
C       -2.1139597063     -3.2499758842     -1.8729144028
H        1.3837529557     -3.1761672773     -0.5967236317
C        3.4602539544     -2.8385132836     -0.1162849660
H        2.1926893971     -2.0530198816     -1.6836695006
H       -1.8610436305     -4.0820124227     -1.2036230239
H       -2.2314012100     -3.6562509696     -2.8841444476
H       -3.0861938761     -2.8513909392     -1.5563845910
H        3.8237923035     -3.6869490581     -0.7072506283
H        3.3930661640     -3.1622515254      0.9299367472
H        4.2143615748     -2.0432781314     -0.1697728742
H       -1.4360910322     -0.3193608625      1.7669296757
H       -0.9492927306      1.2831472759      2.3188105334
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H        0.1989691254     -0.0635636526      2.4301396302
O       -3.1318001490      1.9390068699     -2.0324964379
C       -3.3183182768      0.7873060418     -2.7953115857
H       -3.5573693472     -0.1087634053     -2.1809288695
H       -2.4277251876      0.5125737020     -3.4007573232
H       -4.1542756778      0.8976302101     -3.5119397648

PEPM - 0.05nN Force Path b
B3LYP+D3 Energy:   -682.1106920169
C        0.0125619039    -0.6177180394      0.6512809383
C       -0.1884374592     0.0509784438      2.0160543450
C        0.6534623496     1.3314849518      2.1486898248
H        0.0675897577    -0.6616079269      2.8087917865
H       -1.2503112415     0.2990539701      2.1510422077
C        0.4049475511     2.0867911515      3.4674683121
H        0.4107706950     1.9648770519      1.2909877273
H        1.7173372384     1.0732423495      2.0659981989
C        0.7044314020     1.1752682611      4.6885554989
C       -0.5688692963     0.6524260573      5.3696637889
H        1.3025315275     1.6920780472      5.4429246255
H        1.3190849932     0.3267909270      4.3629568839
C       -0.2637067521    -0.3291704211      6.5050831327
H       -1.2153132018     0.1641583802      4.6298367730
H       -1.1386053435     1.5088940290      5.7563689635
N        1.1535366390     3.4114786013      3.5319936472
H       -0.6606466007     2.3635412061      3.4956690406
C        0.8635937171     4.2353051863      2.3185888689
C        0.7236025987     4.1527928745      4.7639832874
C        1.2642458817     5.5804965014      4.8668514783
H        1.0410981811     3.5796186729      5.6350048151
H       -0.3762880564     4.1793965729      4.7674082406
C        0.9233432713     6.4018300723      3.6227070631
H        2.3503778259     5.5695359607      5.0188605353
H        0.8296151960     6.0274925815      5.7689359148
C        1.4248637265     5.6574350814      2.3841456591
H        1.3690523183     7.4012961546      3.6848223756
H       -0.1658053711     6.5355025182      3.5558629917
H       -0.2279344013     4.2720930338      2.1831542246
H        1.2887338060     3.7243739857      1.4548007554
H        2.5221059341     5.6302525605      2.3838573807
H        1.1229571387     6.1708233505      1.4637217530
C        3.0619026160     3.0512589854      3.5816486599
H        3.1523340315     2.9898999953      2.5095475050
H        2.9405533521     2.1528235441      4.1593424798
H        3.3052003701     3.9701296590      4.0844476740
H       -0.2763079256     0.0557132401     -0.1652744971
H       -0.5886246347    -1.5299310046      0.5630179268
H        1.0637225402    -0.8924554055      0.4990439354
H        0.3504650409     0.1412673129      7.2832248092
H        0.2869730830    -1.2009820372      6.1296046994
H       -1.1840739923    -0.6915058595      6.9772600212
O        5.0565434895     2.6414971166      3.6455878212
C        5.3332984446     2.4636550607      5.0008836698
H        6.4073854107     2.2772716564      5.1846715511
H        4.7867234103     1.6035348152      5.4472731967
H        5.0578133694     3.3469552976      5.6183639523
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PEPM - 0.05nN Force Path d
B3LYP+D3 Energy: -682.1101750523

C	-0.5328698210	0.0750126414	0.1368726972
C	-0.6295489996	0.6281822852	1.5626890029
C	0.5607770600	1.5369765273	1.9127905804
H	-0.6879721064	-0.2049123597	2.2735013265
H	-1.5615900894	1.1988456704	1.6765736494
C	0.4578419349	2.0687790083	3.3517222140
H	0.5851662513	2.3576882981	1.1901312824
H	1.4921768360	0.9702915203	1.7870444123
C	0.6225814228	0.9199205688	4.3857863339
C	-0.6410759604	0.6693912199	5.2190595116
H	1.4610775513	1.1135308952	5.0626412716
H	0.8913999166	-0.0011399433	3.8554124066
C	-0.4689951251	-0.4837648510	6.2126406549
H	-1.4821864503	0.4567013515	4.5453577626
H	-0.9066915149	1.5883643477	5.7591876489
N	1.3791450831	3.2490569082	3.6156373957
H	-0.5413830893	2.5048915016	3.4690873883
C	0.9660081120	4.6050134861	2.5353878588
C	1.1243567383	3.7861305667	5.0019890453
C	1.7984683668	5.1270872344	5.3139548250
H	1.4331177811	3.0287970786	5.7276362591
H	0.0381245160	3.9016834276	5.0817976240
C	1.3474494128	6.2381099246	4.3514051715
H	2.8899937727	5.0214022521	5.2869401230
H	1.5363450781	5.3640150204	6.3548864929
C	1.5911209110	5.8511254981	2.8957664727
H	1.8595159856	7.1759291798	4.6038937873
H	0.2715518325	6.4171172125	4.5166215141
H	-0.1171128104	4.5528064534	2.6811698279
H	1.2595204852	4.1906429115	1.5733033290
H	2.6558472880	5.8866332023	2.6272500786
H	0.9050374664	6.9449160232	1.9870989482
C	2.8085079902	2.9260596597	3.4093772402
H	2.9396577119	2.4746981728	2.4259628472
H	3.1687949592	2.2395623933	4.1806641417
H	3.3858266171	3.8499823059	3.4485038708
H	-0.4858278551	0.8869042140	-0.5996888240
H	-1.4003991428	-0.5491071174	-0.1061120254
H	0.3678110725	-0.5389562203	0.0126415637
H	0.3462264928	-0.2759860459	6.9169546847
H	-0.2282356828	-1.4196266133	5.6928110851
H	-1.3824693846	-0.6492153319	6.7953604382
O	0.4216597152	7.7241297962	1.3589621335
C	-0.4382054747	7.0528359811	0.4554846384
H	-1.4882627018	7.0683325592	0.7909898352
H	-0.1458306170	5.9960335100	0.3359084279
H	-0.3956868245	7.5214807797	-0.5374547847

PEPM - 0.05nN Force Path e
B3LYP+D3 Energy: -682.1106001813

C	-0.4439766041	-0.6027493841	0.4712352440
C	-0.6737638242	0.2603684481	1.7102863898
C	0.5923615392	1.0121095826	2.1602907214
H	-1.0307757288	-0.3638985212	2.5355006221
H	-1.4639884934	0.9969960010	1.5067057659

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C     0.3054508799     1.7111829822     3.4866792579
H     0.8735969895     1.6996200601     1.3547094575
H     1.4215495533     0.3068395661     2.2897104666
C     0.4893817351     0.9234490253     4.6896359299
C    -0.4274097521     1.1723295959     5.8908563933
H     1.5405424121     0.7335302092     4.9421196705
H     0.2031711383    -0.5333440896     4.4284732029
C    -1.8989786442     0.8600085948     5.5592223786
H    -0.3775004569     2.1883325235     6.3154556369
H    -0.1097951256     0.5042423253     6.7043949655
N     1.2797672471     3.2399479649     3.4427635354
H    -0.6713034658     2.2022326950     3.4469919819
C     0.7445083630     4.1589643494     2.3864350102
C     1.1160846082     3.8752824947     4.7909345837
C     1.7406288008     5.2682029440     4.8965073016
H     1.5351394157     3.1809877183     5.5206200585
H     0.0382440231     3.9421641909     4.9644950366
C     1.1917618878     6.2020216280     3.8095065106
H     2.8336454627     5.2093381496     4.8271720696
H     1.5128290294     5.6561202243     5.8962417657
C     1.3613844348     5.5616313124     2.4259340343
H     1.6963816239     7.1740659503     3.8481818475
H     0.1239816392     6.3855132957     3.9948557244
H    -0.3362506240     4.2206659527     2.5552502520
H     0.9094415179     3.6888723295     1.4157616545
H     2.4245459233     5.5128869569     2.1587007922
H     0.8702018024     6.1639723300     1.6527275814
C     2.6956417172     2.8654885410     3.2026771763
H     2.8102582248     2.5094289143     2.1786432858
H     2.9596121484     2.0679358063     3.9003809583
H     3.3644931898     3.7126613915     3.3577231244
H    -0.1152028586     0.0034993152    -0.3830597638
H    -1.3605716507    -1.1265033735     0.1748917402
H     0.3282018381    -1.3587335806     0.6570904456
H    -2.0181542835    -0.1840421172     5.2489772329
H    -2.2698475203     1.4888237638     4.7407824723
H    -2.5522195048     1.0353771010     6.4245270188
O     0.0545074389    -1.6894167268     4.4344558944
C     1.0912203494    -2.2859699506     3.6866099731
H     1.3994546693    -3.2418167926     4.1369975017
H     1.9862476791    -1.6408907145     3.6446715490
H     0.7917948463    -2.4939216344     2.6449147132

PEPM - 0.10nN Force Reactant
B3LYP+D3 Energy:   -682.1460439121
C    -0.3938063837    -0.3559201849     0.4577657239
C    -0.5573673074     0.3259472652     1.8154522896
C     0.4292914612     1.4938653400     1.9964991152
H    -0.4094153303    -0.4243200791     2.5973715844
H    -1.5848623034     0.6974058843     1.9238709871
C     0.3058265865     2.1654150048     3.3740142322
H     0.2363591978     2.2113312120     1.1946949123
H     1.4488088048     1.1121171840     1.8553834449
C     0.4912063423     1.1301798607     4.5043434774
C    -0.8556360991     0.5675995413     5.0130127813
H     1.0311866972     1.5349466097     5.3636545646
H     1.1193036256     0.3123740841     4.1298341024
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C    -0.7264664863    -0.8795138085     5.4912344347
H    -1.6152035428     0.6186831620     4.2270326129
H    -1.2249752138     1.2081921545     5.8237619978
N     1.2721582985     3.3855908884     3.5265706187
H    -0.6693531588     2.6555939502     3.4512834739
C     1.0478872653     4.3451116063     2.3562486337
C     0.8714777089     4.1285950564     4.8071334752
C     1.6000236880     5.4553693232     5.0007011253
H     1.0633393731     3.4593611160     5.6444993302
H    -0.2068101296     4.2887962785     4.6913971661
C     1.3803513989     6.3951249033     3.8111654147
H     2.6715197826     5.2942695130     5.1700931536
H     1.2038839416     5.8930852838     5.9245028136
C     1.7708102856     5.6812713291     2.5136379055
H     1.9626152326     7.3151654202     3.9336792279
H     0.3214296551     6.6826628325     3.7659226480
H    -0.0368719477     4.4838087701     2.3186320823
H     1.3887094362     3.8364907941     1.4562237306
H     2.8571252323     5.5387128951     2.4681960125
H     1.5025012012     6.2836883810     1.6377559263
C     2.7037530430     2.9420652494     3.5727959077
H     2.9556916313     2.4594576246     2.6292616165
H     2.8346606093     2.2438522608     4.3974183906
H     3.3518222481     3.8023032750     3.7207492433
H    -0.5534610896     0.3493260264    -0.3675151608
H    -1.1123195026    -1.1752259839     0.3419959990
H     0.6141073689    -0.7747945106     0.3462987655
H     0.0307498939    -0.9713401195     6.2802086545
H    -0.4254425376    -1.5374458644     4.6666523655
H    -1.6752696334    -1.2544177571     5.8921587454
O    -2.1102447510     4.3996361553     3.4779009454
C    -3.0617407723     3.4963292358     3.9280531085
H    -2.8864769315     3.1471476584     4.9736447855
H    -3.1112117177     2.5589702127     3.3219895535
H    -4.1036796305     3.8928665463     3.9267139614

