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## Supporting Information

# One-Pot Synthesis and AFM Imaging of a Triangular Aramide Macrocycle

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## Materials

Trifluoroacetic acid was purchased from Iris Biotech GmbH. All other reagents and solvents were purchased from Acros or Sigma-Aldrich and used without further purification. The following compounds were prepared according to literature procedures: phenyl 4-aminobenzoate[1], 2,4-bis((2-ethylhexyl)oxy)benzaldehyde[2], 4-(2-ethylhexyl)oxybenzaldehyde[3].

## Characterization

All $^{1}H$ NMR (360 MHz) and $^{13}C$ NMR (90 MHz) spectra were recorded on a Bruker Avance DPX (360 MHz) FT NMR spectrometer. Chemical shifts were given in ppm relative to the residual solvent peak ($CDCl_3$: 7.26 for $^{1}H$; $CDCl_3$: 77.16 for $^{13}C$). HR-MALDI FT-ICR mass spectra were measured on a Bruker FTMS 4.7T BioAPEX II in positive mode using *trans*-2-[3-(*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) as Matrix and silver trifluoroacetate (AgTFA) as counter ion source. HR-MS (ESI+) mass spectra were measured on a Bruker FTMS 4.7T BioAPEX II. Gel permeation chromatography (GPC) with chloroform as eluent and toluene as internal reference was carried out on an instrument consisting of a Jasco PU-2087plus pump and a set of two MZ-Gel SD*plus* Linear columns (length x ID 300 x 8 mm; particle size 5 μm). Signal detection was performed with Applied Biosystems 759A Absorbance Detector (UV 254 nm). The GPC was calibrated using a series of monodisperse polystyrene standards.

## *Synthesis of monomers*

**Phenyl 4-((2,4-dimethoxybenzyl)amino)benzoate (1a)**

Phenyl 4-aminobenzoate (4.00 g, 18.76 mmol) and 2,4-dimethoxybenzaldehyde (3.12 g, 18.76 mmol) were dissolved in 80 mL toluene and refluxed 18 h under Dean-Stark conditions. After removal of the solvent under reduced pressure, the yellow solid was dissolved in a mixture of 60 mL anhydrous THF and 30 mL anhydrous methanol. The solution was cooled with an ice/water-bath and sodium borohydride (0.75 g, 19.70 mmol) was added. After stirring for 18 h and warming to room temperature, a colorless precipitate was formed. The mixture was diluted with 250 mL water, filtered and washed with cold methanol. The resulting colorless solid was recrystallized twice from ethanol/methanol to afford the product as colorless crystals (5.59 g, 82%).

$^{1}$H-NMR (360 MHz, $CDCl_3$): δ (ppm) 8.01 (d, $^{3}J$ = 8.28 Hz, 2H), 7.41 (t, $^{3}J$ = 7.20 Hz, 2H), 7.26 - 7.17 (m, 5H), 6.65 (d, $^{3}J$ = 8.28 Hz, 2H), 6.50 (s, 1H), 6.45 (d, $^{3}J$ = 8.64 Hz, 1H), 4.66 (br-s, 1H), 4.34 (s, 2H), 3.85 (s, 3H), 3.81 (s, 3H).

$^{13}$C-NMR (90 MHz, $CDCl_3$): δ (ppm) 165.48, 160.61, 158.53, 152.65, 151.44, 132.32, 129.74, 129.43, 125.50, 122.06, 118.62, 117.35, 111.96, 104.05, 98.82, 55.51, 55.50, 42.69.

HR-MS (ESI+): calc. for $C_{22}H_{21}N_1O_4Na_1$ $(M+Na)^+$ 386.13628, found 386.13682.

**Phenyl 4-((2,4-bis((2-ethylhexyl)oxy)benzyl)amino)benzoate (1b)**

Phenyl 4-aminobenzoate (5.60 g, 26.26 mmol) and 2,4-bis((2-ethylhexyl)oxy)-benzaldehyde (9.52 g, 26.26 mmol) were dissolved in 80 mL toluene and refluxed 18 h under Dean-Stark conditions. After removal of the solvent under reduced pressure, the yellow solid was dissolved in a mixture of 60 mL anhydrous THF and 30 mL anhydrous methanol. The solution was cooled with an ice/water-bath and sodium borohydride (1.04 g, 27.57 mmol) was added. After stirring for 18 h and warming to room temperature, the solution was evaporated to dryness. The residue was diluted with water and extracted three times with dichloromethane. The combined organic extracts were washed with brine, dried over magnesium sulfate and the solvent was removed under reduced pressure. The residual brown oil was purified by silica gel column chromatography eluted by hexane (containing 3 vol.-% ethylacetate) to afford the product as colorless crystals (11.47 g, 78%).

$^{1}$H-NMR (360 MHz, $CDCl_3$): δ (ppm) 8.00 (d, $^{3}J$ = 8.64 Hz, 2H), 7.40 (t, $^{3}J$ = 7.56 Hz, 2H), 7.25 - 7.14 (m, 5H), 6.63 (d, $^{3}J$ = 8.64 Hz, 2H), 6.49 (d, $^{4}J$ = 1.80 Hz, 1H), 6.42 (dd, $^{4}J$ = 1.80 Hz, $^{3}J$ = 8.28 Hz, 1H), 4.62 (br-s, 1H), 4.34 (s, 2H), 3.89 (d, $^{3}J$ = 5.04 Hz, 2H), 3.83 (d, $^{3}J$ = 5.40 Hz, 2H), 1.75 - 1.68 (m, 2H), 1.53 - 1.39 (m, 8H), 1.37 - 1.26 (m, 8H), 0.95 - 0.88 (m, 12H).

$^{13}$C-NMR (90 MHz, $CDCl_3$): δ (ppm) 165.47, 160.48, 158.22, 152.41, 151.45, 132.33, 129.80, 129.48, 129.44, 125.52, 122.07, 118.19, 117.59, 112.20, 104.51, 99.83, 70.63, 70.22, 43.20, 43.17, 39.55, 30.92, 30.66, 29.26, 29.23, 27.05, 24.25, 23.99, 23.19, 14.24, 11.35, 11.26.

HR-MS (ESI+): calc. for $C_{36}H_{49}N_1O_4Na_1$ $(M+Na)^+$ 582.35538, found 582.35548.

**Phenyl 4-((4-((2-ethylhexyl)oxy)benzyl)amino)benzoate (1c)**

Phenyl 4-aminobenzoate (0.87 g, 4.08 mmol) and 4-(2-ethylhexyl)oxybenzaldehyde (0.95 g, 4.08 mmol) were dissolved in 20 mL toluene and refluxed 18 h under Dean-Stark conditions. After removal of the solvent under reduced pressure, the yellow solid was dissolved in a mixture of 20 mL anhydrous THF and 10 mL anhydrous methanol. The solution was cooled with an ice/water-bath and sodium borohydride (170 mg, 4.49 mmol) was added. After stirring for 5 h and warming to room temperature, the solution was evaporated to dryness. The residue was diluted with water and extracted three times with dichloromethane. The combined organic extracts were washed with brine, dried over magnesium sulfate and the solvent was removed under reduced pressure. The residual yellow solid was purified by silica gel column chromatography eluted by hexane/ethyl acetate (4:1) to afford the product as colorless solid (1.39 g, 79 %).

$^{1}$H-NMR (360 MHz, $CDCl_3$): δ (ppm) 8.03 (d, $^{3}J$ = 8.64 Hz, 2H), 7.42 (t, $^{3}J$ = 7.56 Hz, 2H), 7.29 - 7.18 (m, 5H), 6.91 (d, $^{3}J$ = 8.28 Hz, 2H), 6.65 (d, $^{3}J$ = 8.64 Hz, 2H), 4.53 (br-s, 1H), 4.35 (s, 2H), 3.84 (d, $^{3}J$ = 5.04 Hz, 2H), 1.75 - 1.69 (m, 1H), 1.53 - 1.32 (m, 8H), 0.96 - 0.90 (m, 6H).

$^{13}$C-NMR (90 MHz, $CDCl_3$): δ (ppm) 165.29, 158.91, 152.16, 151.24, 132.25, 129.66, 129.31, 128.71, 125.41, 121.90, 117.55, 114.74, 111.73, 70.49, 47.16, 39.31, 30.47, 29.04, 23.80, 23.04, 14.10, 11.09.

HR-MS (ESI+): calc. for $C_{28}H_{33}N_1O_3Na_1$ $(M+Na)^+$ 454.23527, found 454.23504.

## *Synthesis of cyclic trimers versus linear polymers*

General procedure using LiHMDS as base:

Monomer (**1a-c**; 2 mmol) was dissolved in anhydrous THF (0.06 M or 0.25 M) and stirred for 15 min. To this solution 1.5 eq. of LiHMDS (1 M in THF) was added in one shot. After stirring for 18 h at room temperature, a saturated solution of ammonium chloride was added for quenching. The solution was extracted three times with dichloromethane. The combined organic extracts were washed with brine, dried over magnesium sulfate and the solvent was removed under reduced pressure. See below for purification method.

**Cyclic tris(4-((2,4-dimethoxybenzyl)amino)benzamide) (2a)**

Purification was performed by silica gel column chromatography eluted by dichloromethane (using a gradient from 0 - 5 vol.-% methanol) to afford the product as colorless solid (0.06 M: 177 mg, 33 %; 0.25 M 0 %).

$^{1}$H-NMR (360 MHz, $CDCl_3$): δ (ppm) 7.17 (d, $^{3}J$ = 8.28 Hz, 3H), 6.86 (d, $^{3}J$ = 8.28 Hz, 6H), 6.54 (d, $^{3}J$ = 8.28 Hz, 6H), 6.38 (dd, $^{4}J$ = 2.16 Hz, $^{3}J$ = 8.28 Hz, 3H), 6.32 (d, $^{4}J$ = 1.80 Hz, 3H), 4.92 (s, 6H), 3.77 (s, 9H), 3.57 (s, 9H).

$^{13}$C-NMR (90 MHz, $CDCl_3$): δ (ppm) 170.82, 160.48, 158.55, 142.82, 135.55, 131.45, 128.67, 127.55, 117.13, 104.16, 98.12, 55.28, 55.12, 46.66.

HR-MALDI FT-ICR: calc. for $C_{96}H_{90}N_6O_{18}Ag_1$ $(M+Ag)^+$ 1712.53570, found 1721.53641.

**Cyclic tris(4-((2,4-bis((2-ethylhexyl)oxy)benzyl)amino)benzamide) (2b)**

Purification was performed by silica gel column chromatography eluted by hexane (using a gradient from 5 - 15 vol.-% ethyl acetate) to afford the product as yellow solid (0.06 M: 447 mg, 48 %; 0.25 M: 484 mg, 52 %).
$^1$H-NMR (360 MHz, $CDCl_3$): δ (ppm) 7.08 (d, $^3J$ = 9.00 Hz, 3H), 6.86 (d, $^3J$ = 8.28 Hz, 6H), 6.54 (d, $^3J$ = 7.92 Hz, 6H), 6.35 - 6.33 (m, 6H), 4.95 (s, 6H), 3.78 (d, $^3J$ = 5.40 Hz, 6H), 3.72 - 3.63 (m, 6H), 1.71 - 1.66 (m, 6H), 1.57 - 1.26 (m, 48H), 0.94 - 0.81 (m, 36H).
$^{13}$C-NMR (90 MHz, $CDCl_3$): δ (ppm) 170.94, 160.31, 158.24, 142.98, 135.72, 131.11, 128.75, 127.84, 116.98, 104.74, 99.40, 70.55, 70.26, 46.50, 46.48, 39.55, 39.37, 30.66, 30.56, 29.25, 29.15, 23.98, 23.87, 23.19, 23.13, 14.24, 14.20, 11.27, 11.18.
HR-MALDI FT-ICR: calc. for $C_{90}H_{129}N_3O_9Ag_1$ $(M+Ag)^+$ 1502.87743, found 1502.87770.

*Table SI1*. Molecular weights and PDI after polymerization of monomer **1c** determined by GPC based on polystyrene standards.

| Monomer | Concentration M | $M_n$ g / mol | PDI |
|---|---|---|---|
| **P1a** | 0.06 | 3800 | 1.67 |
| **P1b** | 0.25 | 11100 | 1.49 |

## *Deprotection of cyclic trimers **2***

**Cyclic tris(*p*-benzamide) (7)**

Cyclic tris(4-((2,4-dimethoxybenzyl)amino)benzamide) **2a** respectively cyclic tris(4-((2,4-bis((2-ethylhexyl)oxy)benzyl)amino)benzamide) **2b** was heated at 65°C in trifluoroacetic acid containing excess triisopropylsilane. After stirring for 18h, trifluoroacetic acid was evaporated, chloroform was added and the resulting precipitate was filtered and washed with methanol and dichloromethane. After drying in vacuum, the product was afforded as a colorless solid in quantitative yield.
Analytical data of **7** was identical to that reported previously.[4]

# $^{1}$H- and $^{13}$C-NMR spectra

## Phenyl 4-((2,4-dimethoxybenzyl)amino)benzoate (1a)

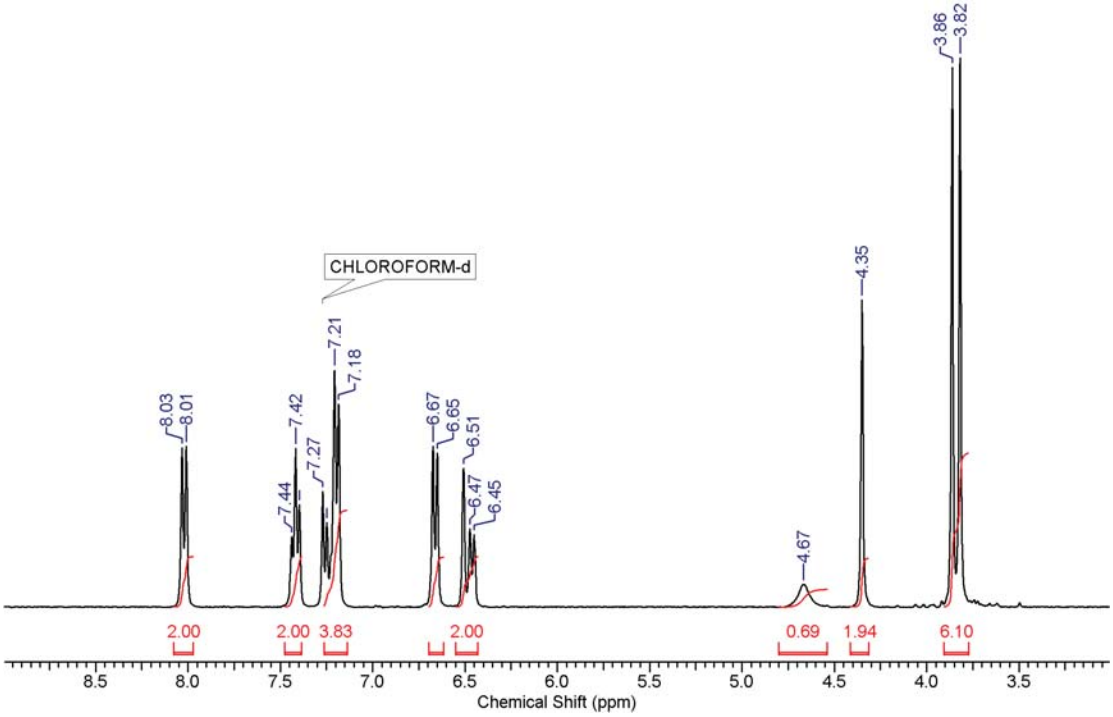



**Figure SI1.** $^{1}$H-NMR spectrum (360 MHz, $CDCl_3$) of **1a**.

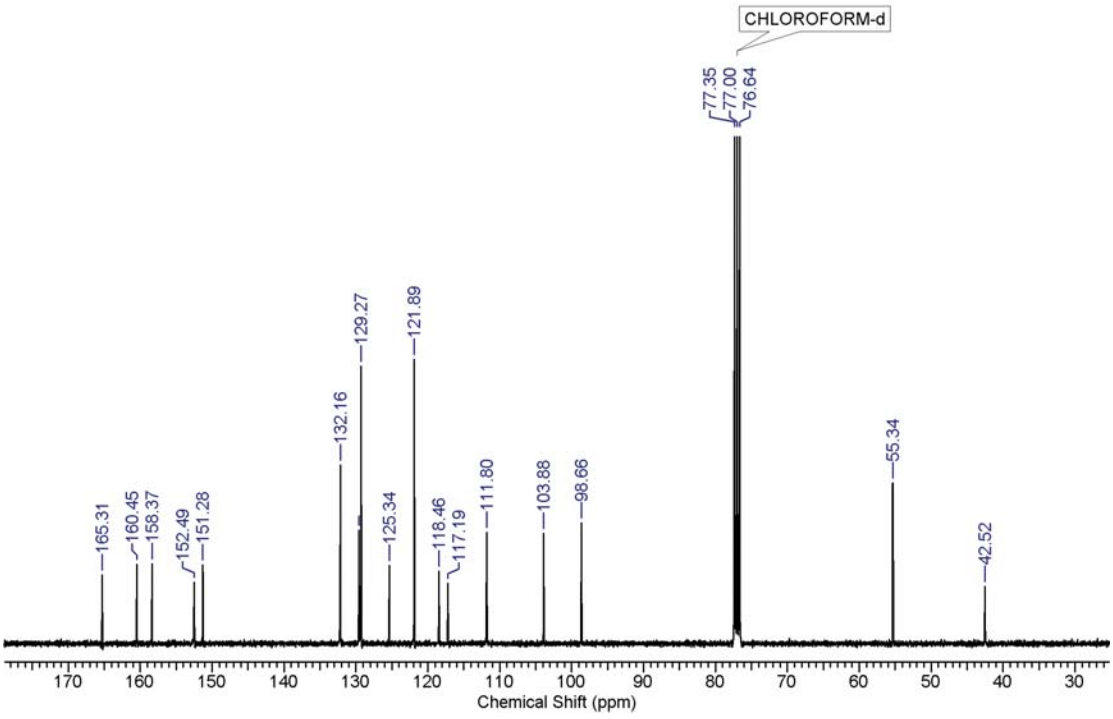



**Figure SI2.** $^{13}$C-NMR spectrum (90 MHz, $CDCl_3$) of **1a**.

**Phenyl 4-((2,4-bis((2-ethylhexyl)oxy)benzyl)amino)benzoate (1b)**

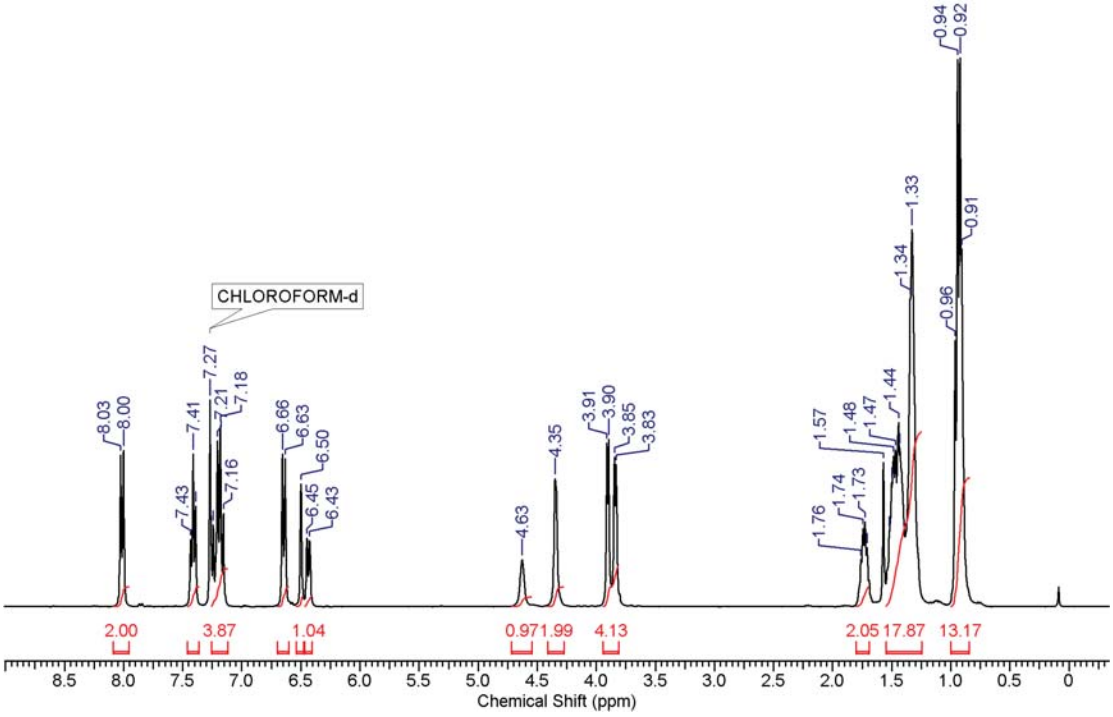



**Figure SI3.** $^{1}$H-NMR spectrum (360 MHz, $CDCl_3$) of **1b**.

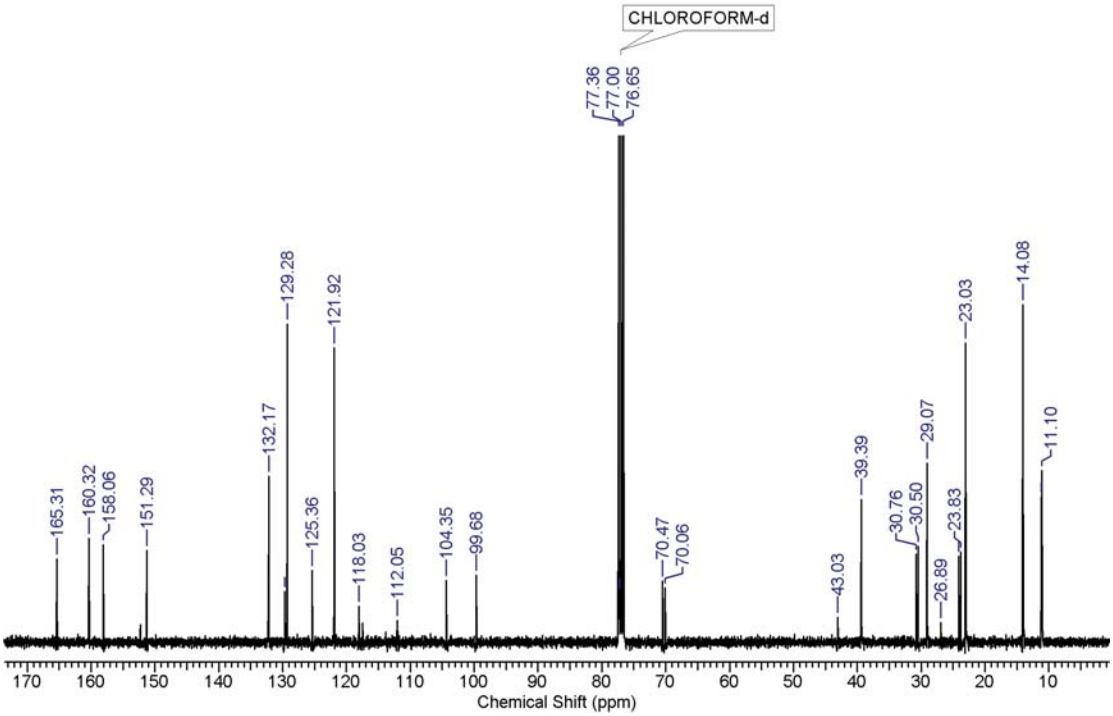



**Figure SI4.** $^{13}$C-NMR spectrum (90 MHz, $CDCl_3$) of **1b**.

**Phenyl 4-((4-((2-ethylhexyl)oxy)benzyl)amino)benzoate (1c)**

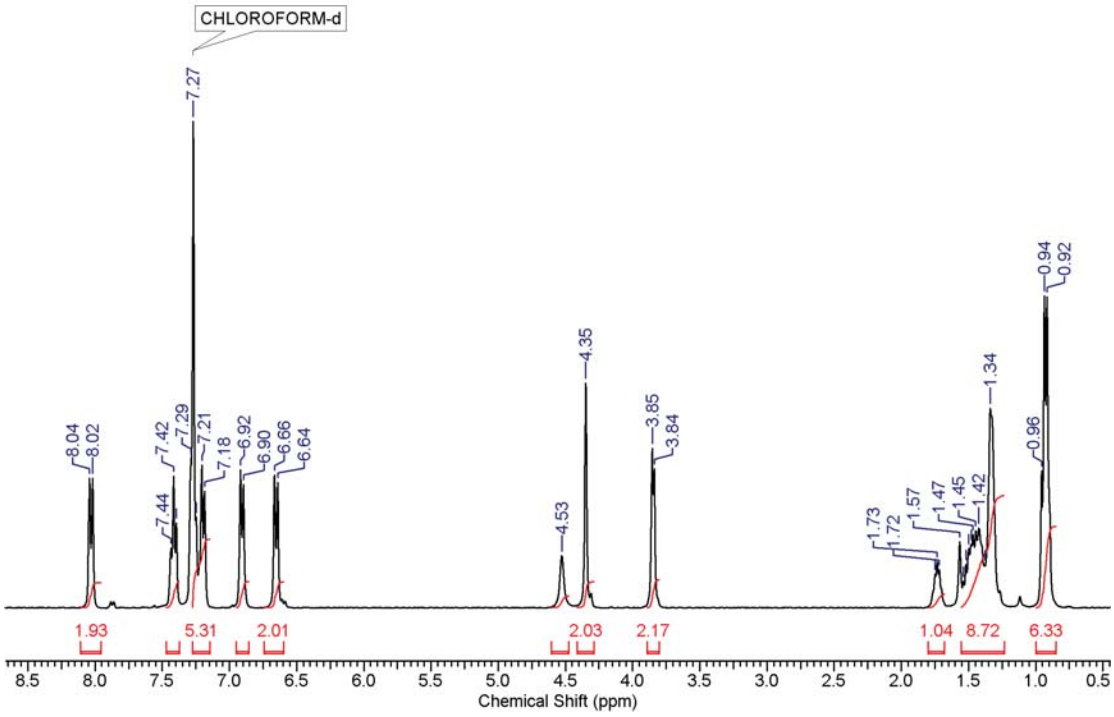



**Figure SI5.** $^{1}$H-NMR spectrum (360 MHz, $CDCl_3$) of **1c**.

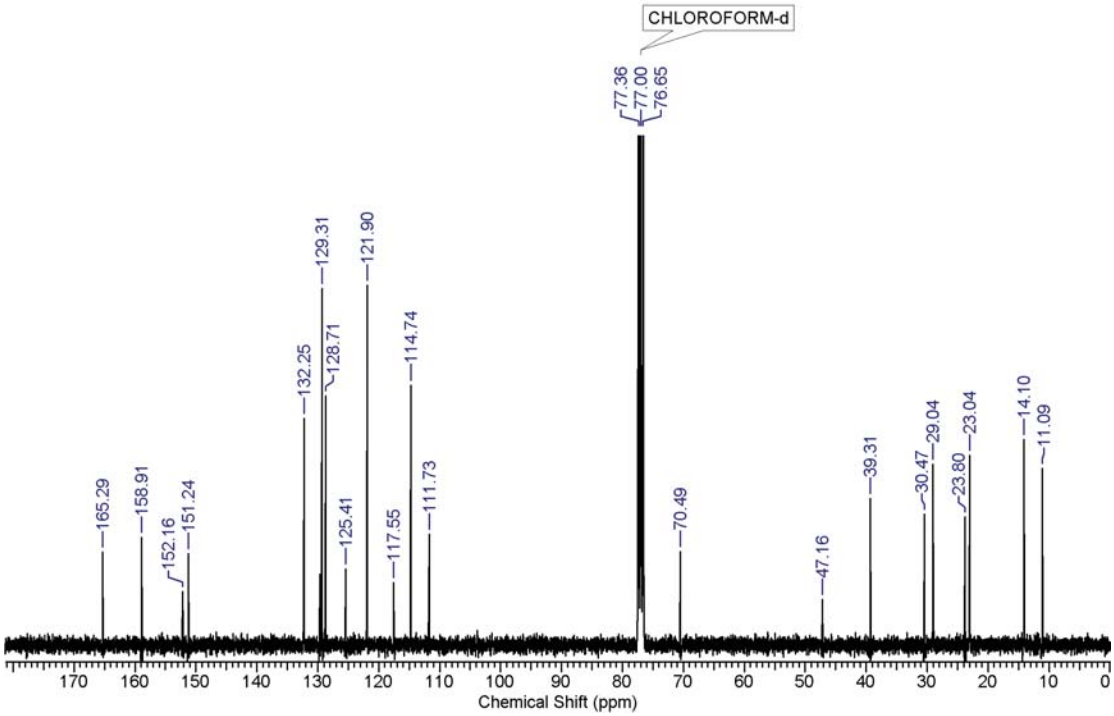



**Figure SI6.** $^{13}$C-NMR spectrum (90 MHz, $CDCl_3$) of **1c**.

## Cyclic tris(4-((2,4-dimethoxybenzyl)amino)benzamide) (2a)

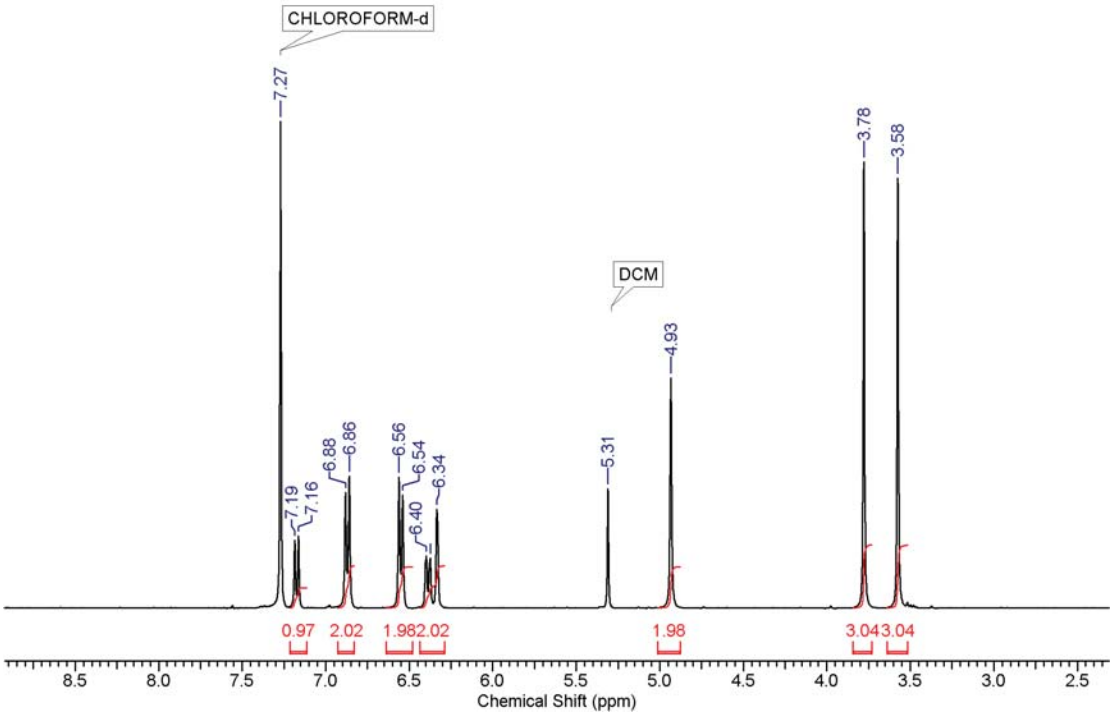



**Figure SI7.** $^{1}$H-NMR spectrum (360 MHz, $CDCl_3$) of **2a**.

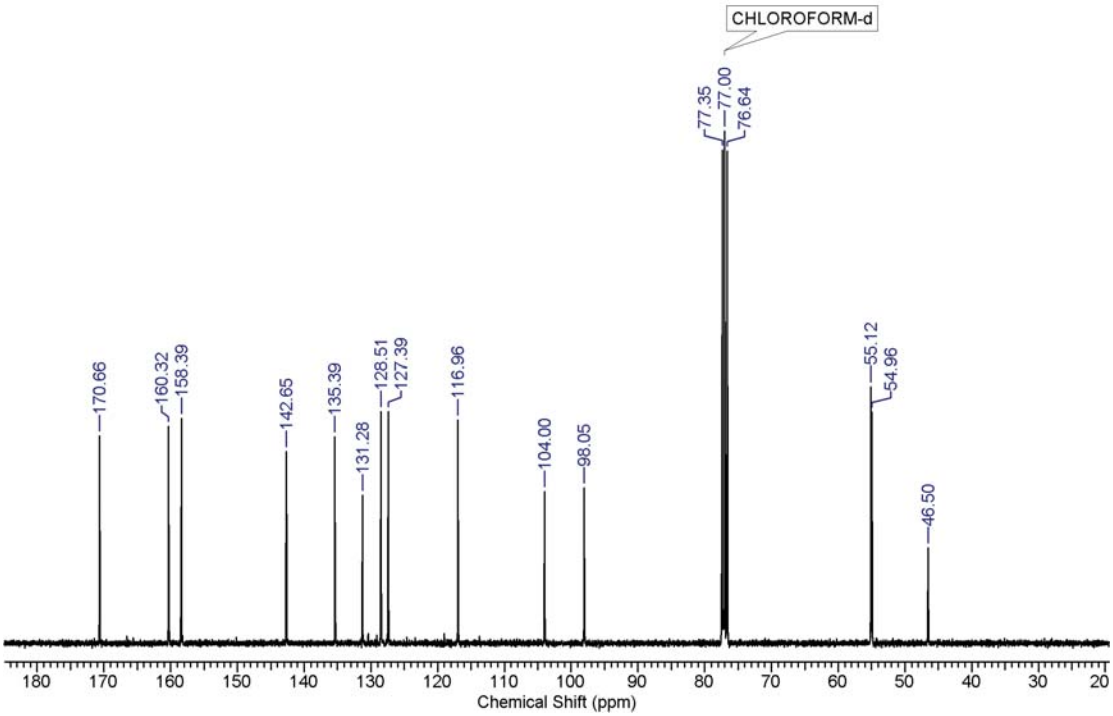