PEPM - 0.10nN Force Path a
B3LYP+D3 Energy:   -682.1117339015
N    -0.1753756380     0.7555525121     0.4573313114
C    -1.1090313587    -2.1978775086    -1.7999852638
C    -1.6477239855     1.6750955396    -0.6040889757
C    -1.8026938247     2.9682657675     0.1462873821
H    -1.0055228914     1.6210314499    -1.4692779926
H    -2.3046270884     0.8497164899    -0.3966315621
C    -0.5167564488     3.7989338544     0.1755383662
H    -2.1536001405     2.7712708146     1.1668082807
H    -2.5995183894     3.5290681556    -0.3502850700
C     1.9093710324    -2.3550878666    -0.7387152106
C     0.5861534514     3.1198663996     0.9901644096
H    -0.7295207812     4.7871686082     0.6004867464
H    -0.1727009379     3.9642827161    -0.8556820869
C     0.9570937975     1.7221815553     0.4849058071
H     0.2884940191     3.0747111271     2.0451335649
H     1.5046265642     3.7185265023     0.9570296161
H     1.7685388792     1.3243645632     1.1052985645
H     1.3280198936     1.7942450292    -0.5439419176
C     0.1710159605    -0.4669640024    -0.3665410853
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C    -0.9826735890    -1.4961776047    -0.4261050901
C     1.4789427670    -1.1456494131     0.1026507773
H     0.3326080632    -0.0689308411    -1.3762747110
C    -0.6494780469     0.4194574758     1.8130502339
H    -0.8198023502    -2.2459397315     0.3581978793
H    -1.9447966176    -1.0349989942    -0.1924511340
H     1.3570333894    -1.4698566135     1.1451805060
H     2.3014296595    -0.4230117780     0.0924088297
H    -0.1735293813    -2.1159142780    -2.3624208971
H    -1.8612095471    -1.6716375540    -2.4000576157
C    -1.4842372688    -3.6769419333    -1.6731430990
H     1.1216846447    -3.1141385458    -0.7480358111
C     3.1908079538    -3.0001449021    -0.2097837571
H     2.0572485994    -2.0423752711    -1.7812250229
H    -0.7202330422    -4.2326910822    -1.1158286733
H    -1.5896137937    -4.1477556236    -2.6577650416
H    -2.4353461430    -3.8027229206    -1.1400864356
H     3.4832956046    -3.8592355735    -0.8244437227
H     3.0573525806    -3.3547925974     0.8201055195
H     4.0265742597    -2.2887448891    -0.2088280132
H    -1.5090875942    -0.2492106885     1.7510771906
H    -0.9667460144     1.3255433640     2.3291228431
H     0.1382567368    -0.0604372714     2.4063423222
O    -3.1013432602     2.1216989575    -2.0438136605
C    -3.2606397415     0.9856649653    -2.8361628330
H    -3.6844845195     0.1198494212    -2.2813984638
H    -2.3058255884     0.6246255606    -3.2770900927
H    -3.9416591910     1.1672890364    -3.6888680829

PEPM - 0.10nN Force Path b
B3LYP+D3 Energy:   -682.1106354321
C     0.0413307573    -0.7331455749     0.9186569572
C    -0.2263743707     0.0599861768     2.1969217411
C     0.5676024053     1.3764803440     2.2414159199
H     0.0273952414    -0.5724793024     3.0536165710
H    -1.2995809768     0.2796023617     2.2776139654
C     0.3633561857     2.1754793301     3.5429166145
H     0.2651739872     1.9679851294     1.3725508665
H     1.6358781308     1.1530757384     2.1223738240
C     0.6778820616     1.2780981158     4.7670861964
C    -0.5850069508     0.6278499903     5.3701990021
H     1.1935346798     1.8257850740     5.5587330263
H     1.3769905548     0.4920234338     4.4545813704
C    -0.2746460497    -0.7037639212     6.0562652494
H    -1.3345569883     0.4576785944     4.5904275109
H    -1.0447783264     1.3280084550     6.0803430784
N     1.1471964726     3.4814127486     3.5503256540
H    -0.6938351828     2.4784679360     3.5956704814
C     0.8671554563     4.2655742494     2.3084486989
C     0.7497781367     4.2767835301     4.7577489059
C     1.3257696810     5.6941576627     4.8031440562
H     1.0644266965     3.7266619200     5.6444015452
H    -0.3489861430     4.3309106839     4.7730976985
C     0.9960246777     6.4758232021     3.5306005781
H     2.4123256778     5.6626533279     4.9488334864
H     0.9076893559     6.1854248785     5.6897064757
C     1.4671573526     5.6735879535     2.3166381835
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H     1.4676993292     7.4650730146     3.5507829657
H    -0.0896979904     6.6358137406     3.4664479661
H    -0.2241605549     4.3281512402     2.1817972640
H     1.2702544677     3.7099842219     1.4617845513
H     2.5631473891     5.6159840417     2.3078942405
H     1.1704367583     6.1605192785     1.3802899115
C     3.0467563784     3.0808386110     3.6035751035
H     3.1241184810     2.9499330191     2.5368022572
H     2.9100398465     2.2255811417     4.2404338819
H     3.3160566698     4.0238558880     4.0444579556
H    -0.2332012087    -0.1591114321     0.0246324923
H    -0.5338119496    -1.6660946246     0.9068133991
H     1.1037892998    -0.9928219064     0.8325900769
H     0.4721318782    -0.5785833552     6.8506981661
H     0.1272797098    -1.4280903161     5.3368042717
H    -1.1726100971    -1.1412027894     6.5081881152
O     5.0319460156     2.6291658849     3.6671114438
C     5.3192306566     2.4970251195     5.0253055722
H     6.3918217573     2.2988985756     5.2057832315
H     4.7626377035     1.6635695055     5.5083224563
H     5.0650674720     3.4073336271     5.6118814635

PEPM - 0.10nN Force Path d
B3LYP+D3 Energy:   -682.1097922962
C    -0.6790612078     0.0196310174     0.5055097661
C    -0.6897458700     0.5536071353     1.9376533401
C     0.3207515403     1.6941060390     2.1395932902
H    -0.4675453316    -0.2778717807     2.6129610739
H    -1.6972594619     0.9074255274     2.1943526330
C     0.3730007822     2.2150954239     3.5888454622
H     0.0538862315     2.5039661314     1.4545083242
H     1.3128292579     1.3342406093     1.8383669688
C     0.6627567306     1.0598259701     4.5806591519
C    -0.6206939664     0.4213528932     5.1587975549
H     1.2860842000     1.3945673665     5.4142488739
H     1.2567457341     0.2991197188     4.0585275721
C    -0.4614091136    -1.0796946467     5.4099945151
H    -1.4644692607     0.5797779671     4.4796857869
H    -0.8870320093     0.9364291637     6.0906834569
N     1.3332773170     3.3854293387     3.7490351198
H    -0.6043208468     2.6505789310     3.8258928972
C     0.9857989631     4.6608497606     2.5548053767
C     1.0956809333     4.0528470085     5.0808707659
C     1.8375187997     5.3790325252     5.2831284807
H     1.3570132708     3.3458173058     5.8738795099
H     0.0161244189     4.2289837169     5.1366559904
C     1.4499481133     6.4266288784     4.2244933002
H     2.9223280375     5.2150431624     5.2738654757
H     1.5836336096     5.7171490943     6.2976166731
C     1.6726096888     5.8994050201     2.8097232963
H     2.0143420490     7.3526361313     4.3976629616
H     0.3861942313     6.6805995216     4.3686580193
H    -0.0992215275     4.6744824465     2.6960633148
H     1.2631887195     4.1505408196     1.6352131674
H     2.7376427766     5.8575071172     2.5443310783
H     1.0356173984     6.9467232573     1.7866432996
C     2.7529076495     2.9935394151     3.5847161911
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H     2.8607374737     2.3945783685     2.6808269965
H     3.1009761275     2.4207005741     4.4483462262
H     3.3549071664     3.8965079016     3.4806214425
H    -0.9182669572     0.8075998578    -0.2198250865
H    -1.4132888978    -0.7843599399     0.3802069177
H     0.3075264893    -0.3832022499     0.2442035147
H     0.3734853076    -1.2827249013     6.0926928662
H    -0.2583578538    -1.6129135490     4.4731186281
H    -1.3671821817    -1.5106478949     5.8524668716
O     0.6012141715     7.6802364791     1.0860479602
C    -0.2385357852     6.9618611541     0.1984131667
H    -1.2898498807     6.9586566775     0.5301676679
H     0.0816168973     5.9108972591     0.1043283039
H    -0.2033392232     7.4097913811    -0.8036559950

PEPM - 0.10nN Force Path e
B3LYP+D3 Energy:   -682.1103899756
C    -0.4439766041    -0.6027493841     0.4712352440
C    -0.6737638242     0.2603684481     1.7102863898
C     0.5923615392     1.0121095826     2.1602907214
H    -1.0307757288    -0.3638985212     2.5355006221
H    -1.4639884934     0.9969960010     1.5067057659
C     0.3054508799     1.7111829822     3.4866792579
H     0.8735969895     1.6996200601     1.3547094575
H     1.4215495533     0.3068395661     2.2897104666
C     0.4893817351     0.9234490253     4.6896359299
C    -0.4274097521     1.1723295959     5.8908563933
H     1.5405424121     0.7335302092     4.9421196705
H     0.2031711383    -0.5333440896     4.4284732029
C    -1.8989786442     0.8600085948     5.5592223786
H    -0.3775004569     2.1883325235     6.3154556369
H    -0.1097951256     0.5042423253     6.7043949655
N     1.2797672471     3.2399479649     3.4427635354
H    -0.6713034658     2.2022326950     3.4469919819
C     0.7445083630     4.1589643494     2.3864350102
C     1.1160846082     3.8752824947     4.7909345837
C     1.7406288008     5.2682029440     4.8965073016
H     1.5351394157     3.1809877183     5.5206200585
H     0.0382440231     3.9421641909     4.9644950366
C     1.1917618878     6.2020216280     3.8095065106
H     2.8336454627     5.2093381496     4.8271720696
H     1.5128290294     5.6561202243     5.8962417657
C     1.3613844348     5.5616313124     2.4259340343
H     1.6963816239     7.1740659503     3.8481818475
H     0.1239816392     6.3855132957     3.9948557244
H    -0.3362506240     4.2206659527     2.5552502520
H     0.9094415179     3.6888723295     1.4157616545
H     2.4245459233     5.5128869569     2.1587007922
H     0.8702018024     6.1639723300     1.6527275814
C     2.6956417172     2.8654885410     3.2026771763
H     2.8102582248     2.5094289143     2.1786432858
H     2.9596121484     2.0679358063     3.9003809583
H     3.3644931898     3.7126613915     3.3577231244
H    -0.1152028586     0.0034993152    -0.3830597638
H    -1.3605716507    -1.1265033735     0.1748917402
H     0.3282018381    -1.3587335806     0.6570904456
H    -2.0181542835    -0.1840421172     5.2489772329
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H    -2.2698475203     1.4888237638     4.7407824723
H    -2.5522195048     1.0353771010     6.4245270188
O     0.0545074389    -1.6894167268     4.4344558944
C     1.0912203494    -2.2859699506     3.6866099731
H     1.3994546693    -3.2418167926     4.1369975017
H     1.9862476791    -1.6408907145     3.6446715490
H     0.7917948463    -2.4939216344     2.6449147132

PEPM - 0.15nN Force Reactant
B3LYP+D3 Energy:   -682.1460074568
C    -0.5905330179    -0.1270578463     0.2758039383
C    -0.5972865763     0.3711111213     1.7261168411
C     0.4143463155     1.5105320708     1.9356392546
H    -0.3721918448    -0.4692005085     2.3917223176
H    -1.6027775913     0.7253040383     1.9876780580
C     0.3348007463     2.1151768375     3.3444406995
H     0.2037918703     2.2726503926     1.1809308325
H     1.4231015959     1.1256452717     1.7386692855
C     0.5500985976     1.0439320067     4.4362492304
C    -0.7800535743     0.5393034713     5.0172446585
H     1.1467525685     1.4161725408     5.2738999772
H     1.1234237315     0.2044297805     4.0231253572
C    -0.5695197487    -0.5863470870     6.0346722326
H    -1.4415314156     0.1960571363     4.2172050161
H    -1.2941980999     1.3844607914     5.4944233104
N     1.3041907751     3.3329076589     3.5196988891
H    -0.6390684052     2.6029829687     3.4748162652
C     1.0212569431     4.3504973112     2.4128157656
C     0.9651692760     4.0029309566     4.8570914992
C     1.6856654268     5.3290600273     5.0829773625
H     1.2113363223     3.2935616097     5.6457976046
H    -0.1202243149     4.1443811429     4.8176131912
C     1.3904259190     6.3261574331     3.9588777344
H     2.7667969416     5.1763015219     5.1856994999
H     1.3346394173     5.7106602452     6.0489604253
C     1.7314420352     5.6877514659     2.6097352604
H     1.9608729659     7.2505671853     4.1022097155
H     0.3251923584     6.5930789078     3.9791580563
H    -0.0658492960     4.4751613695     2.4251004264
H     1.3307776194     3.8962349328     1.4730611330
H     2.8166105572     5.5655333738     2.5093450038
H     1.4153504126     6.3305070967     1.7796265079
C     2.7377690555     2.8960973576     3.4739639075
H     2.9494282012     2.4818955887     2.4889476847
H     2.9063023494     2.1429025965     4.2416379579
H     3.3899786667     3.7475154443     3.6540572947
H    -0.8550817082     0.6771444270    -0.4218427030
H    -1.3097024865    -0.9422649774     0.1370273658
H     0.4009225733    -0.5017799205    -0.0077491170
H     0.0659955908    -0.2532947377     6.8650268893
H    -0.0798580391    -1.4511794203     5.5691739949
H    -1.5223039127    -0.9265776837     6.4559916284
O    -2.0901265352     4.1823961795     3.7147738946
C    -3.1922815194     3.3496965114     3.5869581048
H    -3.8377853981     3.3095943637     4.4954883703
H    -2.9209883989     2.2844884748     3.3845854205
H    -3.8790914088     3.6326521519     2.7554498375
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PEPM - 0.15nN Force Path a
B3LYP+D3 Energy: -682.1116747367

N	-0.1753756380	0.7555525121	0.4573313114
C	-1.1090313587	-2.1978775086	-1.7999852638
C	-1.6477239855	1.6750955396	-0.6040889757
C	-1.8026938247	2.9682657675	0.1462873821
H	-1.0055228914	1.6210314499	-1.4692779926
H	-2.3046270884	0.8497164899	-0.3966315621
C	-0.5167564488	3.7989338544	0.1755383662
H	-2.1536001405	2.7712708146	1.1668082807
H	-2.5995183894	3.5290681556	-0.3502850700
C	1.9093710324	-2.3550878666	-0.7387152106
C	0.5861534514	3.1198663996	0.9901644096
H	-0.7295207812	4.7871686082	0.6004867464
H	-0.1727009379	3.9642827161	-0.8556820869
C	0.9570937975	1.7221815553	0.4849058071
H	0.2884940191	3.0747111271	2.0451335649
H	1.5046265642	3.7185265023	0.9570296161
H	1.7685388792	1.3243645632	1.1052985645
H	1.3280198936	1.7942450292	-0.5439419176
C	0.1710159605	-0.4669640024	-0.3665410853
C	-0.9826735890	-1.4961776047	-0.4261050901
C	1.4789427670	-1.1456494131	0.1026507773
H	0.3326080632	-0.0689308411	-1.3762747110
C	-0.6494780469	0.4194574758	1.8130502339
H	-0.8198023502	-2.2459397315	0.3581978793
H	-1.9447966176	-1.0349989942	-0.1924511340
H	1.3570333894	-1.4698566135	1.1451805060
H	2.3014296595	-0.4230117780	0.0924088297
H	-0.1735293813	-2.1159142780	-2.3624208971
H	-1.8612095471	-1.6716375540	-2.4000576157
C	-1.4842372688	-3.6769419333	-1.6731430990
H	1.1216846447	-3.1141385458	-0.7480358111
C	3.1908079538	-3.0001449021	-0.2097837571
H	2.0572485994	-2.0423752711	-1.7812250229
H	-0.7202330422	-4.2326910822	-1.1158286733
H	-1.5896137937	-4.1477556236	-2.6577650416
H	-2.4353461430	-3.8027229206	-1.1400864356
H	3.4832956046	-3.8592355735	-0.8244437227
H	3.0573525806	-3.3547925974	0.8201055195
H	4.0265742597	-2.2887448891	-0.2088280132
H	-1.5090875942	-0.2492106885	1.7510771906
H	-0.9667460144	1.3255433640	2.3291228431
H	0.1382567368	-0.0604372714	2.4063423222
O	-3.1013432602	2.1216989575	-2.0438136605
C	-3.2606397415	0.9856649653	-2.8361628330
H	-3.6844845195	0.1198494212	-2.2813984638
H	-2.3058255884	0.6246255606	-3.2770900927
H	-3.9416591910	1.1672890364	-3.6888680829

PEPM - 0.15nN Force Path b
B3LYP+D3 Energy: -682.1105579002

C	0.0413307573	-0.7331455749	0.9186569572
C	-0.2263743707	0.0599861768	2.1969217411
C	0.5676024053	1.3764803440	2.2414159199
H	0.0273952414	-0.5724793024	3.0536165710

H	-1.2995809768	0.2796023617	2.2776139654
C	0.3633561857	2.1754793301	3.5429166145
H	0.2651739872	1.9679851294	1.3725508665
H	1.6358781308	1.1530757384	2.1223738240
C	0.6778820616	1.2780981158	4.7670861964
C	-0.5850069508	0.6278499903	5.3701990021
H	1.1935346798	1.8257850740	5.5587330263
H	1.3769905548	0.4920234338	4.4545813704
C	-0.2746460497	-0.7037639212	6.0562652494
H	-1.3345569883	0.4576785944	4.5904275109
H	-1.0447783264	1.3280084550	6.0803430784
N	1.1471964726	3.4814127486	3.5503256540
H	-0.6938351828	2.4784679360	3.5956704814
C	0.8671554563	4.2655742494	2.3084486989
C	0.7497781367	4.2767835301	4.7577489059
C	1.3257696810	5.6941576627	4.8031440562
H	1.0644266965	3.7266619200	5.6444015452
H	-0.3489861430	4.3309106839	4.7730976985
C	0.9960246777	6.4758232021	3.5306005781
H	2.4123256778	5.6626533279	4.9488334864
H	0.9076893559	6.1854248785	5.6897064757
C	1.4671573526	5.6735879535	2.3166381835
H	1.4676993292	7.4650730146	3.5507829657
H	-0.0896979904	6.6358137406	3.4664479661
H	-0.2241605549	4.3281512402	2.1817972640
H	1.2702544677	3.7099842219	1.4617845513
H	2.5631473891	5.6159840417	2.3078942405
H	1.1704367583	6.1605192785	1.3802899115
C	3.0467563784	3.0808386110	3.6035751035
H	3.1241184810	2.9499330191	2.5368022572
H	2.9100398465	2.2255811417	4.2404338819
H	3.3160566698	4.0238558880	4.0444579556
H	-0.2332012087	-0.1591114321	0.0246324923
H	-0.5338119496	-1.6660946246	0.9068133991
H	1.1037892998	-0.9928219064	0.8325900769
H	0.4721318782	-0.5785833552	6.8506981661
H	0.1272797098	-1.4280903161	5.3368042717
H	-1.1726100971	-1.1412027894	6.5081881152
O	5.0319460156	2.6291658849	3.6671114438
C	5.3192306566	2.4970251195	5.0253055722
H	6.3918217573	2.2988985756	5.2057832315
H	4.7626377035	1.6635695055	5.5083224563
H	5.0650674720	3.4073336271	5.6118814635

PEPM - 0.15nN Force Path d
B3LYP+D3 Energy: -682.1096966184

C	-0.6790612078	0.0196310174	0.5055097661
C	-0.6897458700	0.5536071353	1.9376533401
C	0.3207515403	1.6941060390	2.1395932902
H	-0.4675453316	-0.2778717807	2.6129610739
H	-1.6972594619	0.9074255274	2.1943526330
C	0.3730007822	2.2150954239	3.5888454622
H	0.0538862315	2.5039661314	1.4545083242
H	1.3128292579	1.3342406093	1.8383669688
C	0.6627567306	1.0598259701	4.5806591519
C	-0.6206939664	0.4213528932	5.1587975549
H	1.2860842000	1.3945673665	5.4142488739

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H     1.2567457341     0.2991197188     4.0585275721
C    -0.4614091136    -1.0796946467     5.4099945151
H    -1.4644692607     0.5797779671     4.4796857869
H    -0.8870320093     0.9364291637     6.0906834569
N     1.3332773170     3.3854293387     3.7490351198
H    -0.6043208468     2.6505789310     3.8258928972
C     0.9857989631     4.6608497606     2.5548053767
C     1.0956809333     4.0528470085     5.0808707659
C     1.8375187997     5.3790325252     5.2831284807
H     1.3570132708     3.3458173058     5.8738795099
H     0.0161244189     4.2289837169     5.1366559904
C     1.4499481133     6.4266288784     4.2244933002
H     2.9223280375     5.2150431624     5.2738654757
H     1.5836336096     5.7171490943     6.2976166731
C     1.6726096888     5.8994050201     2.8097232963
H     2.0143420490     7.3526361313     4.3976629616
H     0.3861942313     6.6805995216     4.3686580193
H    -0.0992215275     4.6744824465     2.6960633148
H     1.2631887195     4.1505408196     1.6352131674
H     2.7376427766     5.8575071172     2.5443310783
H     1.0356173984     6.9467232573     1.7866432996
C     2.7529076495     2.9935394151     3.5847161911
H     2.8607374737     2.3945783685     2.6808269965
H     3.1009761275     2.4207005741     4.4483462262
H     3.3549071664     3.8965079016     3.4806214425
H    -0.9182669572     0.8075998578    -0.2198250865
H    -1.4132888978    -0.7843599399     0.3802069177
H     0.3075264893    -0.3832022499     0.2442035147
H     0.3734853076    -1.2827249013     6.0926928662
H    -0.2583578538    -1.6129135490     4.4731186281
H    -1.3671821817    -1.5106478949     5.8524668716
O     0.6012141715     7.6802364791     1.0860479602
C    -0.2385357852     6.9618611541     0.1984131667
H    -1.2898498807     6.9586566775     0.5301676679
H     0.0816168973     5.9108972591     0.1043283039
H    -0.2033392232     7.4097913811    -0.8036559950

PEPM - 0.15nN Force Path e
B3LYP+D3 Energy:   -682.1099927791
C    -0.4439766041    -0.6027493841     0.4712352440
C    -0.6737638242     0.2603684481     1.7102863898
C     0.5923615392     1.0121095826     2.1602907214
H    -1.0307757288    -0.3638985212     2.5355006221
H    -1.4639884934     0.9969960010     1.5067057659
C     0.3054508799     1.7111829822     3.4866792579
H     0.8735969895     1.6996200601     1.3547094575
H     1.4215495533     0.3068395661     2.2897104666
C     0.4893817351     0.9234490253     4.6896359299
C    -0.4274097521     1.1723295959     5.8908563933
H     1.5405424121     0.7335302092     4.9421196705
H     0.2031711383    -0.5333440896     4.4284732029
C    -1.8989786442     0.8600085948     5.5592223786
H    -0.3775004569     2.1883325235     6.3154556369
H    -0.1097951256     0.5042423253     6.7043949655
N     1.2797672471     3.2399479649     3.4427635354
H    -0.6713034658     2.2022326950     3.4469919819
C     0.7445083630     4.1589643494     2.3864350102
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C	1.1160846082	3.8752824947	4.7909345837
C	1.7406288008	5.2682029440	4.8965073016
H	1.5351394157	3.1809877183	5.5206200585
H	0.0382440231	3.9421641909	4.9644950366
C	1.1917618878	6.2020216280	3.8095065106
H	2.8336454627	5.2093381496	4.8271720696
H	1.5128290294	5.6561202243	5.8962417657
C	1.3613844348	5.5616313124	2.4259340343
H	1.6963816239	7.1740659503	3.8481818475
H	0.1239816392	6.3855132957	3.9948557244
H	-0.3362506240	4.2206659527	2.5552502520
H	0.9094415179	3.6888723295	1.4157616545
H	2.4245459233	5.5128869569	2.1587007922
H	0.8702018024	6.1639723300	1.6527275814
C	2.6956417172	2.8654885410	3.2026771763
H	2.8102582248	2.5094289143	2.1786432858
H	2.9596121484	2.0679358063	3.9003809583
H	3.3644931898	3.7126613915	3.3577231244
H	-0.1152028586	0.0034993152	-0.3830597638
H	-1.3605716507	-1.1265033735	0.1748917402
H	0.3282018381	-1.3587335806	0.6570904456
H	-2.0181542835	-0.1840421172	5.2489772329
H	-2.2698475203	1.4888237638	4.7407824723
H	-2.5522195048	1.0353771010	6.4245270188
O	0.0545074389	-1.6894167268	4.4344558944
C	1.0912203494	-2.2859699506	3.6866099731
H	1.3994546693	-3.2418167926	4.1369975017
H	1.9862476791	-1.6408907145	3.6446715490
H	0.7917948463	-2.4939216344	2.6449147132