**Figure SI8.** $^{13}$C-NMR spectrum (90 MHz, $CDCl_3$) of **2a**.

**Cyclic tris(4-((2,4-bis((2-ethylhexyl)oxy)benzyl)amino)benzamide) (2b)**

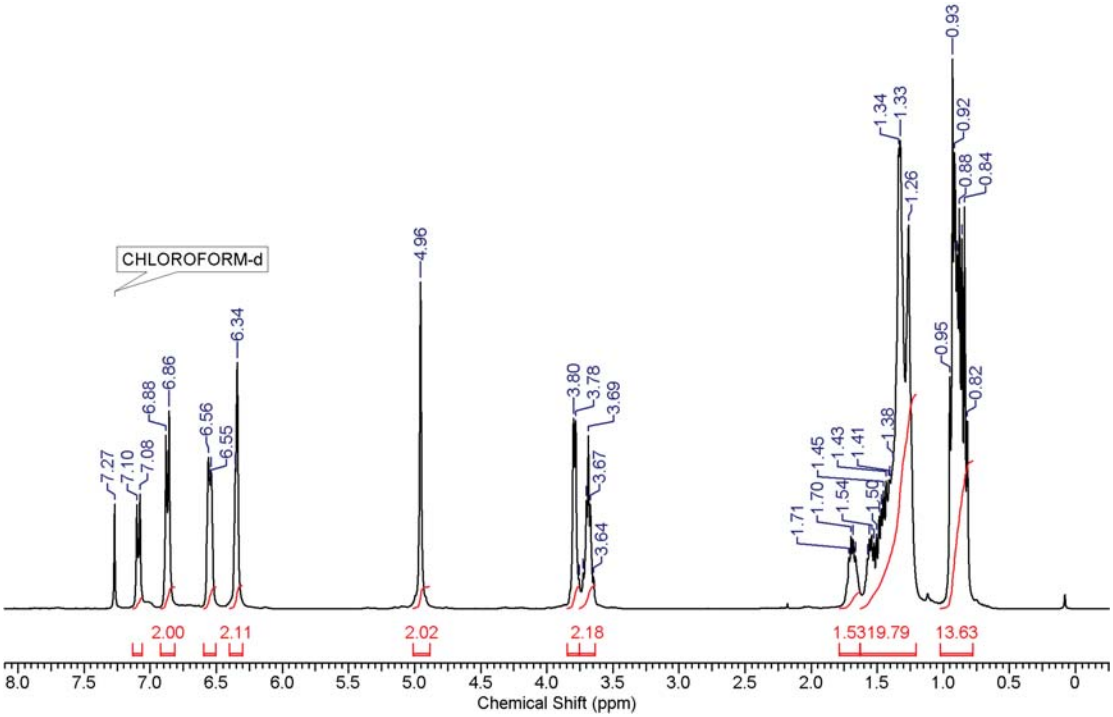



**Figure SI9.** $^{1}$H-NMR spectrum (360 MHz, $CDCl_3$) of **2b**.

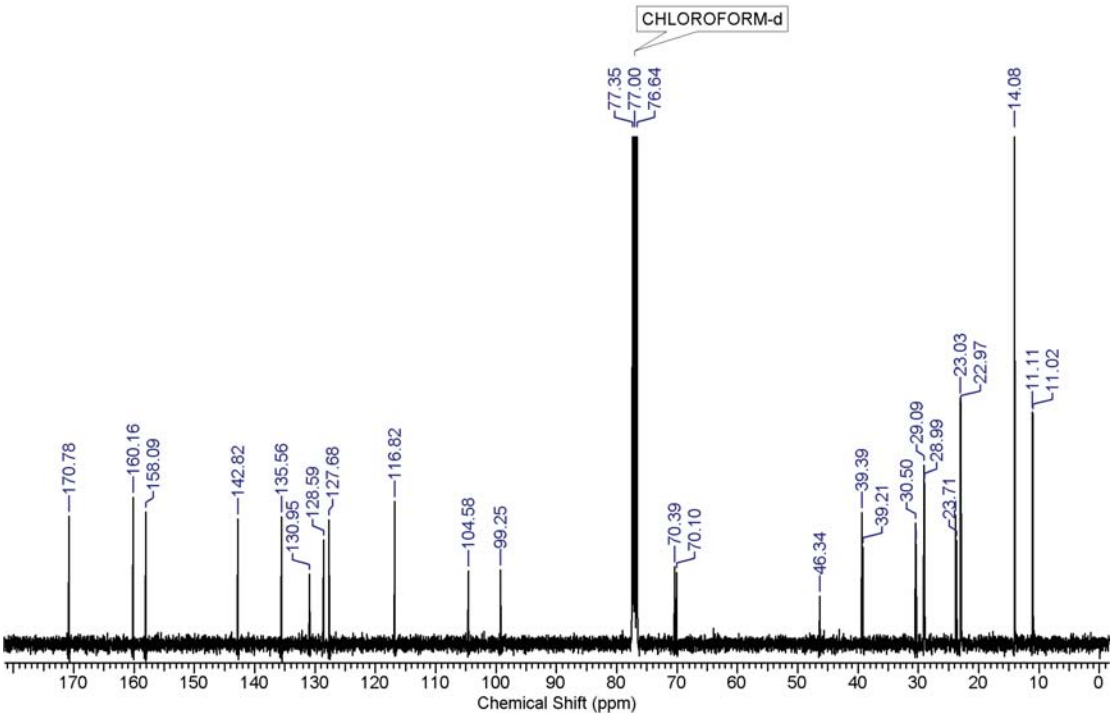



**Figure SI10.** $^{13}$C-NMR spectrum (90 MHz, $CDCl_3$) of **2b**.

## Gel permeation chromatography elugrams

### P1a

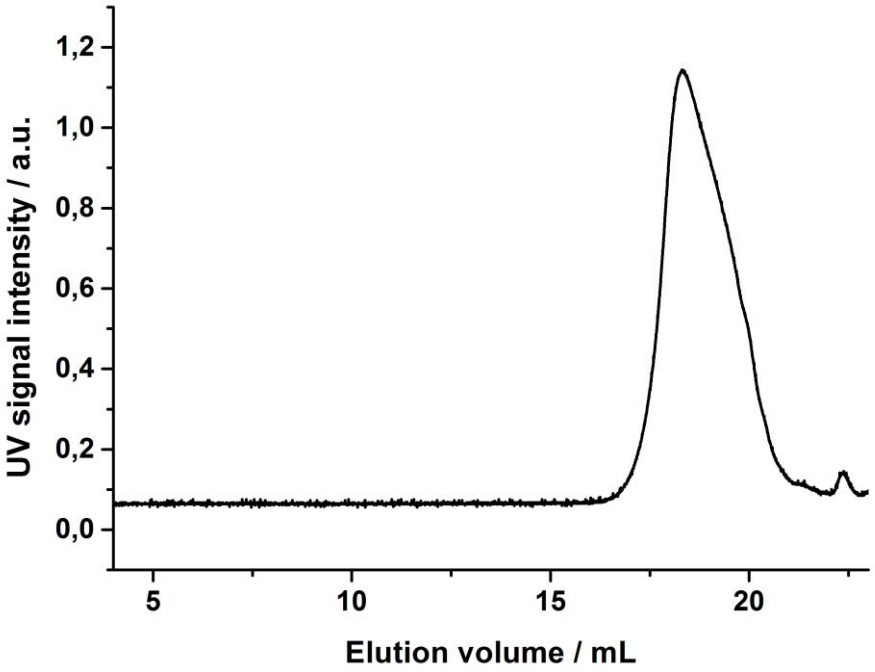



**Figure SI11.** GPC elugram of **P1a** in chloroform.

### P1b

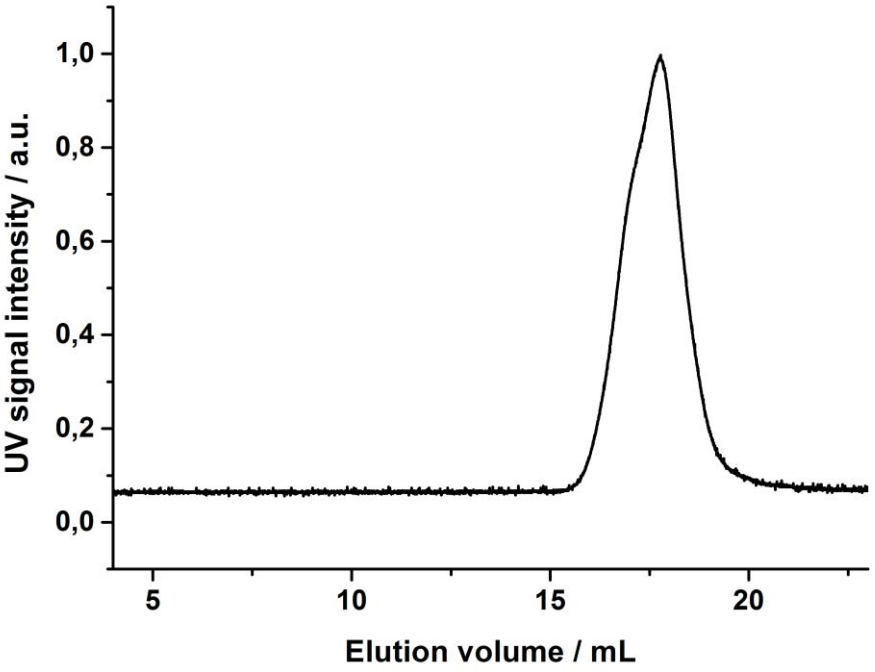



**Figure SI12.** GPC elugram of **P1b** in chloroform.

## Mass spectra - HR-MS (ESI+)

### Phenyl 4-((2,4-dimethoxybenzyl)amino)benzoate (1a)

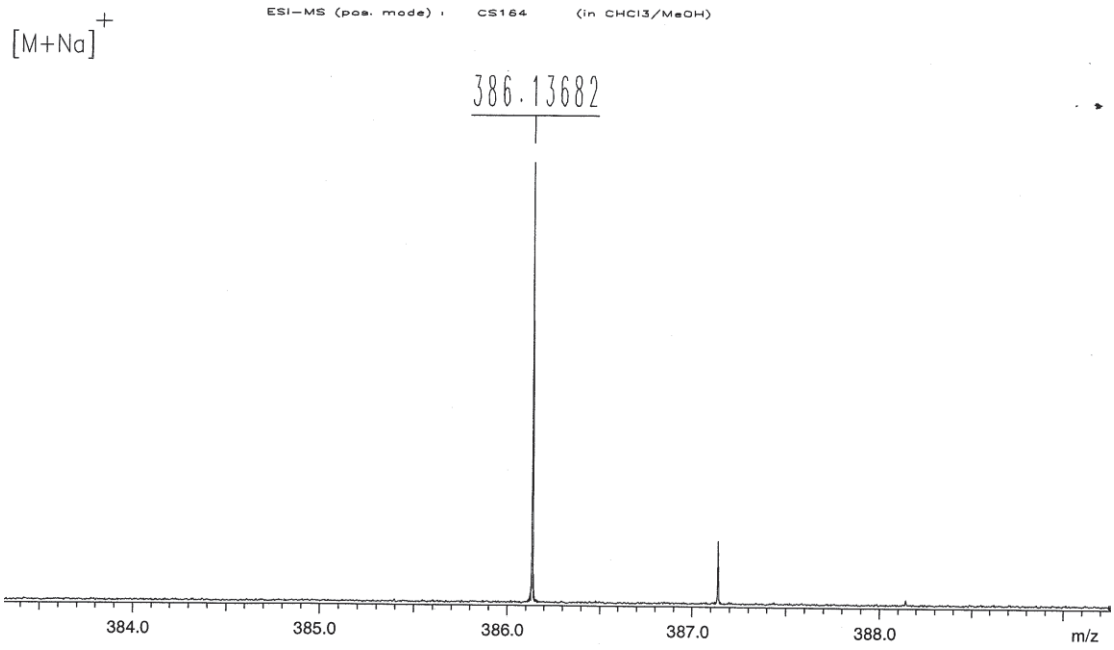



**Figure SI13.** High-resolution mass spectrum (ESI+) of **1a**.

### Phenyl 4-((2,4-bis((2-ethylhexyl)oxy)benzyl)amino)benzoate (1b)

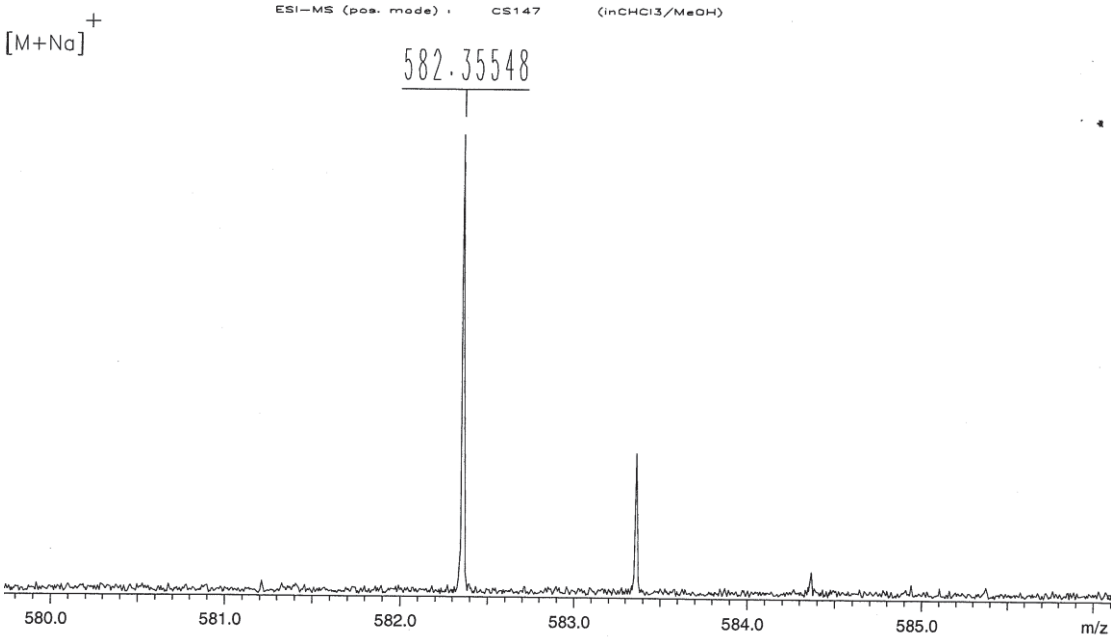



**Figure SI14.** High-resolution mass spectrum (ESI+) of **1b**.

### Phenyl 4-((4-((2-ethylhexyl)oxy)benzyl)amino)benzoate (1c)

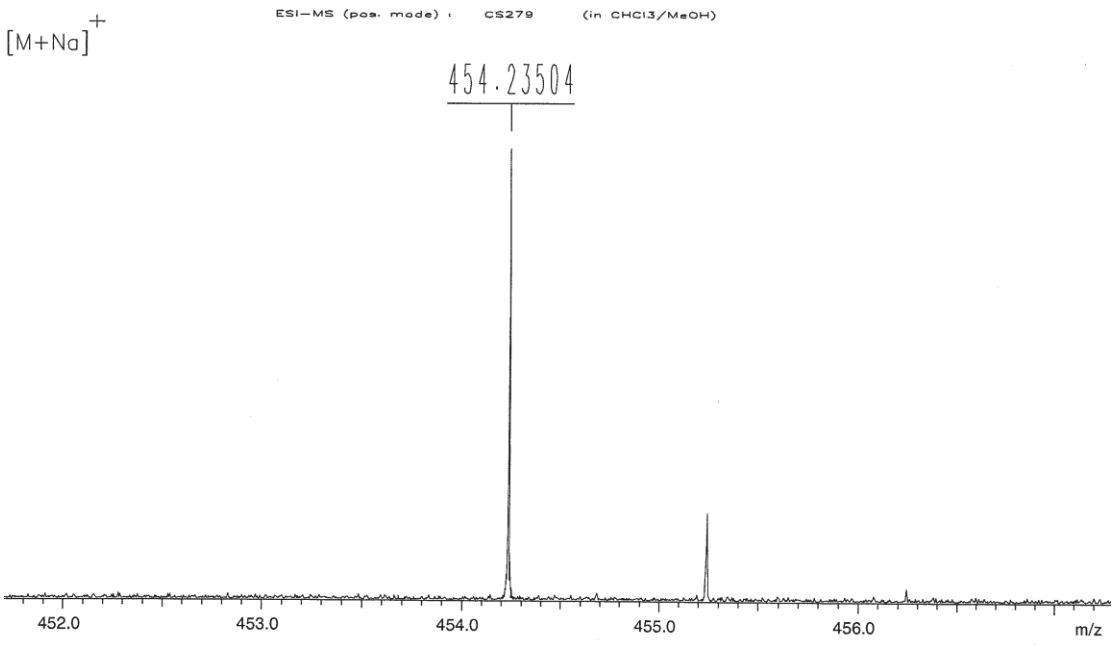



**Figure SI15.** High-resolution mass spectrum (ESI+) of **1c**.

## Mass spectra - MALDI FT-ICR

### Cyclic tris(4-((2,4-dimethoxybenzyl)amino)benzamide) (2a)

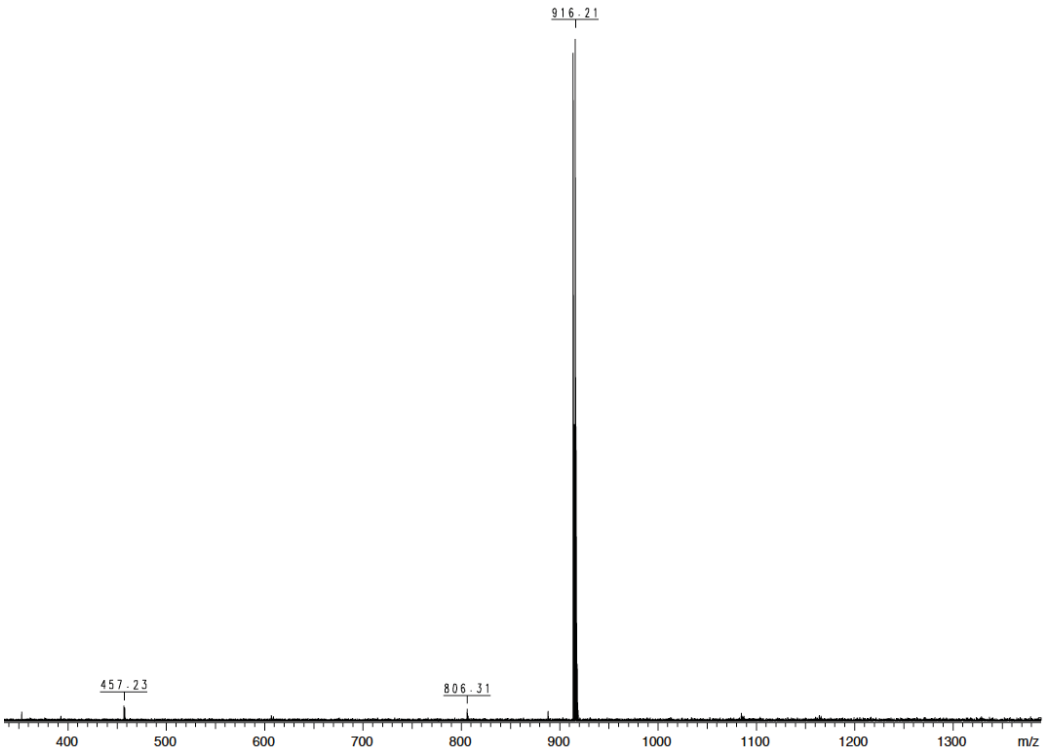



**Figure SI16.** High-resolution MALDI FT-ICR mass spectrum of **2a** as $Ag^+$-adduct.

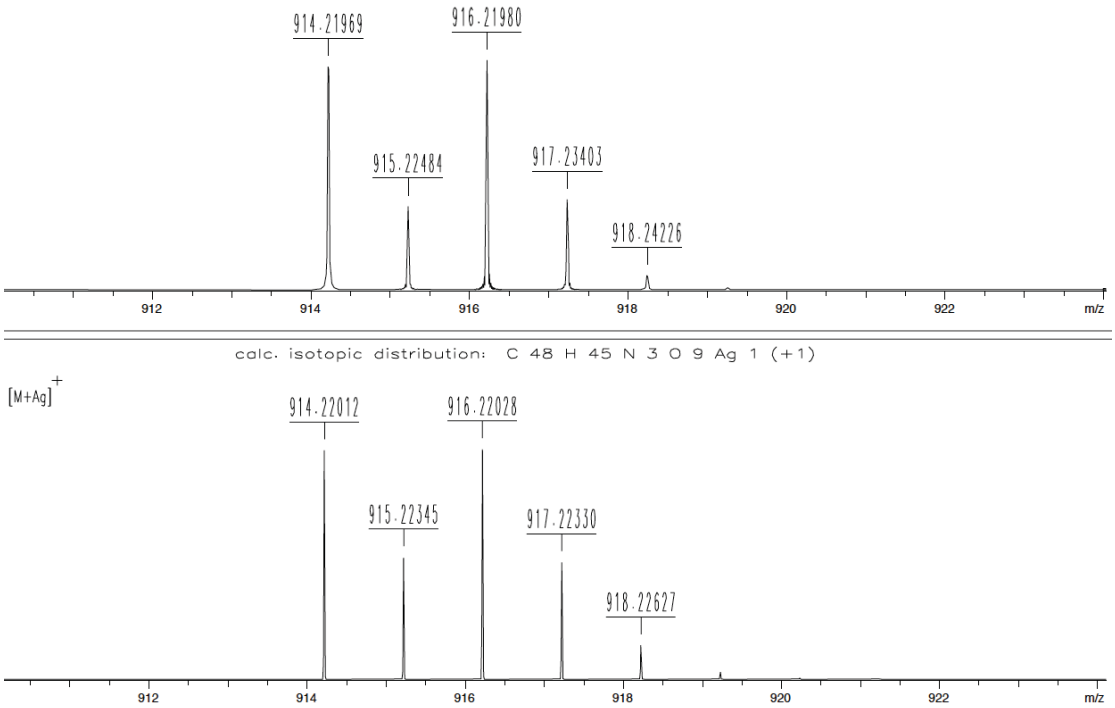



**Figure SI17.** High-resolution MALDI FT-ICR mass spectrum of **2a** as $Ag^+$-adduct. Measured isotope pattern (bottom) in comparison to the calculated isotope pattern (top).

## Cyclic tris(4-((2,4-bis((2-ethylhexyl)oxy)benzyl)amino)benzamide) (2b)

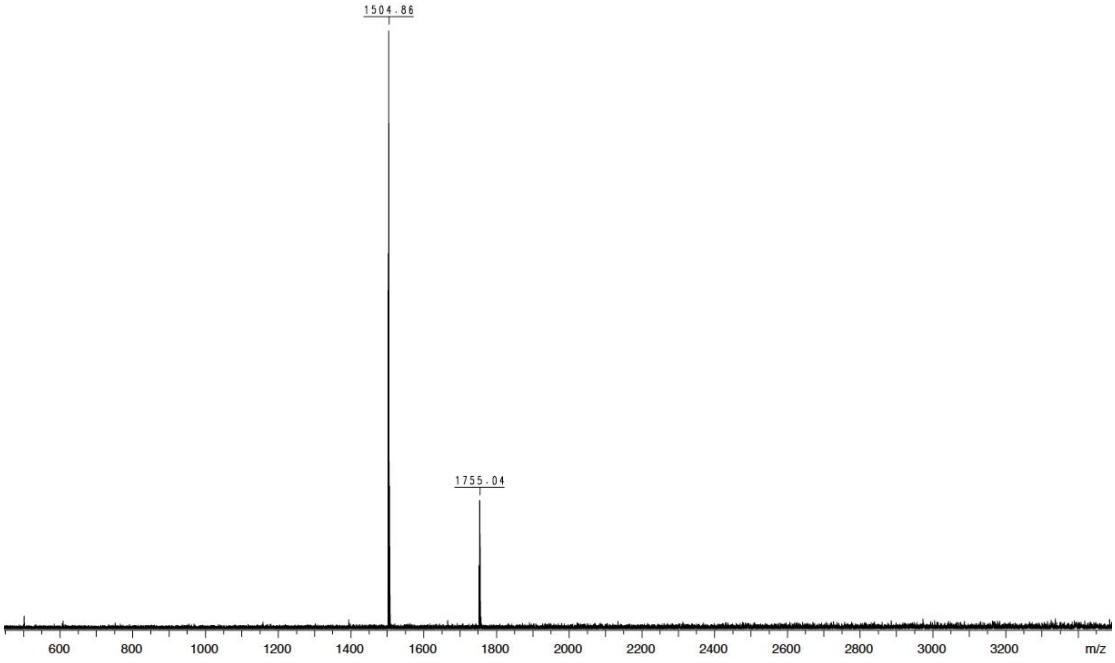



**Figure SI18.** High-resolution MALDI FT-ICR mass spectrum of **2b** as $Ag^+$-adduct.

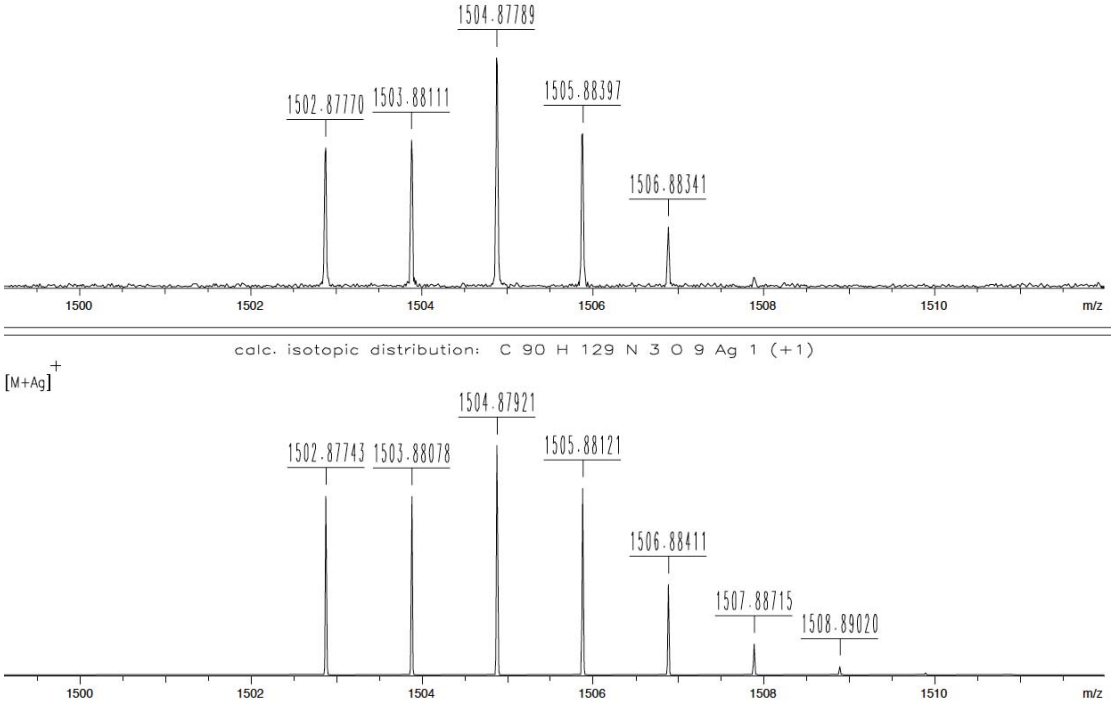