PEPM - 0.20nN Force Reactant
B3LYP+D3 Energy: -682.1459061815

C	-0.5905330179	-0.1270578463	0.2758039383
C	-0.5972865763	0.3711111213	1.7261168411
C	0.4143463155	1.5105320708	1.9356392546
H	-0.3721918448	-0.4692005085	2.3917223176
H	-1.6027775913	0.7253040383	1.9876780580
C	0.3348007463	2.1151768375	3.3444406995
H	0.2037918703	2.2726503926	1.1809308325
H	1.4231015959	1.1256452717	1.7386692855
C	0.5500985976	1.0439320067	4.4362492304
C	-0.7800535743	0.5393034713	5.0172446585
H	1.1467525685	1.4161725408	5.2738999772
H	1.1234237315	0.2044297805	4.0231253572
C	-0.5695197487	-0.5863470870	6.0346722326
H	-1.4415314156	0.1960571363	4.2172050161
H	-1.2941980999	1.3844607914	5.4944233104
N	1.3041907751	3.3329076589	3.5196988891
H	-0.6390684052	2.6029829687	3.4748162652
C	1.0212569431	4.3504973112	2.4128157656
C	0.9651692760	4.0029309566	4.8570914992
C	1.6856654268	5.3290600273	5.0829773625
H	1.2113363223	3.2935616097	5.6457976046
H	-0.1202243149	4.1443811429	4.8176131912
C	1.3904259190	6.3261574331	3.9588777344
H	2.7667969416	5.1763015219	5.1856994999
H	1.3346394173	5.7106602452	6.0489604253

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C     1.7314420352     5.6877514659     2.6097352604
H     1.9608729659     7.2505671853     4.1022097155
H     0.3251923584     6.5930789078     3.9791580563
H    -0.0658492960     4.4751613695     2.4251004264
H     1.3307776194     3.8962349328     1.4730611330
H     2.8166105572     5.5655333738     2.5093450038
H     1.4153504126     6.3305070967     1.7796265079
C     2.7377690555     2.8960973576     3.4739639075
H     2.9494282012     2.4818955887     2.4889476847
H     2.9063023494     2.1429025965     4.2416379579
H     3.3899786667     3.7475154443     3.6540572947
H    -0.8550817082     0.6771444270    -0.4218427030
H    -1.3097024865    -0.9422649774     0.1370273658
H     0.4009225733    -0.5017799205    -0.0077491170
H     0.0659955908    -0.2532947377     6.8650268893
H    -0.0798580391    -1.4511794203     5.5691739949
H    -1.5223039127    -0.9265776837     6.4559916284
O    -2.0901265352     4.1823961795     3.7147738946
C    -3.1922815194     3.3496965114     3.5869581048
H    -3.8377853981     3.3095943637     4.4954883703
H    -2.9209883989     2.2844884748     3.3845854205
H    -3.8790914088     3.6326521519     2.7554498375

PEPM - 0.20nN Force Path a
B3LYP+D3 Energy:   -682.1115976520
N    -0.1753756380     0.7555525121     0.4573313114
C    -1.1090313587    -2.1978775086    -1.7999852638
C    -1.6477239855     1.6750955396    -0.6040889757
C    -1.8026938247     2.9682657675     0.1462873821
H    -1.0055228914     1.6210314499    -1.4692779926
H    -2.3046270884     0.8497164899    -0.3966315621
C    -0.5167564488     3.7989338544     0.1755383662
H    -2.1536001405     2.7712708146     1.1668082807
H    -2.5995183894     3.5290681556    -0.3502850700
C     1.9093710324    -2.3550878666    -0.7387152106
C     0.5861534514     3.1198663996     0.9901644096
H    -0.7295207812     4.7871686082     0.6004867464
H    -0.1727009379     3.9642827161    -0.8556820869
C     0.9570937975     1.7221815553     0.4849058071
H     0.2884940191     3.0747111271     2.0451335649
H     1.5046265642     3.7185265023     0.9570296161
H     1.7685388792     1.3243645632     1.1052985645
H     1.3280198936     1.7942450292    -0.5439419176
C     0.1710159605    -0.4669640024    -0.3665410853
C    -0.9826735890    -1.4961776047    -0.4261050901
C     1.4789427670    -1.1456494131     0.1026507773
H     0.3326080632    -0.0689308411    -1.3762747110
C    -0.6494780469     0.4194574758     1.8130502339
H    -0.8198023502    -2.2459397315     0.3581978793
H    -1.9447966176    -1.0349989942    -0.1924511340
H     1.3570333894    -1.4698566135     1.1451805060
H     2.3014296595    -0.4230117780     0.0924088297
H    -0.1735293813    -2.1159142780    -2.3624208971
H    -1.8612095471    -1.6716375540    -2.4000576157
C    -1.4842372688    -3.6769419333    -1.6731430990
H     1.1216846447    -3.1141385458    -0.7480358111
C     3.1908079538    -3.0001449021    -0.2097837571
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H     2.0572485994    -2.0423752711    -1.7812250229
H    -0.7202330422    -4.2326910822    -1.1158286733
H    -1.5896137937    -4.1477556236    -2.6577650416
H    -2.4353461430    -3.8027229206    -1.1400864356
H     3.4832956046    -3.8592355735    -0.8244437227
H     3.0573525806    -3.3547925974     0.8201055195
H     4.0265742597    -2.2887448891    -0.2088280132
H    -1.5090875942    -0.2492106885     1.7510771906
H    -0.9667460144     1.3255433640     2.3291228431
H     0.1382567368    -0.0604372714     2.4063423222
O    -3.1013432602     2.1216989575    -2.0438136605
C    -3.2606397415     0.9856649653    -2.8361628330
H    -3.6844845195     0.1198494212    -2.2813984638
H    -2.3058255884     0.6246255606    -3.2770900927
H    -3.9416591910     1.1672890364    -3.6888680829

PEPM - 0.20nN Force Path b
B3LYP+D3 Energy:   -682.1104621469
C     0.0413307573    -0.7331455749     0.9186569572
C    -0.2263743707     0.0599861768     2.1969217411
C     0.5676024053     1.3764803440     2.2414159199
H     0.0273952414    -0.5724793024     3.0536165710
H    -1.2995809768     0.2796023617     2.2776139654
C     0.3633561857     2.1754793301     3.5429166145
H     0.2651739872     1.9679851294     1.3725508665
H     1.6358781308     1.1530757384     2.1223738240
C     0.6778820616     1.2780981158     4.7670861964
C    -0.5850069508     0.6278499903     5.3701990021
H     1.1935346798     1.8257850740     5.5587330263
H     1.3769905548     0.4920234338     4.4545813704
C    -0.2746460497    -0.7037639212     6.0562652494
H    -1.3345569883     0.4576785944     4.5904275109
H    -1.0447783264     1.3280084550     6.0803430784
N     1.1471964726     3.4814127486     3.5503256540
H    -0.6938351828     2.4784679360     3.5956704814
C     0.8671554563     4.2655742494     2.3084486989
C     0.7497781367     4.2767835301     4.7577489059
C     1.3257696810     5.6941576627     4.8031440562
H     1.0644266965     3.7266619200     5.6444015452
H    -0.3489861430     4.3309106839     4.7730976985
C     0.9960246777     6.4758232021     3.5306005781
H     2.4123256778     5.6626533279     4.9488334864
H     0.9076893559     6.1854248785     5.6897064757
C     1.4671573526     5.6735879535     2.3166381835
H     1.4676993292     7.4650730146     3.5507829657
H    -0.0896979904     6.6358137406     3.4664479661
H    -0.2241605549     4.3281512402     2.1817972640
H     1.2702544677     3.7099842219     1.4617845513
H     2.5631473891     5.6159840417     2.3078942405
H     1.1704367583     6.1605192785     1.3802899115
C     3.0467563784     3.0808386110     3.6035751035
H     3.1241184810     2.9499330191     2.5368022572
H     2.9100398465     2.2255811417     4.2404338819
H     3.3160566698     4.0238558880     4.0444579556
H    -0.2332012087    -0.1591114321     0.0246324923
H    -0.5338119496    -1.6660946246     0.9068133991
H     1.1037892998    -0.9928219064     0.8325900769
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H     0.4721318782    -0.5785833552     6.8506981661
H     0.1272797098    -1.4280903161     5.3368042717
H    -1.1726100971    -1.1412027894     6.5081881152
O     5.0319460156     2.6291658849     3.6671114438
C     5.3192306566     2.4970251195     5.0253055722
H     6.3918217573     2.2988985756     5.2057832315
H     4.7626377035     1.6635695055     5.5083224563
H     5.0650674720     3.4073336271     5.6118814635

PEPM - 0.20nN Force Path d
B3LYP+D3 Energy:   -682.1095823441
C       -0.7536040034      0.1962941939      0.2795180990
C       -0.6631285162      0.5520828953      1.7686075218
C        0.3554628694      1.6751458654      2.0200297399
H       -0.3895665712     -0.3455002738      2.3348825447
H       -1.6515006418      0.8652314079      2.1311330903
C        0.3834286643      2.1456663029      3.4842629468
H        0.0982800167      2.5108108149      1.3631897822
H        1.3484504214      1.3215920014      1.7148657852
C        0.6609707955      0.9701914592      4.4565936100
C       -0.6172096092      0.4083456061      5.0962214142
H        1.3325204339      1.2717846109      5.2660780585
H        1.1899214867      0.1756616318      3.9150797668
C       -0.3393490843     -0.8315860211      5.9526933401
H       -1.3546360020      0.1653416767      4.3249038038
H       -1.0712767257      1.1927886573      5.7177948295
N        1.3273809099      3.3209429995      3.7010407585
H       -0.6027521651      2.5661236913      3.7122520095
C        0.9935673181      4.6299458600      2.5428770081
C        1.0534948620      3.9388151751      5.0503716961
C        1.7742658271      5.2654937609      5.3136487436
H        1.3050761595      3.2067796344      5.8234892398
H       -0.0290028723      4.1012691300      5.0884044668
C        1.3941915229      6.3427216538      4.2830245627
H        2.8609784579      5.1146982605      5.3215211749
H        1.4956380696      5.5663523274      6.3335258071
C        1.6574326112      5.8689304264      2.8565202152
H        1.9397092759      7.2705662493      4.5004479334
H        0.3234398184      6.5750951586      4.4111699564
H       -0.0949233728      4.6268757652      2.6553568394
H        1.3015076053      4.1556877854      1.6133842810
H        2.7292936944      5.8491226461      2.6168616784
H        1.0331570202      6.9375538905      1.8567307392
C        2.7540690130      2.9494473429      3.5515980885
H        2.8850709554      2.3807025262      2.6312233626
H        3.0944191214      2.3546906906      4.4032433414
H        3.3470260092      3.8621269431      3.4873171926
H       -1.0734504059      1.0605180479     -0.3157771870
H       -1.4717340694     -0.6138578590      0.1089553839
H        0.2197111707     -0.1312670359     -0.1069243837
H        0.3920035869     -0.6103748949      6.7401541085
H        0.0664734704     -1.6474055210      5.3415908362
H       -1.2535160626     -1.1962561002      6.4349179662
O        0.6014490619      7.6873380709      1.1673662851
C       -0.2119603880      6.9837819486      0.2448591408
H       -1.2716141419      6.9706977540      0.5489250801
H        0.1143835012      5.9356341511      0.1396734714
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H       -0.1527843877      7.4497517969     -0.7480019604