**Figure SI19.** High-resolution MALDI FT-ICR mass spectrum of **2b** as $Ag^+$-adduct. Measured isotope pattern (bottom) in comparison to the calculated isotope pattern (top).

## AFM Experiments

NC-AFM experiments were performed at room temperature (RT) under ultra-high vacuum conditions (base pressure < 1 x $10^{-10}$ mbar). The system is equipped with an atomic force microscope (VT AFM XA from Omicron Nanotechnology, Taunusstein, Germany) operated in the frequency modulation mode.[5] Signal demodulation and oscillation excitation is realized using a phase locked loop and amplitude controller (easyPLL Plus from Nanosurf, Liestal, Switzerland). Standard n-doped cantilevers with resonance frequencies around 300 kHz were used (type PPP-NCH from Nanossensors, Neuchâtel, Switzerland) and bombarded with Ar ions prior use to remove contaminants.

The sample used here is the calcite(10.4) cleavage plane. Calcite crystal of the highest available quality and a cross-section of 2 x 4 mm² were purchased from Korth Kristalle GmbH (Altenholz, Germany). The crystals were degassed for two hours at 550 K to removed contaminants, cleaved *in situ*[6] and annealed at 500 K for one hour to remove surface charges.

Molecular material was sublimed onto the sample using a home-built Knudsen cell at a temperature of 539 K. The substrate is held at RT during the deposition process.

A color scale is used for data representation, with bright colors corresponding to highly attractive interactions while darker colors correspond to less attractive or even repulsive interactions. Depending on feedback-loop settings, either frequency shift ($\Delta f$) or topography ($z$) images are obtained (Image type is given in the upper right corner of the image). The presented data are raw data except for a plane substraction to account for tilted samples and a correction for the effects of linear thermal drift.

## Quantum Chemical Calculations

All quantum chemical calculations were performed with the Gaussian 09 package (revision D.01) of electronic structure programs.[7] The conformational search was carried out with the MM3 molecular mechanics force field using the default algorithms implemented in the Spartan'10 suite of programs.[8] Ring strain calculations were carried out using HF/6- 31G* using Spartan 8.[9]

Geometries obtained from the conformational search were fully optimized at the M06-2X/6-31G(d) level of theory using the default integration grid in Gaussian.

Frequency analyses were performed to check the nature of stationary points and to provide zero-point vibrational energies (ZPVEs) which were used without scaling. Single point energies at the optimized geometries were computed with the M06-2X, M06L and B97D functionals using the 6-311+G(2d,p) basis set and the collective effects of surrounding solvent were modeled by polarizable continuum model (PCM; tetrahydrofurane).

The final energies are sums of total energies and ZPVEs (0 K, ideal gas). The entropy effects, which may be associated with a significant error when several vibrational modes with very low frequencies are present, were assumed to be of similar importance among different conformers in all series of conformers, and were neglected in the calculations of Boltzmann distributions, i.e. the computed final energies (0 K) were considered to represent the free energies at 298.15 K.
In the case of transition state optimizations, we had to resort to a finer integration grid (Int=Ultrafine option in Gaussian) due to the very low vibrational frequencies of a number of normal modes that prevented the geometry optimization from converging to the corresponding transition states. The PCM solvation model was used both in the geometry optimizations and in the single point energy calculations. Starting from the transition states, intrinsic reaction coordinate (IRC) calculations, followed by full geometry optimizations at the end of each IRC path, were used to identify the energy minima corresponding to the reactants, the tetrahedral intermediates, and the products that are connected by these transition states. Finally, single point energies were computed at the same level of theory as described above but with the finer integration grid.

## Ring strain calculations

*N*-methylated oligo(*p*-benzamide)s were used as models for *N*-benzylated oligomers (Figure SI20/21).