PEPM - 0.20nN Force Path e
B3LYP+D3 Energy:   -682.1095263085
C    -0.4439766041    -0.6027493841     0.4712352440
C    -0.6737638242     0.2603684481     1.7102863898
C     0.5923615392     1.0121095826     2.1602907214
H    -1.0307757288    -0.3638985212     2.5355006221
H    -1.4639884934     0.9969960010     1.5067057659
C     0.3054508799     1.7111829822     3.4866792579
H     0.8735969895     1.6996200601     1.3547094575
H     1.4215495533     0.3068395661     2.2897104666
C     0.4893817351     0.9234490253     4.6896359299
C    -0.4274097521     1.1723295959     5.8908563933
H     1.5405424121     0.7335302092     4.9421196705
H     0.2031711383    -0.5333440896     4.4284732029
C    -1.8989786442     0.8600085948     5.5592223786
H    -0.3775004569     2.1883325235     6.3154556369
H    -0.1097951256     0.5042423253     6.7043949655
N     1.2797672471     3.2399479649     3.4427635354
H    -0.6713034658     2.2022326950     3.4469919819
C     0.7445083630     4.1589643494     2.3864350102
C     1.1160846082     3.8752824947     4.7909345837
C     1.7406288008     5.2682029440     4.8965073016
H     1.5351394157     3.1809877183     5.5206200585
H     0.0382440231     3.9421641909     4.9644950366
C     1.1917618878     6.2020216280     3.8095065106
H     2.8336454627     5.2093381496     4.8271720696
H     1.5128290294     5.6561202243     5.8962417657
C     1.3613844348     5.5616313124     2.4259340343
H     1.6963816239     7.1740659503     3.8481818475
H     0.1239816392     6.3855132957     3.9948557244
H    -0.3362506240     4.2206659527     2.5552502520
H     0.9094415179     3.6888723295     1.4157616545
H     2.4245459233     5.5128869569     2.1587007922
H     0.8702018024     6.1639723300     1.6527275814
C     2.6956417172     2.8654885410     3.2026771763
H     2.8102582248     2.5094289143     2.1786432858
H     2.9596121484     2.0679358063     3.9003809583
H     3.3644931898     3.7126613915     3.3577231244
H    -0.1152028586     0.0034993152    -0.3830597638
H    -1.3605716507    -1.1265033735     0.1748917402
H     0.3282018381    -1.3587335806     0.6570904456
H    -2.0181542835    -0.1840421172     5.2489772329
H    -2.2698475203     1.4888237638     4.7407824723
H    -2.5522195048     1.0353771010     6.4245270188
O     0.0545074389    -1.6894167268     4.4344558944
C     1.0912203494    -2.2859699506     3.6866099731
H     1.3994546693    -3.2418167926     4.1369975017
H     1.9862476791    -1.6408907145     3.6446715490
H     0.7917948463    -2.4939216344     2.6449147132

PEPM - 0.25nN Force Reactant
B3LYP+D3 Energy:   -682.1457873326
C    -0.3938063837    -0.3559201849     0.4577657239
C    -0.5573673074     0.3259472652     1.8154522896
C     0.4292914612     1.4938653400     1.9964991152
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H    -0.4094153303    -0.4243200791     2.5973715844
H    -1.5848623034     0.6974058843     1.9238709871
C     0.3058265865     2.1654150048     3.3740142322
H     0.2363591978     2.2113312120     1.1946949123
H     1.4488088048     1.1121171840     1.8553834449
C     0.4912063423     1.1301798607     4.5043434774
C    -0.8556360991     0.5675995413     5.0130127813
H     1.0311866972     1.5349466097     5.3636545646
H     1.1193036256     0.3123740841     4.1298341024
C    -0.7264664863    -0.8795138085     5.4912344347
H    -1.6152035428     0.6186831620     4.2270326129
H    -1.2249752138     1.2081921545     5.8237619978
N     1.2721582985     3.3855908884     3.5265706187
H    -0.6693531588     2.6555939502     3.4512834739
C     1.0478872653     4.3451116063     2.3562486337
C     0.8714777089     4.1285950564     4.8071334752
C     1.6000236880     5.4553693232     5.0007011253
H     1.0633393731     3.4593611160     5.6444993302
H    -0.2068101296     4.2887962785     4.6913971661
C     1.3803513989     6.3951249033     3.8111654147
H     2.6715197826     5.2942695130     5.1700931536
H     1.2038839416     5.8930852838     5.9245028136
C     1.7708102856     5.6812713291     2.5136379055
H     1.9626152326     7.3151654202     3.9336792279
H     0.3214296551     6.6826628325     3.7659226480
H    -0.0368719477     4.4838087701     2.3186320823
H     1.3887094362     3.8364907941     1.4562237306
H     2.8571252323     5.5387128951     2.4681960125
H     1.5025012012     6.2836883810     1.6377559263
C     2.7037530430     2.9420652494     3.5727959077
H     2.9556916313     2.4594576246     2.6292616165
H     2.8346606093     2.2438522608     4.3974183906
H     3.3518222481     3.8023032750     3.7207492433
H    -0.5534610896     0.3493260264    -0.3675151608
H    -1.1123195026    -1.1752259839     0.3419959990
H     0.6141073689    -0.7747945106     0.3462987655
H     0.0307498939    -0.9713401195     6.2802086545
H    -0.4254425376    -1.5374458644     4.6666523655
H    -1.6752696334    -1.2544177571     5.8921587454
O    -2.1102447510     4.3996361553     3.4779009454
C    -3.0617407723     3.4963292358     3.9280531085
H    -2.8864769315     3.1471476584     4.9736447855
H    -3.1112117177     2.5589702127     3.3219895535
H    -4.1036796305     3.8928665463     3.9267139614

PEPM - 0.25nN Force Path a
B3LYP+D3 Energy:   -682.1115055456
N    -0.1753756380     0.7555525121     0.4573313114
C    -1.1090313587    -2.1978775086    -1.7999852638
C    -1.6477239855     1.6750955396    -0.6040889757
C    -1.8026938247     2.9682657675     0.1462873821
H    -1.0055228914     1.6210314499    -1.4692779926
H    -2.3046270884     0.8497164899    -0.3966315621
C    -0.5167564488     3.7989338544     0.1755383662
H    -2.1536001405     2.7712708146     1.1668082807
H    -2.5995183894     3.5290681556    -0.3502850700
C     1.9093710324    -2.3550878666    -0.7387152106
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C     0.5861534514     3.1198663996     0.9901644096
H    -0.7295207812     4.7871686082     0.6004867464
H    -0.1727009379     3.9642827161    -0.8556820869
C     0.9570937975     1.7221815553     0.4849058071
H     0.2884940191     3.0747111271     2.0451335649
H     1.5046265642     3.7185265023     0.9570296161
H     1.7685388792     1.3243645632     1.1052985645
H     1.3280198936     1.7942450292    -0.5439419176
C     0.1710159605    -0.4669640024    -0.3665410853
C    -0.9826735890    -1.4961776047    -0.4261050901
C     1.4789427670    -1.1456494131     0.1026507773
H     0.3326080632    -0.0689308411    -1.3762747110
C    -0.6494780469     0.4194574758     1.8130502339
H    -0.8198023502    -2.2459397315     0.3581978793
H    -1.9447966176    -1.0349989942    -0.1924511340
H     1.3570333894    -1.4698566135     1.1451805060
H     2.3014296595    -0.4230117780     0.0924088297
H    -0.1735293813    -2.1159142780    -2.3624208971
H    -1.8612095471    -1.6716375540    -2.4000576157
C    -1.4842372688    -3.6769419333    -1.6731430990
H     1.1216846447    -3.1141385458    -0.7480358111
C     3.1908079538    -3.0001449021    -0.2097837571
H     2.0572485994    -2.0423752711    -1.7812250229
H    -0.7202330422    -4.2326910822    -1.1158286733
H    -1.5896137937    -4.1477556236    -2.6577650416
H    -2.4353461430    -3.8027229206    -1.1400864356
H     3.4832956046    -3.8592355735    -0.8244437227
H     3.0573525806    -3.3547925974     0.8201055195
H     4.0265742597    -2.2887448891    -0.2088280132
H    -1.5090875942    -0.2492106885     1.7510771906
H    -0.9667460144     1.3255433640     2.3291228431
H     0.1382567368    -0.0604372714     2.4063423222
O    -3.1013432602     2.1216989575    -2.0438136605
C    -3.2606397415     0.9856649653    -2.8361628330
H    -3.6844845195     0.1198494212    -2.2813984638
H    -2.3058255884     0.6246255606    -3.2770900927
H    -3.9416591910     1.1672890364    -3.6888680829

PEPM - 0.25nN Force Path b
B3LYP+D3 Energy:   -682.1103498809
C     0.0413307573    -0.7331455749     0.9186569572
C    -0.2263743707     0.0599861768     2.1969217411
C     0.5676024053     1.3764803440     2.2414159199
H     0.0273952414    -0.5724793024     3.0536165710
H    -1.2995809768     0.2796023617     2.2776139654
C     0.3633561857     2.1754793301     3.5429166145
H     0.2651739872     1.9679851294     1.3725508665
H     1.6358781308     1.1530757384     2.1223738240
C     0.6778820616     1.2780981158     4.7670861964
C    -0.5850069508     0.6278499903     5.3701990021
H     1.1935346798     1.8257850740     5.5587330263
H     1.3769905548     0.4920234338     4.4545813704
C    -0.2746460497    -0.7037639212     6.0562652494
H    -1.3345569883     0.4576785944     4.5904275109
H    -1.0447783264     1.3280084550     6.0803430784
N     1.1471964726     3.4814127486     3.5503256540
H    -0.6938351828     2.4784679360     3.5956704814
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C     0.8671554563     4.2655742494     2.3084486989
C     0.7497781367     4.2767835301     4.7577489059
C     1.3257696810     5.6941576627     4.8031440562
H     1.0644266965     3.7266619200     5.6444015452
H    -0.3489861430     4.3309106839     4.7730976985
C     0.9960246777     6.4758232021     3.5306005781
H     2.4123256778     5.6626533279     4.9488334864
H     0.9076893559     6.1854248785     5.6897064757
C     1.4671573526     5.6735879535     2.3166381835
H     1.4676993292     7.4650730146     3.5507829657
H    -0.0896979904     6.6358137406     3.4664479661
H    -0.2241605549     4.3281512402     2.1817972640
H     1.2702544677     3.7099842219     1.4617845513
H     2.5631473891     5.6159840417     2.3078942405
H     1.1704367583     6.1605192785     1.3802899115
C     3.0467563784     3.0808386110     3.6035751035
H     3.1241184810     2.9499330191     2.5368022572
H     2.9100398465     2.2255811417     4.2404338819
H     3.3160566698     4.0238558880     4.0444579556
H    -0.2332012087    -0.1591114321     0.0246324923
H    -0.5338119496    -1.6660946246     0.9068133991
H     1.1037892998    -0.9928219064     0.8325900769
H     0.4721318782    -0.5785833552     6.8506981661
H     0.1272797098    -1.4280903161     5.3368042717
H    -1.1726100971    -1.1412027894     6.5081881152
O     5.0319460156     2.6291658849     3.6671114438
C     5.3192306566     2.4970251195     5.0253055722
H     6.3918217573     2.2988985756     5.2057832315
H     4.7626377035     1.6635695055     5.5083224563
H     5.0650674720     3.4073336271     5.6118814635

PEPM - 0.25nN Force Path d
B3LYP+D3 Energy:   -682.1094495951
C    -0.6790612078     0.0196310174     0.5055097661
C    -0.6897458700     0.5536071353     1.9376533401
C     0.3207515403     1.6941060390     2.1395932902
H    -0.4675453316    -0.2778717807     2.6129610739
H    -1.6972594619     0.9074255274     2.1943526330
C     0.3730007822     2.2150954239     3.5888454622
H     0.0538862315     2.5039661314     1.4545083242
H     1.3128292579     1.3342406093     1.8383669688
C     0.6627567306     1.0598259701     4.5806591519
C    -0.6206939664     0.4213528932     5.1587975549
H     1.2860842000     1.3945673665     5.4142488739
H     1.2567457341     0.2991197188     4.0585275721
C    -0.4614091136    -1.0796946467     5.4099945151
H    -1.4644692607     0.5797779671     4.4796857869
H    -0.8870320093     0.9364291637     6.0906834569
N     1.3332773170     3.3854293387     3.7490351198
H    -0.6043208468     2.6505789310     3.8258928972
C     0.9857989631     4.6608497606     2.5548053767
C     1.0956809333     4.0528470085     5.0808707659
C     1.8375187997     5.3790325252     5.2831284807
H     1.3570132708     3.3458173058     5.8738795099
H     0.0161244189     4.2289837169     5.1366559904
C     1.4499481133     6.4266288784     4.2244933002
H     2.9223280375     5.2150431624     5.2738654757
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H     1.5836336096     5.7171490943     6.2976166731
C     1.6726096888     5.8994050201     2.8097232963
H     2.0143420490     7.3526361313     4.3976629616
H     0.3861942313     6.6805995216     4.3686580193
H    -0.0992215275     4.6744824465     2.6960633148
H     1.2631887195     4.1505408196     1.6352131674
H     2.7376427766     5.8575071172     2.5443310783
H     1.0356173984     6.9467232573     1.7866432996
C     2.7529076495     2.9935394151     3.5847161911
H     2.8607374737     2.3945783685     2.6808269965
H     3.1009761275     2.4207005741     4.4483462262
H     3.3549071664     3.8965079016     3.4806214425
H    -0.9182669572     0.8075998578    -0.2198250865
H    -1.4132888978    -0.7843599399     0.3802069177
H     0.3075264893    -0.3832022499     0.2442035147
H     0.3734853076    -1.2827249013     6.0926928662
H    -0.2583578538    -1.6129135490     4.4731186281
H    -1.3671821817    -1.5106478949     5.8524668716
O     0.6012141715     7.6802364791     1.0860479602
C    -0.2385357852     6.9618611541     0.1984131667
H    -1.2898498807     6.9586566775     0.5301676679
H     0.0816168973     5.9108972591     0.1043283039
H    -0.2033392232     7.4097913811    -0.8036559950

PEPM - 0.25nN Force Path e
B3LYP+D3 Energy:   -682.1092959094
C    -0.4439766041    -0.6027493841     0.4712352440
C    -0.6737638242     0.2603684481     1.7102863898
C     0.5923615392     1.0121095826     2.1602907214
H    -1.0307757288    -0.3638985212     2.5355006221
H    -1.4639884934     0.9969960010     1.5067057659
C     0.3054508799     1.7111829822     3.4866792579
H     0.8735969895     1.6996200601     1.3547094575
H     1.4215495533     0.3068395661     2.2897104666
C     0.4893817351     0.9234490253     4.6896359299
C    -0.4274097521     1.1723295959     5.8908563933
H     1.5405424121     0.7335302092     4.9421196705
H     0.2031711383    -0.5333440896     4.4284732029
C    -1.8989786442     0.8600085948     5.5592223786
H    -0.3775004569     2.1883325235     6.3154556369
H    -0.1097951256     0.5042423253     6.7043949655
N     1.2797672471     3.2399479649     3.4427635354
H    -0.6713034658     2.2022326950     3.4469919819
C     0.7445083630     4.1589643494     2.3864350102
C     1.1160846082     3.8752824947     4.7909345837
C     1.7406288008     5.2682029440     4.8965073016
H     1.5351394157     3.1809877183     5.5206200585
H     0.0382440231     3.9421641909     4.9644950366
C     1.1917618878     6.2020216280     3.8095065106
H     2.8336454627     5.2093381496     4.8271720696
H     1.5128290294     5.6561202243     5.8962417657
C     1.3613844348     5.5616313124     2.4259340343
H     1.6963816239     7.1740659503     3.8481818475
H     0.1239816392     6.3855132957     3.9948557244
H    -0.3362506240     4.2206659527     2.5552502520
H     0.9094415179     3.6888723295     1.4157616545
H     2.4245459233     5.5128869569     2.1587007922
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H     0.8702018024     6.1639723300     1.6527275814
C     2.6956417172     2.8654885410     3.2026771763
H     2.8102582248     2.5094289143     2.1786432858
H     2.9596121484     2.0679358063     3.9003809583
H     3.3644931898     3.7126613915     3.3577231244
H    -0.1152028586     0.0034993152    -0.3830597638
H    -1.3605716507    -1.1265033735     0.1748917402
H     0.3282018381    -1.3587335806     0.6570904456
H    -2.0181542835    -0.1840421172     5.2489772329
H    -2.2698475203     1.4888237638     4.7407824723
H    -2.5522195048     1.0353771010     6.4245270188
O     0.0545074389    -1.6894167268     4.4344558944
C     1.0912203494    -2.2859699506     3.6866099731
H     1.3994546693    -3.2418167926     4.1369975017
H     1.9862476791    -1.6408907145     3.6446715490
H     0.7917948463    -2.4939216344     2.6449147132

PEPE No Force Reactant
B3LYP+D3 Energy:   -721.4616415901
N    -0.2269838676     0.6006274484     0.1482355449
C    -1.4890469404     1.3024541953    -0.3559230099
C    -1.5991902379     2.7477964130     0.1312175010
H    -2.3333874240     0.7013398646    -0.0169609615
H    -1.4525769249     1.2969775534    -1.4526208278
C    -0.3628350477     3.5683560109    -0.2575951627
H    -1.7697963240     2.7932404380     1.2128320631
H    -2.4976095397     3.1635614499    -0.3396875352
C     0.9202851450     2.8837937437     0.2314061812
H    -0.4344035839     4.5815090609     0.1526364814
H    -0.3235656319     3.6625947961    -1.3510097277
C     0.9882099205     1.4350499149    -0.2473241440
H     1.0069489422     2.9469630291     1.3219339038
H     1.8051729830     3.3857588848    -0.1762677860
H     1.8702372227     0.9179644406     0.1310416070
H     1.0231556342     1.4215395909    -1.3353825869
C    -0.0862737786    -0.8141073288    -0.4892201286
C     0.1391918583    -0.7701765201    -2.0204364662
C    -1.2562979046    -1.7368656336    -0.1149009005
H     0.8227408846    -1.1965517647    -0.0190932276
C    -0.3070646356     0.4938428981     1.6739316650
H    -0.5505607554    -1.4842047467    -2.4818208215
C     1.5693238955    -1.1335988507    -2.4475745803
H    -0.1503720234     0.1953717771    -2.4491975259
H    -2.1299436696    -1.4917701682    -0.7313213314
H    -1.5554444294    -1.6066355891     0.9289050482
C    -0.8789230520    -3.2140816920    -0.3159812741
H     1.8137782955    -2.1363210049    -2.0702290396
H     2.2896269450    -0.4491445066    -1.9807524287
C     1.7380329871    -1.0946877323    -3.9696394136
H    -0.5738300893    -3.3879744799    -1.3554341496
C    -2.0318308277    -4.1582158022     0.0402685565
H    -0.0039226120    -3.4466088877     0.3065972621
H     1.0490860468    -1.7930324379    -4.4609335440
H     2.7581835618    -1.3638672612    -4.2664122139
H     1.5274287529    -0.0913208748    -4.3602810350
H    -1.7406232352    -5.2052787327    -0.1003789824
H    -2.9083411810    -3.9651082326    -0.5902159056
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H    -2.3379851894    -4.0315041575     1.0859924571
H    -1.3048644847     0.1208297588     1.9036205367
C     0.7611266824    -0.3644052966     2.3397409168
H    -0.2528759530     1.5123197007     2.0481360954
H     0.6394233879    -1.4294422094     2.1280307037
H     0.6572492686    -0.2270310091     3.4209380663
H     1.7762333533    -0.0633445066     2.0659783099
O    -1.7618897095     1.6781096058    -3.5649508042
C    -2.5145785724     0.5312402464    -3.7556112398
H    -2.7891016742     0.0126955281    -2.8034951252
H    -1.9999395049    -0.2501626317    -4.3631816062
H    -3.4863050619     0.7096538090    -4.2719627601

PEPE No Force Path a
B3LYP+D3 Energy:   -721.4263119625
N    -0.0493848573     0.6413680401     0.0913283075
C    -1.5707784651     1.6373218138    -0.8428092095
C    -1.4271112252     3.0110099281    -0.2457283801
H    -2.2385067767     0.9115738603    -0.4120097271
H    -1.1258187068     1.4242587788    -1.7980969370
C    -0.0340673923     3.6284257491    -0.4318858682
H    -1.6957573592     2.9929169426     0.8170730372
H    -2.1717467541     3.6414663498    -0.7396835766
C     1.0577656186     2.9028339028     0.3616435279
H    -0.0699449782     4.6800399158    -0.1231650089
H     0.2212017001     3.6228107361    -1.5014380057
C     1.2049734725     1.4332401615    -0.0367465214
H     0.8649110229     3.0035923970     1.4368948922
H     2.0286387551     3.3808863490     0.1820777721
H     2.0062211771     0.9514394823     0.5397328044
H     1.5061561144     1.4004788915    -1.0847739931
C     0.1203366841    -0.7105189545    -0.5740265082
C     0.4838239715    -0.5996679870    -2.0841147902
C    -1.0890836627    -1.6496188599    -0.3855824447
H     0.9742536846    -1.1788370958    -0.0624556767
C    -0.4794671036     0.5224420911     1.5157341091
H    -0.2696807034    -1.1379268683    -2.6713508770
C     1.8724912759    -1.1581094818    -2.4238921798
H     0.4286671360     0.4340790477    -2.4374054405
H    -1.9252608317    -1.3155683155    -1.0131622896
H    -1.4463055996    -1.6363222767     0.6479725692
C    -0.7323367232    -3.1050049706    -0.7288743933
H     1.9313723285    -2.2071964547    -2.1033179983
H     2.6331372583    -0.6187126743    -1.8428095061
C     2.1948530614    -1.0527063486    -3.9176711799
H    -0.4107683351    -3.1844173165    -1.7749899916
C    -1.9015885878    -4.0659036551    -0.4882629251
H     0.1284183028    -3.4115112636    -0.1175913863
H     1.4716428487    -1.6180656219    -4.5188013742
H     3.1943251105    -1.4444134370    -4.1388447541
H     2.1601573453    -0.0082745185    -4.2523483358
H    -1.6239744943    -5.0968503563    -0.7366148160
H    -2.7685851412    -3.7942941946    -1.1029841467
H    -2.2193237373    -4.0480547581     0.5617218277
H    -1.5109317377     0.1623903848     1.5192130443
C     0.3894230952    -0.3541610271     2.4221876279
H    -0.5169550570     1.5314151943     1.9259632749
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H     0.3923474442    -1.4034645584     2.1124537472
H    -0.0139226895    -0.3076954630     3.4395125979
H     1.4258512676    -0.0042135542     2.4603420983
O    -3.2434444983     2.0851722289    -1.9937269031
C    -3.6704818082     0.8834153147    -2.5607536428
H    -2.8998532672     0.4042809647    -3.2030775898
H    -4.5612891163     1.0240129784    -3.2009485042
H    -3.9531833661     0.1196002088    -1.8036170557

PEPE No Force Path b
B3LYP+D3 Energy:   -721.4276251749
N    -0.0330095383     0.7490319921     0.0495568792
C    -1.2228103198     1.4781752078    -0.4856698841
C    -1.3245187262     2.9273499521     0.0002087219
H    -2.1131663314     0.9156964155    -0.1940243595
H    -1.1750401444     1.4727538377    -1.5818063721
C    -0.0331318234     3.7044522326    -0.2742683210
H    -1.5591582704     2.9579744390     1.0699055232
H    -2.1743687360     3.3879084254    -0.5174562994
C     1.1581344173     2.9691597809     0.3499005793
H    -0.1087499828     4.7242692395     0.1200325196
H     0.1204357454     3.7879643031    -1.3597546898
C     1.2270230964     1.5256169309    -0.1530330252
H     1.0888413278     2.9996784519     1.4436408070
H     2.1027549927     3.4569224748     0.0826925955
H     2.0334761123     0.9745259447     0.3388568400
H     1.4610076311     1.5499452271    -1.2237393135
C     0.1115233145    -0.6242648469    -0.5746995008
C     0.4265166505    -0.5915541153    -2.1018655223
C    -1.0938903186    -1.5381670495    -0.2891328126
H     0.9799958753    -1.0503660013    -0.0609801826
C    -0.3975764082     0.5815865244     2.0277534732
H    -0.3413189992    -1.1641539396    -2.6358494406
C     1.8062965421    -1.1601216150    -2.4582680447
H     0.3500871485     0.4260202388    -2.4993884474
H    -1.9394651340    -1.2529433851    -0.9284806963
H    -1.4319043549    -1.4286078042     0.7448753266
C    -0.7578889392    -3.0187687064    -0.5260665952
H     1.8772411704    -2.1939026405    -2.0929905648
H     2.5829058293    -0.5935185103    -1.9265433410
C     2.0798304519    -1.1239430652    -3.9654912130
H    -0.4410876860    -3.1739027950    -1.5655547676
C    -1.9417070851    -3.9407803213    -0.2138081044
H     0.1004486520    -3.2950171299     0.1022347848
H     1.3320559981    -1.7088021124    -4.5160343539
H     3.0678965036    -1.5347684208    -4.2027091193
H     2.0419114739    -0.0953401814    -4.3455734810
H    -1.6810415642    -4.9919413198    -0.3827242638
H    -2.8052078386    -3.7030017195    -0.8473809762
H    -2.2577233177    -3.8369674146     0.8316644396
H    -1.3964314301     0.2644870172     1.7932575754
C     0.6493621366    -0.3917744408     2.4818467761
H    -0.2380071303     1.6316575235     2.1854054397
H     0.3450949812    -1.4269942058     2.3067349998
H     0.8120683119    -0.2574496864     3.5534968525
H     1.6086969477    -0.2232637198     1.9837762111
O    -1.3671007716     0.7319542335     3.9425467752
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C    -2.5186171409     1.4655062663     3.6688594713
H    -3.2317467486     1.4650600651     4.5155025793
H    -3.0882177240     1.0738592201     2.7947200959
H    -2.3157028846     2.5341610222     3.4347060088