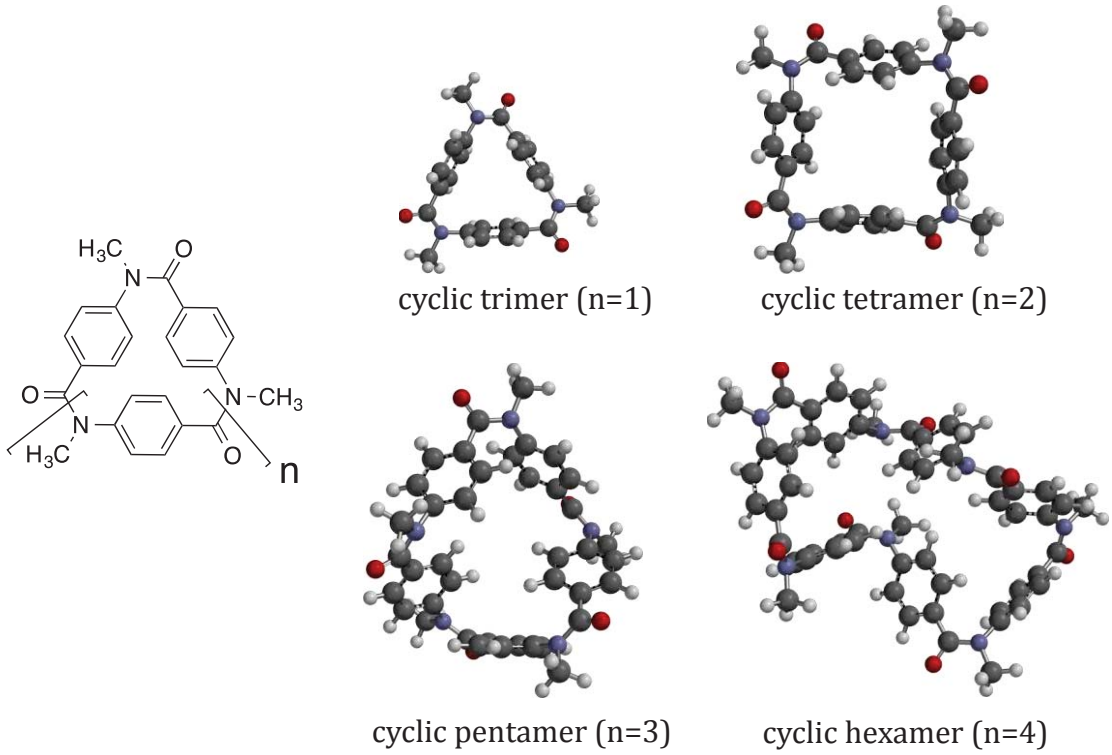



**Figure SI20.** Structures of the cyclic *N*-methylated oligo(*p*-benzamide)s.

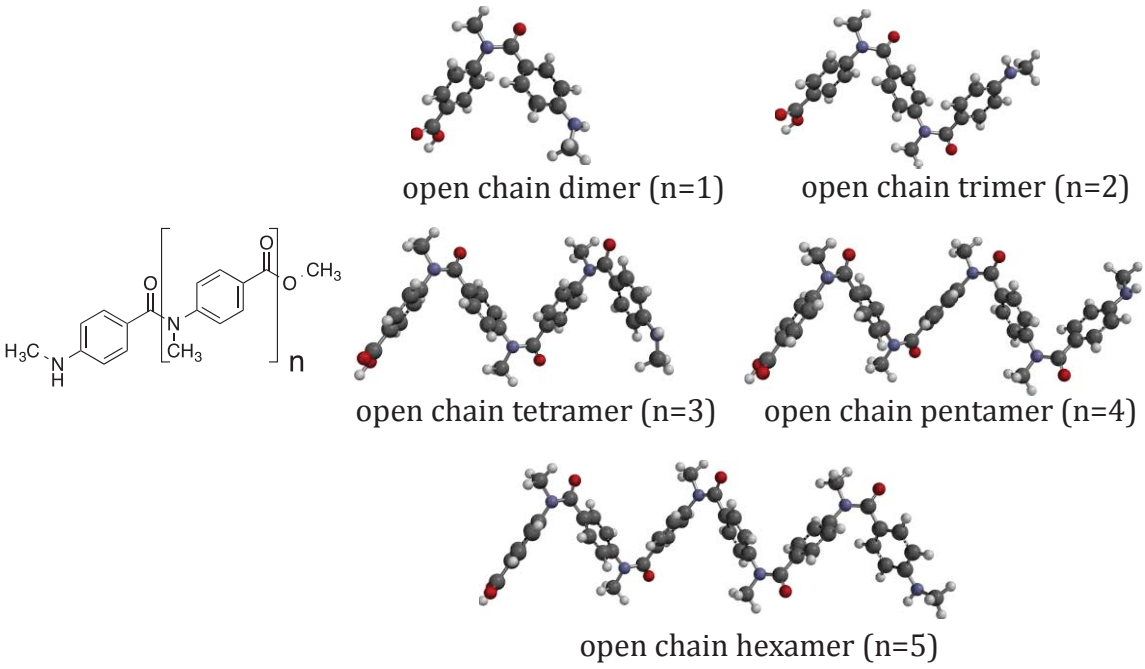



**Figure SI21.** Structures of the linear *N*-methylated oligo(*p*-benzamide)s.

*Table SI2*. Ring strain calculations.[a]

| | open chain / hartree | cyclic strained / hartree | cyclic strain free / hartree | ring strain / hartree | ring strain / kcal mol$^{-1}$ |
|---|---|---|---|---|---|
| Dimer | -948.731028 | N/A | N/A | N/A | N/A |
| Trimer | -1385.079419 | -1309.036793 | -1309.045628 | 0.0088345 | **5.57** |
| Tetramer | -1821.427864 | -1745.390016 | -1745.39417 | 0.004154 | **2.62** |
| Pentamer | -2257.776612 | -2181.725689 | -2181.742713 | 0.0170235 | **10.72** |
| Hexamer | -2694.125198 | -2618.078917 | -2618.091255 | 0.012338 | **7.77** |

[a] HF/6-31G* energies and geometries in the gas phase.

From the calculations of the open chain oligomer energies, an average incremental energy ΔE (from oligomer *n* to oligomer *n*+1) of -436.3485425 hartrees was calculated. Hypothetical cyclic strain free oligomers were calculated by multiplying this energy increment with the number of ring constituting monomers.

The difference in energy between the cyclic strained oligomer and the cyclic strain free oligomer is reported as the ring strain.

## Cartesian Coordinates (HF 6-31G*))

**open chain dimer**

| | | | |
|---|---|---|---|
| H | 2.151663 | -1.726391 | 1.825738 |
| C | 2.357703 | -1.045539 | 1.022626 |
| C | 2.871070 | 0.767051 | -1.000256 |
| C | 3.380777 | -1.311988 | 0.111844 |
| C | 1.599987 | 0.105700 | 0.905938 |
| C | 1.830334 | 1.024989 | -0.107090 |
| C | 3.622070 | -0.379099 | -0.906620 |
| H | 0.828771 | 0.283181 | 1.630803 |
| H | 4.416990 | -0.558488 | -1.609738 |
| H | 3.084016 | 1.484833 | -1.769770 |
| N | 4.174968 | -2.434140 | 0.202557 |
| C | 1.106207 | 2.322750 | -0.240909 |
| O | 1.658023 | 3.285486 | -0.700851 |
| C | -4.068847 | -1.729619 | -0.092657 |
| O | -4.790660 | -2.010029 | 0.811762 |
| C | -3.039104 | -0.660831 | -0.049411 |
| C | -1.129992 | 1.356342 | 0.125210 |
| C | -2.219936 | -0.377824 | -1.133846 |
| C | -2.902157 | 0.074736 | 1.122948 |
| C | -1.953703 | 1.072484 | 1.210649 |
| C | -1.277775 | 0.631897 | -1.050115 |
| H | -2.323881 | -0.935454 | -2.044293 |
| H | -3.536841 | -0.150624 | 1.958476 |
| H | -1.836421 | 1.631539 | 2.120951 |
| H | -0.655267 | 0.855355 | -1.896304 |
| N | -0.192864 | 2.422008 | 0.225238 |
| C | -0.764419 | 3.768245 | 0.209494 |
| H | -1.659694 | 3.775463 | 0.814051 |
| H | -1.015621 | 4.081937 | -0.798316 |
| H | -0.050470 | 4.465220 | 0.617862 |
| C | 3.819092 | -3.569685 | 1.019078 |
| H | 4.548499 | -4.351351 | 0.853434 |
| H | 2.830548 | -3.965478 | 0.792160 |
| H | 3.850512 | -3.310505 | 2.070784 |
| O | -4.121807 | -2.368548 | -1.258594 |
| H | -4.804904 | -3.028751 | -1.196578 |
| H | 4.665881 | -2.657335 | -0.633022 |

**open chain trimer:**

| | | | |
|---|---|---|---|
| H | 0.020843 | -1.259551 | 1.927465 |
| C | 0.083454 | -0.715671 | 1.002481 |
| C | 0.303747 | 0.715364 | -1.348772 |
| C | 0.952870 | -1.155841 | 0.011689 |
| C | -0.686043 | 0.415652 | 0.809592 |
| C | -0.585110 | 1.141840 | -0.371071 |
| C | 1.047745 | -0.436918 | -1.172378 |
| H | -1.345277 | 0.740126 | 1.591567 |
| H | 1.712954 | -0.769556 | -1.947404 |
| H | 0.405231 | 1.289097 | -2.250329 |
| N | 1.687477 | -2.358401 | 0.213803 |
| C | 3.028208 | -2.481475 | -0.101444 |
| O | 3.464611 | -3.535005 | -0.480392 |
| C | 3.932572 | -1.309515 | 0.088518 |
| C | 5.798883 | 0.770411 | 0.411781 |
| C | 3.745818 | -0.324512 | 1.057259 |
| C | 5.079583 | -1.245452 | -0.691412 |
| C | 5.994200 | -0.219164 | -0.553351 |
| C | 4.659111 | 0.689978 | 1.222318 |
| H | 2.888542 | -0.354999 | 1.701819 |
| H | 5.253308 | -2.014874 | -1.419892 |
| H | 6.858985 | -0.199130 | -1.188084 |
| H | 4.502576 | 1.429908 | 1.987913 |
| C | -1.317296 | 2.429671 | -0.610682 |
| O | -0.784408 | 3.321686 | -1.210667 |
| N | 6.700322 | 1.793962 | 0.614196 |
| C | -6.377442 | -1.593094 | 0.582133 |
| O | -7.002013 | -1.741872 | 1.584336 |
| C | -5.371982 | -0.520074 | 0.368813 |
| C | -3.501756 | 1.514783 | 0.063081 |
| C | -4.669221 | -0.390966 | -0.820896 |
| C | -5.139213 | 0.378402 | 1.404607 |
| C | -4.209043 | 1.385900 | 1.254292 |
| C | -3.746063 | 0.628429 | -0.976443 |
| H | -4.848467 | -1.075587 | -1.626938 |
| H | -5.685355 | 0.271098 | 2.322116 |
| H | -4.017251 | 2.072622 | 2.058463 |
| H | -3.215327 | 0.733494 | -1.904401 |
| N | -2.579856 | 2.590140 | -0.084287 |
| C | -3.167457 | 3.920438 | -0.243673 |
| H | -4.023524 | 4.004105 | 0.409493 |
| H | -3.484267 | 4.093183 | -1.266655 |
| H | -2.438071 | 4.668843 | 0.021442 |
| C | 0.909533 | -3.594065 | 0.140058 |
| H | 1.448837 | -4.387851 | 0.631433 |
| H | 0.725400 | -3.887689 | -0.888251 |
| H | -0.037380 | -3.441460 | 0.637388 |
| C | 7.726460 | 2.116868 | -0.348383 |
| H | 8.244254 | 3.004638 | -0.010245 |
| H | 7.332850 | 2.305124 | -1.345912 |
| H | 8.455210 | 1.317661 | -0.413225 |
| O | -6.525635 | -2.395764 | -0.467651 |
| H | -7.183081 | -3.047786 | -0.245799 |
| H | 6.322843 | 2.578269 | 1.095711 |