PEPE No Force Path c
B3LYP+D3 Energy:   -721.4297944376
N     0.1082586249     0.7599453888     0.1341574171
C    -1.2137364215     1.3593470574    -0.2505179152
C    -1.3784578846     2.8119132900     0.1999839802
H    -1.9895253891     0.7250846072     0.1829631330
H    -1.3044979663     1.3039743121    -1.3399174787
C    -0.2221129669     3.6833288765    -0.3015431766
H    -1.4482322038     2.8688993204     1.2924729128
H    -2.3372741623     3.1686509833    -0.1939259052
C     1.1128596965     3.0992935364     0.1735158756
H    -0.3374569923     4.7140255334     0.0521223065
H    -0.2382710147     3.7139582054    -1.4003147779
C     1.2663178916     1.6389340680    -0.2559987694
H     1.1980891561     3.1939398319     1.2618273139
H     1.9568800858     3.6517606221    -0.2554394063
H     2.1514665593     1.1818475042     0.1948331787
H     1.3787408049     1.5979998944    -1.3411593002
C     0.3027817100    -0.6190337208    -0.4919454654
C     0.4057813657    -0.5922835750    -2.0417315349
C    -0.7488363485    -1.6411177931    -0.0243846115
H     1.2668794877    -0.9300051384    -0.0788870163
C     0.1748671298     0.5780910815     1.8603170024
H    -0.4064230563    -1.1997161085    -2.4586488401
C     1.7494556906    -1.1213951734    -2.5658705169
H     0.2442222760     0.4130092107    -2.4445173993
H    -1.7093337856    -1.4511041875    -0.5199775362
H    -0.9222117219    -1.5571807980     1.0513321583
C    -0.3049877829    -3.0851566063    -0.3124920569
H     1.9322845195    -2.1199460451    -2.1479467996
H     2.5612808531    -0.4805289154    -2.1948541835
C     1.7943383555    -1.1831033764    -4.0954692716
H    -0.1622034395    -3.2341358065    -1.3903962586
C    -1.3145984802    -4.1116546136     0.2128145182
H     0.6736898583    -3.2561112019     0.1569476923
H     1.0216250446    -1.8584516001    -4.4838471532
H     2.7658342189    -1.5426580703    -4.4533789055
H     1.6195653220    -0.1924069908    -4.5337593075
H    -0.9765361677    -5.1358957321     0.0181184409
H    -2.2932945571    -3.9844110864    -0.2664049865
H    -1.4570030378    -4.0041543664     1.2954585644
H    -0.8174830609     0.1593633216     2.0242944204
C     1.2754103489    -0.1844900544     2.4151244959
H     0.1686957932     1.6236556905     2.1590743249
H     1.3342860590    -1.2254119903     2.0793660616
H     0.8782280027    -0.3735049588     3.9203616970
H     2.2529488105     0.3051598255     2.3476266562
O     0.5424202395    -0.6270103584     4.9558942709
C    -0.6417557118    -1.3911516143     4.8106257369
H    -0.6220279116    -1.9913038923     3.8847646750
H    -1.5463012281    -0.7605860966     4.7748972831
H    -0.7519753414    -2.0858857879     5.6540372192
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PEPE No Force Path d
B3LYP+D3 Energy: -721.4239995614

N	0.0754311781	0.8157010998	0.2207584160
C	-1.1649904836	1.9532436028	-0.4281878261
C	-1.0480756395	3.2750150612	0.1190845558
H	-2.0686323927	1.3911346471	-0.1931032966
H	-0.9016303903	1.8622629314	-1.4815382389
C	0.3542593412	3.8546630850	-0.0580401470
H	-1.4092353236	3.3550446771	1.1525787729
H	-2.0838305199	4.1834687075	-0.7469729750
C	1.4414719254	2.9550586634	0.5662699335
H	0.4273726943	4.8615264515	0.3745622891
H	0.5799673717	3.9633808189	-1.1323372850
C	1.3952666457	1.5170942460	0.0307158047
H	1.3574618459	2.9667212564	1.6602805295
H	2.4472727584	3.3312857975	0.3326199663
H	2.1784493629	0.8979337156	0.4817027452
H	1.5884331838	1.5463520712	-1.0425388737
C	0.0955957233	-0.5269087908	-0.5015620540
C	0.3016386563	-0.3805244844	-2.0350989175
C	-1.1491329485	-1.3786511625	-0.1965958033
H	0.9695615625	-1.0511190184	-0.0914415072
C	-0.2474438459	0.6832545829	1.6785009023
H	-0.6191020269	-0.6810332576	-2.5495349490
C	1.4808216170	-1.2106572465	-2.5629473983
H	0.4657474741	0.6589710415	-2.3294943559
H	-2.0403558714	-0.8914742431	-0.6129026322
H	-1.3076725457	-1.4639712860	0.8816993473
C	-1.0445023328	-2.8104367188	-0.7487015191
H	1.3582582641	-2.2604261724	-2.2670835481
H	2.4045094469	-0.8622200255	-2.0797680176
C	1.6233912517	-1.1161663886	-4.0849653566
H	-0.9327211964	-2.7974469262	-1.8396354636
C	-2.2687081868	-3.6550977923	-0.3783291588
H	-0.1353732777	-3.2816489522	-0.3497015346
H	0.7244933403	-1.4941199235	-4.5879911971
H	2.4787348136	-1.7007016118	-4.4425363725
H	1.7693012999	-0.0761466162	-4.4029470257
H	-2.1784301630	-4.6746194611	-0.7702975964
H	-3.1873315704	-3.2177349593	-0.7889435359
H	-2.3896384127	-3.7227741282	0.7098595848
H	-1.2766657030	0.3278551771	1.7498128236
C	0.6883291786	-0.2029475672	2.4976698333
H	-0.2536906629	1.6953963250	2.0815020584
H	0.7036038008	-1.2377595537	2.1419449668
H	0.3315231063	-0.2125003232	3.5330566273
H	1.7153449264	0.1739945515	2.5055249790
O	-2.7775372958	4.7967091029	-1.3211518463
C	-3.5728058655	3.9155297486	-2.0976098702
H	-3.5522261497	2.8934729466	-1.6859528260
H	-3.2277093618	3.8599421028	-3.1423776711
H	-4.6186389992	4.2508198774	-2.1042717617

PEPE No Force Path e
B3LYP+D3 Energy: -721.4233560689

N	-0.0950565430	0.7154295063	0.1669665646

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C      -1.2737829415     1.3977784566    -0.4498244441
C      -1.4426672182     2.8562599036    -0.0086144202
H      -2.1625150208     0.8097297989    -0.2113358895
H      -1.1199204237     1.3512741177    -1.5325223815
C      -0.1679080536     3.6685866053    -0.2718701297
H      -1.7060184886     2.9021543683     1.0554078072
H      -2.2931416474     3.2758607729    -0.5590842007
C       1.0473104582     2.9751942320     0.3607412024
H      -0.2773244928     4.6880018632     0.1154878022
H      -0.0099138519     3.7509387070    -1.3566278621
C       1.1364168470     1.5191709033    -0.1089054079
H       0.9918605518     3.0329043338     1.4546241294
H       1.9771596319     3.4766416932     0.0679213196
H       1.9886446417     0.9983160487     0.3320203064
H       1.2600585848     1.5054574198    -1.1901586593
C       0.1232616731    -0.9244685798    -0.7460760780
C       0.4542836658    -0.8017289321    -2.1530997914
C      -1.1548495514    -1.6961947617    -0.4093081665
H       0.9718836305    -1.2543041970    -0.1454188524
C      -0.3098055258     0.5079391384     1.6381902441
H       0.0676127972    -2.0140120108    -2.7387743992
C       1.8937964364    -0.4889135697    -2.5820683793
H      -0.2944905116    -0.2399414143    -2.7297236640
H      -1.8454225133    -1.6312508971    -1.2578039911
H      -1.6845913993    -1.2880462774     0.4554987036
C      -0.8501103017    -3.1754216004    -0.1012968339
H       2.5834540769    -0.8310504602    -1.7959083228
H       2.0777395351     0.5913763454    -2.6846206213
C       2.3070074780    -1.1405334304    -3.9133121054
H      -0.2094798547    -3.5900134236    -0.8829701714
C      -2.1230341486    -4.0199361228     0.0170506180
H      -0.2797016188    -3.2349208869     0.8358449293
H       2.3286440310    -2.2319044903    -3.8399287014
H       3.3050611740    -0.8023853865    -4.2207523006
H       1.6063349220    -0.8796424607    -4.7165908992
H      -1.8866424041    -5.0609104893     0.2672377508
H      -2.6802730217    -4.0197294379    -0.9279791378
H      -2.7901624975    -3.6302873447     0.7964974010
H      -1.3283069438     0.1372198302     1.7674570491
C       0.6806016077    -0.4356646458     2.3171094641
H      -0.2759942648     1.4831802317     2.1316521060
H       0.5614240106    -1.4713967571     1.9907705555
H       0.4932338945    -0.4037047332     3.3955487008
H       1.7210968010    -0.1378534299     2.1559613028
O      -0.3770644880    -2.9591516771    -3.4350389498
C       0.4413247148    -4.0920259353    -3.2978892353
H      -0.1231587574    -4.9725851004    -2.9421651035
H       1.2566861131    -3.9270397782    -2.5676762172
H       0.9252745069    -4.3796815456    -4.2485969402

PEQ No Force Reactant
B3LYP+D3 Energy:   -720.2517244915
N     -0.1435004149     0.7793995409     0.5030217578
C     -1.3195109515     1.4519996929    -0.1994139925
C     -1.9058405278     2.5653918302     0.6935751547
H     -2.0583729120     0.6861561358    -0.4254218841
H     -0.9043014546     1.8272592049    -1.1377581698
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C    -0.8597694429     2.9526252456     1.7509984045
H    -2.8271688581     2.2236341083     1.1776715156
H    -2.1597616538     3.4248331019     0.0651526745
C     0.4816752499     3.1605282589     1.0306810304
C     0.9950507194     1.7979610445     0.5192292909
H     1.2269459311     3.5876649768     1.7089019697
H     0.3568365042     3.8584736525     0.1954412533
H     1.7598681104     1.3957494617     1.1820791088
H     1.3655873193     1.8460682756    -0.5082882145
C     0.2694487969    -0.4786021295    -0.3105790399
C    -0.8412365958    -1.5560755095    -0.3042694334
C     1.6252337236    -1.0468139667     0.1361995182
H     0.3917296565    -0.0578836965    -1.3153436129
C    -0.5223185209     0.4669975301     1.9395379237
H    -0.4962306444    -2.4216594613     0.2739428631
C    -1.2490040822    -2.0027737331    -1.7164745181
H    -1.7413964905    -1.2110937594     0.2116673963
H     1.5582212230    -1.4474845567     1.1560123989
H     2.3863572809    -0.2620918173     0.1460487059
C     2.1219207534    -2.1574994678    -0.8063840694
H    -0.3646063464    -2.3420641452    -2.2695464161
H    -1.6378076340    -1.1342926168    -2.2655095525
C    -2.3000072801    -3.1167694016    -1.6938404028
H     1.4194570720    -2.9995910149    -0.8067589638
C     3.5139096222    -2.6605762398    -0.4084533759
H     2.1478397707    -1.7704239513    -1.8339885529
H    -1.9214938997    -4.0060358031    -1.1747333554
H    -2.5807516204    -3.4160760061    -2.7100522843
H    -3.2105051728    -2.7906569809    -1.1759085614
H     3.8561289566    -3.4502640362    -1.0868748985
H     3.5086540123    -3.0709133325     0.6090146348
H     4.2513832388    -1.8489431772    -0.4368774891
H    -1.4444304895    -0.1127534643     1.9081691050
C    -0.7044801089     1.7798029345     2.7357232266
H     0.2679675778    -0.1602490111     2.3517534471
O     1.0277185420     1.6136913233    -2.6860812698
C     1.4018157992     1.9879841036    -3.9721090010
H    -1.1617032032     3.8604421376     2.2809009833
H     0.1572980565     1.9513441264     3.3890780737
H    -1.5895506271     1.6861708455     3.3725245323
H     1.8147340238     1.1500884870    -4.5814651539
H     2.1893205280     2.7773510197    -3.9989206462
H     0.5632686914     2.3986577242    -4.5819967481