**open chain tetramer:**

| | | | |
|---|---|---|---|
| H | -6.969507 | -0.934518 | 3.816848 |
| C | -6.742199 | -0.580675 | 2.826020 |
| C | -6.181913 | 0.306188 | 0.274995 |
| C | -6.989762 | 0.760085 | 2.500566 |
| C | -6.235475 | -1.447903 | 1.888875 |
| C | -5.925659 | -1.018336 | 0.597905 |
| C | -6.706152 | 1.187693 | 1.203223 |
| H | -6.074858 | -2.478110 | 2.144834 |
| H | -6.895078 | 2.202121 | 0.909583 |
| H | -5.985331 | 0.668564 | -0.715568 |
| N | -7.532657 | 1.597756 | 3.451592 |
| C | -5.436990 | -2.041540 | -0.373413 |
| O | -5.762559 | -3.192735 | -0.258812 |
| H | 1.596445 | 1.295947 | 1.364979 |
| C | 1.734635 | 0.764933 | 0.440666 |
| C | 2.029479 | -0.628462 | -1.926084 |
| C | 1.130061 | 1.240961 | -0.715745 |
| C | 2.498852 | -0.385969 | 0.408761 |
| C | 2.656384 | -1.092517 | -0.777567 |
| C | 1.292835 | 0.542018 | -1.903490 |
| H | 2.950645 | -0.739865 | 1.315207 |
| H | 0.834969 | 0.905356 | -2.805030 |
| H | 2.125421 | -1.187592 | -2.837253 |
| N | 0.398377 | 2.463276 | -0.668578 |
| C | -0.848227 | 2.613892 | -1.232068 |
| O | -1.206152 | 3.678318 | -1.656193 |
| C | -1.787300 | 1.443307 | -1.257764 |
| C | -3.697985 | -0.589292 | -1.345292 |
| C | -1.859071 | 0.499796 | -0.243212 |
| C | -2.691535 | 1.368530 | -2.311924 |
| C | -3.629591 | 0.357174 | -2.361603 |
| C | -2.803135 | -0.511665 | -0.288201 |
| H | -1.184922 | 0.546525 | 0.589961 |
| H | -2.662304 | 2.117175 | -3.080620 |
| H | -4.327808 | 0.305000 | -3.177255 |
| H | -2.846110 | -1.237861 | 0.502103 |
| C | 3.391935 | -2.398651 | -0.867632 |
| O | 2.991876 | -3.261709 | -1.598158 |
| N | -4.650087 | -1.644329 | -1.437556 |
| C | 8.132618 | 1.443698 | 1.573613 |
| O | 8.502456 | 1.560583 | 2.698764 |
| C | 7.177400 | 0.406024 | 1.105626 |
| C | 5.378330 | -1.564108 | 0.322964 |
| C | 6.775227 | 0.314867 | -0.219438 |
| C | 6.679945 | -0.498215 | 2.038019 |
| C | 5.784891 | -1.473712 | 1.650535 |
| C | 5.887580 | -0.672472 | -0.610566 |
| H | 7.160846 | 1.003551 | -0.945764 |
| H | 6.994896 | -0.420499 | 3.060933 |
| H | 5.388571 | -2.165052 | 2.371670 |
| H | 5.591216 | -0.749246 | -1.640232 |
| N | 4.488104 | -2.607186 | -0.061202 |
| C | 5.059373 | -3.953739 | -0.105849 |
| H | 5.733091 | -4.074354 | 0.729587 |
| H | 5.604923 | -4.121405 | -1.028222 |
| H | 4.267049 | -4.681651 | -0.037333 |
| C | 1.198418 | 3.683128 | -0.566767 |
| H | 0.587021 | 4.482789 | -0.180538 |
| H | 1.589101 | 3.983028 | -1.533550 |
| H | 2.023760 | 3.502945 | 0.106421 |
| C | -4.342168 | -2.686619 | -2.415788 |
| H | -5.241684 | -3.230117 | -2.656249 |
| H | -3.606937 | -3.386970 | -2.033432 |
| H | -3.953033 | -2.221588 | -3.310058 |
| C | -7.536167 | 3.033443 | 3.302865 |

| | | | |
|---|---|---|---|
| H | -6.545729 | 3.446173 | 3.118322 |
| H | -7.926633 | 3.469991 | 4.212596 |
| H | -8.187804 | 3.332987 | 2.490588 |
| O | 8.550614 | 2.253359 | 0.605157 |
| H | 9.155165 | 2.880493 | 0.989650 |
| H | -7.426098 | 1.276252 | 4.386689 |

**open chain pentamer:**

| | | | |
|---|---|---|---|
| H | 5.125601 | -2.366927 | -0.780557 |
| C | 4.826483 | -1.373016 | -0.503636 |
| C | 4.031980 | 1.180522 | 0.209689 |
| C | 5.046621 | -0.316920 | -1.377648 |
| C | 4.241248 | -1.146159 | 0.728583 |
| C | 3.818569 | 0.126288 | 1.089656 |
| C | 4.649393 | 0.961913 | -1.007091 |
| H | 4.104193 | -1.957959 | 1.417345 |
| H | 4.833284 | 1.784484 | -1.674042 |
| H | 3.738676 | 2.177569 | 0.475655 |
| N | 5.621924 | -0.522214 | -2.664022 |
| C | 6.736621 | -1.313010 | -2.870833 |
| O | 6.854861 | -1.935293 | -3.892277 |
| C | 7.815393 | -1.339375 | -1.839800 |
| C | 9.972432 | -1.483023 | -0.039887 |
| C | 8.626057 | -2.473418 | -1.778942 |
| C | 8.122089 | -0.275645 | -1.003965 |
| C | 9.181734 | -0.336128 | -0.117203 |
| C | 9.672268 | -2.554319 | -0.892488 |
| H | 8.422586 | -3.292440 | -2.442609 |
| H | 7.540504 | 0.625290 | -1.041486 |
| H | 9.387807 | 0.511301 | 0.507561 |
| H | 10.280273 | -3.441886 | -0.859759 |
| C | 3.239212 | 0.301117 | 2.463629 |
| O | 3.654634 | -0.357770 | 3.377029 |
| N | 11.049507 | -1.580673 | 0.815393 |
| H | -3.546486 | -0.293128 | -1.706815 |
| C | -3.808851 | 0.170400 | -0.773143 |
| C | -4.422770 | 1.348782 | 1.649002 |
| C | -3.390447 | 1.469597 | -0.516057 |
| C | -4.547067 | -0.525806 | 0.164917 |
| C | -4.863527 | 0.058999 | 1.385368 |
| C | -3.713757 | 2.059611 | 0.697704 |
| H | -4.853843 | -1.530934 | -0.050860 |
| H | -3.401983 | 3.067257 | 0.902665 |
| H | -4.641649 | 1.792490 | 2.601492 |
| N | -2.681352 | 2.186885 | -1.523483 |
| C | -1.531130 | 2.896608 | -1.269218 |
| O | -1.251464 | 3.869661 | -1.913763 |
| C | -0.586587 | 2.406466 | -0.209291 |
| C | 1.322982 | 1.629176 | 1.668824 |
| C | -0.351362 | 1.062487 | 0.039952 |
| C | 0.153570 | 3.360255 | 0.481382 |
| C | 1.090931 | 2.976737 | 1.419214 |
| C | 0.592946 | 0.675677 | 0.975925 |
| H | -0.896750 | 0.308053 | -0.492998 |
| H | -0.001274 | 4.400168 | 0.265229 |
| H | 1.661444 | 3.717159 | 1.950178 |
| H | 0.762497 | -0.368408 | 1.163812 |
| C | -5.576518 | -0.669643 | 2.488352 |
| O | -5.267175 | -0.474489 | 3.630756 |
| N | 2.270783 | 1.256810 | 2.666506 |
| C | -9.992286 | -1.256793 | -2.344207 |
| O | -10.194510 | -2.177470 | -3.070572 |
| C | -9.093204 | -1.300354 | -1.161641 |
| C | -7.385620 | -1.473242 | 1.025645 |

| | | | |
|---|---|---|---|
| C | -8.890122 | -0.196169 | -0.346053 |
| C | -8.442441 | -2.495431 | -0.874254 |
| C | -7.592686 | -2.580529 | 0.209195 |
| C | -8.047848 | -0.285668 | 0.748772 |
| H | -9.394982 | 0.726488 | -0.556659 |
| H | -8.603964 | -3.344473 | -1.510343 |
| H | -7.078466 | -3.499114 | 0.425610 |
| H | -7.906033 | 0.566871 | 1.386795 |
| N | -6.539145 | -1.598348 | 2.164447 |
| C | -7.084626 | -2.363571 | 3.286227 |
| H | -7.621648 | -3.216462 | 2.898161 |
| H | -7.760364 | -1.761319 | 3.883931 |
| H | -6.277269 | -2.702447 | 3.915140 |
| C | -3.478760 | 2.656350 | -2.656145 |
| H | -2.831600 | 2.846318 | -3.497265 |
| H | -4.009734 | 3.571166 | -2.414772 |
| H | -4.195102 | 1.891454 | -2.917814 |
| C | 1.844824 | 1.444825 | 4.052966 |
| H | 2.711901 | 1.489889 | 4.692120 |
| H | 1.210376 | 0.630486 | 4.386386 |
| H | 1.294801 | 2.371711 | 4.125275 |
| C | 4.694032 | -0.438416 | -3.790680 |
| H | 4.121444 | -1.353382 | -3.903534 |
| H | 5.247663 | -0.266664 | -4.699711 |
| H | 4.013854 | 0.384047 | -3.623213 |
| C | 11.237686 | -0.673463 | 1.922516 |
| H | 10.372554 | -0.618330 | 2.580989 |
| H | 11.460475 | 0.325216 | 1.565753 |
| H | 12.088350 | -1.011118 | 2.499559 |
| O | -10.566390 | -0.071754 | -2.528793 |
| H | -11.121541 | -0.133145 | -3.299961 |
| H | 11.346915 | -2.513812 | 0.988887 |

**open chain hexamer**

| | | | |
|---|---|---|---|
| H | 3.045962 | -1.826260 | 0.387586 |
| C | 2.667310 | -0.830361 | 0.248949 |
| C | 1.663863 | 1.724366 | -0.108505 |
| C | 2.866571 | -0.176964 | -0.959042 |
| C | 1.997586 | -0.196488 | 1.279964 |
| C | 1.471337 | 1.076297 | 1.105686 |
| C | 2.364015 | 1.106903 | -1.127375 |
| H | 1.875830 | -0.688369 | 2.226192 |
| H | 2.529515 | 1.620829 | -2.056833 |
| H | 1.288859 | 2.718101 | -0.258611 |
| N | 3.531748 | -0.813914 | -2.047127 |
| C | 4.726972 | -1.481904 | -1.910661 |
| O | 4.998836 | -2.407661 | -2.625028 |
| C | 5.720762 | -1.003317 | -0.892752 |
| C | 7.709417 | -0.236520 | 0.909743 |
| C | 6.546404 | -1.952367 | -0.304997 |
| C | 5.911127 | 0.337971 | -0.582870 |
| C | 6.902576 | 0.717392 | 0.301449 |
| C | 7.515541 | -1.577590 | 0.607685 |
| H | 6.421132 | -2.986756 | -0.562972 |
| H | 5.303587 | 1.092689 | -1.043663 |
| H | 7.061115 | 1.757654 | 0.520541 |
| H | 8.129912 | -2.324688 | 1.074886 |
| C | 0.805355 | 1.719964 | 2.288489 |
| O | 1.217510 | 1.505206 | 3.394934 |
| N | 8.679699 | 0.179766 | 1.865055 |
| H | -5.705051 | -1.022092 | -1.434826 |
| C | -6.043534 | -0.245190 | -0.773522 |
| C | -6.854849 | 1.752973 | 0.953015 |
| C | -5.721530 | 1.076518 | -1.053352 |

| | | | |
|---|---|---|---|
| C | -6.784016 | -0.562670 | 0.349322 |
| C | -7.199335 | 0.435436 | 1.222684 |
| C | -6.143625 | 2.076162 | -0.188377 |
| H | -7.015505 | -1.590699 | 0.550647 |
| H | -5.907173 | 3.102614 | -0.400662 |
| H | -7.150193 | 2.522563 | 1.640414 |
| N | -5.007723 | 1.383453 | -2.248793 |
| C | -3.916314 | 2.218802 | -2.276558 |
| O | -3.659866 | 2.868221 | -3.252823 |
| C | -3.001640 | 2.269038 | -1.086011 |
| C | -1.151838 | 2.459723 | 0.991819 |
| C | -2.692703 | 1.158016 | -0.315553 |
| C | -2.365693 | 3.476101 | -0.815485 |
| C | -1.458673 | 3.574436 | 0.220420 |
| C | -1.777505 | 1.252916 | 0.719370 |
| H | -3.157718 | 0.212309 | -0.515917 |
| H | -2.576950 | 4.328892 | -1.432167 |
| H | -0.969583 | 4.509333 | 0.426420 |
| H | -1.550181 | 0.386786 | 1.313085 |
| C | -7.921317 | 0.156944 | 2.510108 |
| O | -7.683035 | 0.817075 | 3.482886 |
| N | -0.237356 | 2.590955 | 2.077915 |
| H | 13.145071 | -2.677066 | -0.433507 |
| C | 12.380507 | -1.927229 | -0.499563 |
| C | 10.397642 | 0.000520 | -0.608106 |
| C | 12.117619 | -1.286123 | -1.711254 |
| C | 11.665678 | -1.590927 | 0.634035 |
| C | 10.651445 | -0.643191 | 0.602037 |
| C | 11.116552 | -0.306826 | -1.739352 |
| H | 11.894304 | -2.072261 | 1.566161 |
| H | 10.914392 | 0.215152 | -2.658513 |
| H | 9.643020 | 0.760808 | -0.668841 |
| N | 12.828822 | -1.557863 | -2.861674 |
| C | -12.026853 | -2.669693 | -1.773532 |
| O | -12.131182 | -3.817580 | -2.069504 |
| C | -11.192127 | -2.162732 | -0.653250 |
| C | -9.597447 | -1.305747 | 1.456713 |
| C | -11.101911 | -0.811361 | -0.351012 |
| C | -10.485378 | -3.085939 | 0.110005 |
| C | -9.691588 | -2.660658 | 1.155036 |
| C | -10.315887 | -0.386061 | 0.706005 |
| H | -11.650776 | -0.094306 | -0.929908 |
| H | -10.559802 | -4.129085 | -0.130584 |
| H | -9.134139 | -3.370949 | 1.737970 |
| H | -10.261664 | 0.659473 | 0.946687 |
| C | 9.971005 | -0.311524 | 1.888963 |
| O | 10.554246 | -0.426057 | 2.933575 |
| N | -8.806690 | -0.894804 | 2.567901 |
| C | 13.655870 | -2.733537 | -2.993522 |
| H | 13.119742 | -3.659114 | -2.789969 |
| H | 14.507949 | -2.678049 | -2.326520 |
| H | 14.035461 | -2.771968 | -4.006007 |
| C | -9.360689 | -1.184655 | 3.891126 |
| H | -9.827163 | -2.158408 | 3.867984 |
| H | -10.098887 | -0.444741 | 4.181083 |
| H | -8.566656 | -1.183188 | 4.620357 |
| C | -5.773392 | 1.297728 | -3.492048 |
| H | -5.096724 | 1.184633 | -4.323735 |
| H | -6.371242 | 2.188973 | -3.651061 |
| H | -6.427031 | 0.439428 | -3.439533 |
| C | -0.752286 | 3.266394 | 3.268886 |
| H | 0.072530 | 3.629539 | 3.860620 |
| H | -1.347568 | 2.595164 | 3.878657 |
| H | -1.367134 | 4.098326 | 2.957914 |
| C | 2.676423 | -1.264037 | -3.144502 |
| H | 2.206853 | -2.215137 | -2.915995 |
| H | 3.268611 | -1.379630 | -4.038045 |
| H | 1.908538 | -0.523680 | -3.314279 |

| | | | |
|---|---|---|---|
| C | 8.148622 | 0.612753 | 3.157163 |
| H | 7.908952 | -0.233636 | 3.792311 |
| H | 7.252170 | 1.191929 | 2.990406 |
| H | 8.881791 | 1.222156 | 3.660724 |
| H | 12.366629 | -1.282006 | -3.698252 |
| O | -12.663452 | -1.708439 | -2.435835 |
| H | -13.171585 | -2.118457 | -3.128928 |