PEQ No Force Path a
B3LYP+D3 Energy:   -720.2221186559
N    -0.0124544577     0.7960565001     0.4411425893
C    -1.0247474975     1.6064025410    -0.2961600075
C    -1.5343244078     2.7643163016     0.5845876067
H    -1.8522317881     0.9678001431    -0.6231892882
H    -0.5247918076     1.9803147349    -1.1950709255
C    -0.5162268346     3.0313589977     1.7021765167
H    -2.5059514156     2.5095300294     1.0242668310
H    -1.6831253945     3.6549065060    -0.0351876774
C     0.8894966947     3.2594153246     1.1087625535
C     1.5408455889     2.0075508610     0.5533224636
H     1.5481563844     3.6452532184     1.8918866329
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H     0.8377360886     4.0206544659     0.3228689735
H     2.0722749896     1.3595817325     1.2300490012
H     1.7039454342     1.8844763112    -0.5057484491
C     0.3371301657    -0.4451366169    -0.3508696836
C    -0.8269950390    -1.4717113607    -0.3843422782
C     1.6533886501    -1.0777896100     0.1319136634
H     0.5012624900    -0.0689355758    -1.3687993957
C    -0.4740618282     0.5110394713     1.8286680652
H    -0.6176389767    -2.2736168033     0.3353082508
C    -1.0882843474    -2.0781408789    -1.7721695777
H    -1.7611408362    -1.0096589475    -0.0472474585
H     1.5506110713    -1.4093505285     1.1735607565
H     2.4420202906    -0.3223439160     0.1179856506
C     2.1328984952    -2.2653925825    -0.7164541161
H    -0.1596519886    -2.4765745385    -2.1968037332
H    -1.4176685095    -1.2788441104    -2.4504975724
C    -2.1409585630    -3.1908004430    -1.7237114700
H     1.4210283765    -3.0970791651    -0.6471121430
C     3.5212847452    -2.7465430825    -0.2788161427
H     2.1647627426    -1.9692693619    -1.7739623874
H    -1.8094937127    -4.0114475668    -1.0749516838
H    -2.3298130848    -3.6058645316    -2.7203842793
H    -3.0942822191    -2.8190489798    -1.3276708690
H     3.8586783485    -3.5918899370    -0.8893005064
H     3.5152105289    -3.0703358167     0.7695275207
H     4.2638439138    -1.9443269209    -0.3740338364
H    -1.4675062590     0.0514772970     1.7860029827
C    -0.5116352230     1.8195374180     2.6508305105
H     0.2064635075    -0.2164111462     2.2728250582
O     3.4457070585     2.9594570217     0.3854089434
C     4.2070328117     2.0485098039    -0.3420107167
H    -0.8043229167     3.9308589296     2.2570214282
H     0.3508764737     1.8750342981     3.3241031792
H    -1.4121271422     1.8255458973     3.2737326686
H     4.4176969855     1.1071492401     0.2126074460
H     5.1923533911     2.4613559121    -0.6321797215
H     3.7200769421     1.7318662358    -1.2925988530

PEQ No Force Path b
B3LYP+D3 Energy:   -720.2207331329
N    -0.0877472308     0.7502666925     0.4543115884
C    -1.2404822014     1.4511303029    -0.1810056687
C    -1.8541110282     2.4665606432     0.8073788929
H    -1.9783802254     0.7116681501    -0.4912382803
H    -0.8739566542     1.9443628843    -1.0918113633
C    -0.8160350160     2.8117882632     1.8893070398
H    -2.7590978112     2.0537322887     1.2680576949
H    -2.1490192799     3.3676550398     0.2594638345
C     0.5303529587     3.0450833651     1.1900423463
C     1.0393232569     1.7127931391     0.6016933739
H     1.2752603047     3.4411640642     1.8881310535
H     0.4019508448     3.7892143834     0.3953904161
H     1.7702212338     1.2605375643     1.2735169804
H     1.5218931560     1.8638559657    -0.3731193579
C     0.2921658879    -0.4789478354    -0.3426053013
C    -0.8121477793    -1.5681993173    -0.2761055515
C     1.6661213390    -1.0466488869     0.0630973910
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H     0.3767885383    -0.1283692789    -1.3842711460
C    -0.5958439830     0.2847770071     2.3142256343
H    -0.4801262441    -2.3785091859     0.3847212860
C    -1.1924875996    -2.1446062008    -1.6479457885
H    -1.7266020558    -1.1805940732     0.1815038730
H     1.6440538005    -1.3477505282     1.1184321799
H     2.4353494940    -0.2742348605    -0.0325964294
C     2.1130881608    -2.2476961724    -0.7847508525
H    -0.2999869870    -2.5216653811    -2.1619018634
H    -1.5865219482    -1.3324868069    -2.2750513619
C    -2.2291318788    -3.2668795156    -1.5324286588
H     1.4151940259    -3.0841640765    -0.6585139576
C     3.5268131560    -2.7102319950    -0.4136666076
H     2.0817453844    -1.9743927121    -1.8484946044
H    -1.8410846033    -4.0969764409    -0.9285326140
H    -2.4985825482    -3.6657869601    -2.5171008101
H    -3.1477768082    -2.9084474931    -1.0513009384
H     3.8333245826    -3.5704528980    -1.0196257389
H     3.5805773121    -3.0065906665     0.6414405766
H     4.2597059017    -1.9091839066    -0.5713757622
H    -1.4829751102    -0.2168936609     1.9695456966
C    -0.7180527174     1.6682605764     2.9210563811
H     0.3054886856    -0.2937653917     2.4205687101
O    -1.0802139954    -0.6971776036     4.1103364828
C    -1.1154017834    -2.0402256831     3.7366904977
H    -1.1201572125     3.7226523182     2.4160064781
H     0.1281228831     1.8470859671     3.5930222691
H    -1.6244692635     1.6694160284     3.5329394258
H    -1.9359528397    -2.2765221608     3.0236057714
H    -1.2579000371    -2.7104865832     4.6049993923
H    -0.1803199980    -2.3796872573     3.2373951747

PEQ No Force Path c
B3LYP+D3 Energy:   -720.2079493528
N    -0.0935524118     0.8088761148     0.5350366883
C    -1.2814846660     1.5371912600    -0.0241132854
C    -1.8317566689     2.5565572058     1.0059597998
H    -2.0431023102     0.8080288766    -0.3004793089
H    -0.9532931220     2.0317211600    -0.9457605332
C    -0.7222611823     2.9320149923     2.0140245837
H    -2.7016145440     2.1447015665     1.5280619384
H    -2.1699442843     3.4462839366     0.4636603252
C     0.5526675005     3.1500071001     1.1691583709
C     1.0406261222     1.7820683649     0.6349531669
H     1.3542600385     3.5909845750     1.7717095427
H     0.3568135277     3.8408004505     0.3377284988
H     1.7707508602     1.3543333403     1.3220858515
H     1.5076513731     1.8787749359    -0.3519068609
C     0.2409312191    -0.4164378981    -0.2771067767
C    -0.8767780801    -1.4887158295    -0.1720592544
C     1.6154365671    -0.9997450136     0.0978434809
H     0.2996451155    -0.0646386691    -1.3194252619
C    -0.5937248677     0.5156614181     2.3023437811
H    -0.5153575652    -2.3259191073     0.4378181592
C    -1.3462748517    -2.0122512942    -1.5366038298
H    -1.7508055498    -1.1028260630     0.3598974232
H     1.6048861311    -1.3067148357     1.1526683473
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H     2.3895150228    -0.2329104387    -0.0029507138
C     2.0305499093    -2.1930435214    -0.7764644134
H    -0.4872696571    -2.3849997515    -2.1081311807
H    -1.7562691287    -1.1726575709    -2.1152840136
C    -2.3980748240    -3.1178057122    -1.4025273468
H     1.3293406658    -3.0263020382    -0.6450844264
C     3.4501282234    -2.6728165957    -0.4527102176
H     1.9725260971    -1.9032579574    -1.8347589732
H    -1.9966135847    -3.9769816300    -0.8504816054
H    -2.7304073914    -3.4753634392    -2.3838760679
H    -3.2805798145    -2.7577398496    -0.8589192809
H     3.7317399957    -3.5268916753    -1.0792386996
H     3.5320446589    -2.9846502273     0.5960734693
H     4.1850742221    -1.8757570689    -0.6207358144
H    -1.5979573024     0.1845501771     2.0416752059
C    -0.4475331716     1.7669074548     2.9847009775
H     0.0259748542    -0.3236782263     2.6215308308
O    -2.3346272082     1.8085619132     4.9987030240
C    -3.5991664493     1.7062645076     4.3581346596
H    -0.9907090153     3.8632962486     2.5293024535
H     0.5463245315     1.8770058991     3.4395095154
H    -1.5918529397     1.7704967623     4.2428692865
H    -4.3733916831     1.5823826736     5.1235986661
H    -3.6475149228     0.8390311826     3.6811772216
H    -3.8411931392     2.6063076963     3.7713681971

PEQ No Force Path d
B3LYP+D3 Energy:   -720.2087918877
N       2.3032950171     0.7861460790     0.0439519992
C       3.2444943638     1.8584878487     0.4912113741
C       1.0051292743     0.8986577830     0.7770088490
C       0.2588356260     2.1991343726     0.3660941656
H       1.2136039493     0.8911773387     1.8516238751
H       0.4088267322     0.0121654427     0.5495580011
C       2.4963668193     3.1962744492     0.6914686862
H       3.9967648886     1.9460403493    -0.2969486062
H       3.7500279906     1.5496734224     1.4096401881
C       1.2530386230     3.2219391905    -0.2286752411
H       3.1805607169     4.0177563582     0.4522649018
H       2.2031751683     3.3157753979     1.7436361285
H      -0.2220014219     2.6155495878     1.2579389198
H      -0.5368166322     1.9756822670    -0.3536337072
C       1.8212967782     1.3600034697    -1.6829882085
C       1.7162743162     2.7836427110    -1.6299489635
H       0.9038857295     0.7755581839    -1.6909711737
H       2.5835688565     0.9188393415    -2.3271700721
H       0.6079276382     3.2142314073    -2.7852136958
H       2.6549508438     3.2861417196    -1.8977834466
H       0.8032787560     4.2230796059    -0.2199852774
O      -0.0938851568     3.4935036921    -3.5460389744
C      -0.0241511126     2.5043314416    -4.5622912390
H       0.1707402077     2.9631058693    -5.5416393681
H      -0.9621152820     1.9338788403    -4.6321525272
H       0.7895631876     1.7895941492    -4.3582449183
H       1.9295914170    -4.0503243640    -2.1530195316
H       1.3601009155    -2.7742433284    -3.2417027190
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PEQ No Force Path e
B3LYP+D3 Energy:   -720.2140750992
N    -0.0474006914     0.6720005245     0.3496461980
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C    -0.8201851101     2.8354105605     1.5539863978
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C     1.7160759424    -1.3266870947     0.2307352024
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H	0.1472652233	-4.6386679290	0.7147907968
H	1.8471600292	-4.6625725172	0.2025616616

References

1. A. B. Pangborn, M. A. Giardello, R. H. Grubbs, R. K. Rosen and F. J. Timmers, *Organometallics*, 1996, **15**, 1518–1520.
2. A. J. Musacchio, B. C. Lainhart, X. Zhang, S. G. Naguib, T. C. Sherwood and R. R. Knowles, *Science*, 2017, **355**, 727–730.
3. A. Triolo, O. Russina, B. Fazio, G. B. Appetecchi, M. Carewska and S. Passerini, *J. Chem. Phys.*, 2009, **130**, 164521|1–6.
4. C. H. Fujimoto, M. A. Hickner, C. J. Cornelius and D. A. Loy, *Macromolecules*, 2005, **38**, 5010–5016.
5. K. J. T. Noonan, K. M. Hugar, H. A. Kostalik IV, E. B. Lobkovsky, H. D. Abruña and G. W. Coates, *J. Am. Chem. Soc.*, 2012, **134**, 18161–18164.
6. J. A. Porras, I. N. Mills, W. J. Transue and S. Bernhard, *J. Am. Chem. Soc.*, 2016, **138**, 9460–9472.
7. S. Ladouceur, D. Fortin and E. Zysman-Colman, *Inorg. Chem.*, 2011, **50**, 11514–11526.
8. W. You, K. M. Hugar and G. W. Coates, *Macromolecules*, 2018, **51**, 3212–3218.
9. K. M. Meeka, C. M. Antunesa, D. J. Strassera, Z. R. Owczarczyka, A. C. Yang-Neyerlina and B. S. Pivovar, *ECS Transactions*, 2019, **92**, 723–731.