**cyclic trimer**

| | | | |
|---|---|---|---|
| C | -2.293270 | -1.581596 | 1.186707 |
| C | -2.281822 | -0.471653 | -1.347171 |
| C | -2.831340 | -0.324063 | 0.978343 |
| C | -1.679965 | -2.258241 | 0.143098 |
| C | -1.700495 | -1.708146 | -1.130450 |
| C | -2.801133 | 0.250548 | -0.284631 |
| H | -3.262859 | 0.220075 | 1.799468 |
| H | -1.251841 | -2.236261 | -1.951412 |
| H | -2.298046 | -0.046151 | -2.333266 |
| C | -1.024342 | -3.584611 | 0.420840 |
| O | -1.637850 | -4.483135 | 0.922961 |
| N | 0.291788 | -3.718105 | 0.050814 |
| C | 1.167566 | -2.590135 | 0.005029 |
| C | 2.777610 | -0.322856 | -0.128709 |
| C | 1.899900 | -2.320129 | -1.142267 |
| C | 1.308070 | -1.763328 | 1.110058 |
| C | 2.087363 | -0.624105 | 1.035524 |
| C | 2.717110 | -1.204736 | -1.199568 |
| H | 1.811945 | -2.972389 | -1.992292 |
| H | 0.782333 | -1.993753 | 2.018300 |
| H | 2.152765 | 0.028457 | 1.885257 |
| H | 3.285913 | -0.997238 | -2.086903 |
| C | 3.612848 | 0.921147 | -0.256924 |
| N | 3.051458 | 2.102129 | 0.169831 |
| O | 4.728830 | 0.871242 | -0.691736 |
| C | 1.639571 | 2.313461 | 0.106289 |
| C | -1.130371 | 2.573084 | 0.018710 |
| C | 0.938091 | 2.708027 | 1.237016 |
| C | 0.957217 | 2.134397 | -1.087460 |
| C | -0.420028 | 2.242514 | -1.125190 |
| C | -0.437376 | 2.854461 | 1.188003 |
| H | 1.468329 | 2.873860 | 2.157479 |
| H | 1.500387 | 1.876705 | -1.978299 |
| H | -0.939418 | 2.068428 | -2.048302 |
| H | -0.978424 | 3.156156 | 2.065815 |
| C | -2.631625 | 2.666598 | 0.002176 |
| N | -3.314622 | 1.574368 | -0.484406 |
| O | -3.195139 | 3.659020 | 0.366065 |
| H | -2.321002 | -2.025319 | 2.164921 |
| C | 3.897888 | 3.290050 | 0.107346 |
| H | 4.882554 | 3.048463 | 0.474616 |
| H | 3.460291 | 4.060343 | 0.726469 |
| H | 3.988404 | 3.662650 | -0.908019 |
| C | 0.906620 | -5.024391 | 0.269054 |
| H | 1.155475 | -5.177328 | 1.314261 |
| H | 1.810695 | -5.085938 | -0.319832 |
| H | 0.222191 | -5.798525 | -0.039200 |
| C | -4.765950 | 1.697105 | -0.575804 |
| H | -5.136213 | 0.914157 | -1.223197 |
| H | -5.017296 | 2.659143 | -0.993734 |
| H | -5.243110 | 1.608551 | 0.395099 |

**cyclic tetramer:**

| | | | |
|---|---|---|---|
| C | 4.300654 | 1.225850 | 1.031553 |
| O | 5.197678 | 1.199947 | 1.828917 |
| C | 3.627017 | -0.060465 | 0.643751 |
| C | 2.728122 | -2.611315 | -0.040111 |
| C | 3.095834 | -0.305897 | -0.613978 |
| C | 3.691401 | -1.104643 | 1.562771 |
| C | 3.235750 | -2.362908 | 1.230226 |
| C | 2.656438 | -1.575300 | -0.957377 |
| H | 3.057709 | 0.472485 | -1.350109 |
| H | 4.124150 | -0.923070 | 2.527400 |
| H | 3.292387 | -3.167429 | 1.941010 |
| H | 2.286591 | -1.763304 | -1.948927 |
| N | 2.399053 | -3.950517 | -0.405596 |
| H | 1.763304 | 2.286591 | 1.948927 |
| C | 1.575300 | 2.656438 | 0.957377 |
| C | 1.104643 | 3.691401 | -1.562771 |
| C | 2.611315 | 2.728122 | 0.040111 |
| C | 0.305897 | 3.095834 | 0.613978 |
| C | 0.060465 | 3.627017 | -0.643751 |
| C | 2.362908 | 3.235750 | -1.230226 |
| H | -0.472485 | 3.057709 | 1.350109 |
| H | 3.167429 | 3.292387 | -1.941010 |
| H | 0.923070 | 4.124150 | -2.527400 |
| N | 3.950517 | 2.399053 | 0.405596 |
| C | -1.225850 | 4.300654 | -1.031553 |
| O | -1.199947 | 5.197678 | -1.828917 |
| H | -3.167429 | -3.292387 | -1.941010 |
| C | -2.362908 | -3.235750 | -1.230226 |
| C | -0.305897 | -3.095834 | 0.613978 |
| C | -2.611315 | -2.728122 | 0.040111 |
| C | -1.104643 | -3.691401 | -1.562771 |
| C | -0.060465 | -3.627017 | -0.643751 |
| C | -1.575300 | -2.656438 | 0.957377 |
| H | -0.923070 | -4.124150 | -2.527400 |
| H | -1.763304 | -2.286591 | 1.948927 |
| H | 0.472485 | -3.057709 | 1.350109 |
| N | -3.950517 | -2.399053 | 0.405596 |
| C | -4.300654 | -1.225850 | 1.031553 |
| O | -5.197678 | -1.199947 | 1.828917 |
| C | -3.627017 | 0.060465 | 0.643751 |
| C | -2.728122 | 2.611315 | -0.040111 |
| C | -3.095834 | 0.305897 | -0.613978 |
| C | -3.691401 | 1.104643 | 1.562771 |
| C | -3.235750 | 2.362908 | 1.230226 |
| C | -2.656438 | 1.575300 | -0.957377 |
| H | -3.057709 | -0.472485 | -1.350109 |
| H | -4.124150 | 0.923070 | 2.527400 |
| H | -3.292387 | 3.167429 | 1.941010 |
| H | -2.286591 | 1.763304 | -1.948927 |
| C | 1.225850 | -4.300654 | -1.031553 |
| O | 1.199947 | -5.197678 | -1.828917 |
| N | -2.399053 | 3.950517 | -0.405596 |
| C | -4.802083 | -3.549587 | 0.714233 |
| H | -4.609578 | -3.929924 | 1.711750 |
| H | -4.602773 | -4.329695 | -0.005611 |
| H | -5.837764 | -3.256796 | 0.650898 |
| C | -3.549587 | 4.802083 | -0.714233 |
| H | -4.329695 | 4.602773 | 0.005611 |
| H | -3.929924 | 4.609578 | -1.711750 |
| H | -3.256796 | 5.837764 | -0.650898 |
| C | 4.802083 | 3.549587 | 0.714233 |
| H | 5.837764 | 3.256796 | 0.650898 |
| H | 4.609578 | 3.929924 | 1.711750 |
| H | 4.602773 | 4.329695 | -0.005611 |
| C | 3.549587 | -4.802083 | -0.714233 |

| | | | |
|---|---|---|---|
| H | 4.329695 | -4.602773 | 0.005611 |
| H | 3.929924 | -4.609578 | -1.711750 |
| H | 3.256796 | -5.837764 | -0.650898 |

**cyclic pentamer:**

| | | | |
|---|---|---|---|
| H | 1.549809 | -5.611873 | -1.667916 |
| C | 0.999324 | -4.773312 | -1.281849 |
| C | -0.381058 | -2.619128 | -0.234022 |
| C | 1.345196 | -3.484748 | -1.672048 |
| C | -0.007732 | -4.975302 | -0.361809 |
| C | -0.694230 | -3.900845 | 0.203255 |
| C | 0.611963 | -2.416450 | -1.180747 |
| H | -0.239133 | -5.967098 | -0.029063 |
| H | 0.849513 | -1.419527 | -1.501325 |
| H | -0.884278 | -1.761652 | 0.162672 |
| N | 2.442619 | -3.296839 | -2.555773 |
| C | 3.582003 | -2.582945 | -2.291304 |
| O | 4.414756 | -2.450636 | -3.147859 |
| C | 3.785155 | -1.917568 | -0.954648 |
| C | 4.075036 | -0.420486 | 1.383038 |
| C | 3.404513 | -2.447109 | 0.272918 |
| C | 4.422792 | -0.682192 | -0.975975 |
| C | 4.577776 | 0.057629 | 0.182334 |
| C | 3.541360 | -1.702127 | 1.429354 |
| H | 2.968485 | -3.424036 | 0.339870 |
| H | 4.782343 | -0.298709 | -1.911248 |
| H | 5.043659 | 1.024233 | 0.146821 |
| H | 3.192409 | -2.101404 | 2.364135 |
| C | -1.605610 | -4.258270 | 1.352479 |
| O | -1.553731 | -5.374912 | 1.795050 |
| N | 4.088924 | 0.372943 | 2.562313 |
| H | -4.098987 | -3.387176 | -0.094800 |
| C | -3.945484 | -2.403050 | 0.309468 |
| C | -3.589951 | 0.124025 | 1.390399 |
| C | -3.041369 | -2.216575 | 1.345546 |
| C | -4.686697 | -1.333626 | -0.163095 |
| C | -4.519730 | -0.064602 | 0.375365 |
| C | -2.861139 | -0.945580 | 1.875386 |
| H | -5.426689 | -1.486656 | -0.925594 |
| H | -2.164881 | -0.807342 | 2.682497 |
| H | -3.457881 | 1.094660 | 1.827670 |
| N | -2.394059 | -3.321526 | 1.974299 |
| C | -5.475950 | 1.017272 | -0.038326 |
| O | -6.613630 | 0.742481 | -0.295115 |
| H | 2.294480 | 5.363031 | 0.414814 |
| C | 2.194367 | 4.294894 | 0.471190 |
| C | 1.900554 | 1.558263 | 0.665451 |
| C | 1.483730 | 3.616522 | -0.513524 |
| C | 2.793849 | 3.603715 | 1.504872 |
| C | 2.693049 | 2.218696 | 1.594158 |
| C | 1.317506 | 2.244040 | -0.386861 |
| H | 3.353635 | 4.133794 | 2.250961 |
| H | 0.756354 | 1.698482 | -1.121435 |
| H | 1.754405 | 0.498000 | 0.725355 |
| N | 1.026316 | 4.335700 | -1.653796 |
| C | -0.117665 | 4.024386 | -2.352741 |
| O | -0.181363 | 4.216980 | -3.535482 |
| C | -1.330077 | 3.509241 | -1.632342 |
| C | -3.750395 | 2.669463 | -0.541089 |
| C | -1.709518 | 3.929583 | -0.364095 |
| C | -2.170370 | 2.665650 | -2.347451 |
| C | -3.367188 | 2.240875 | -1.804326 |
| C | -2.915774 | 3.516485 | 0.174829 |
| H | -1.078966 | 4.591800 | 0.198709 |
| H | -1.893639 | 2.370832 | -3.341424 |
| H | -4.019196 | 1.602893 | -2.373196 |

| | | | |
|---|---|---|---|
| H | -3.218591 | 3.856968 | 1.148389 |
| C | 3.456296 | 1.576223 | 2.725580 |
| O | 3.545571 | 2.160093 | 3.773324 |
| N | -5.034720 | 2.324135 | -0.018948 |
| C | 2.065577 | 4.979748 | -2.464390 |
| H | 2.835130 | 5.364005 | -1.814652 |
| H | 1.631407 | 5.792170 | -3.024330 |
| H | 2.507422 | 4.277368 | -3.162111 |
| C | -6.069466 | 3.339137 | -0.219838 |
| H | -6.398232 | 3.377235 | -1.253014 |
| H | -5.665755 | 4.302062 | 0.058489 |
| H | -6.918566 | 3.111743 | 0.404969 |
| C | -3.059910 | -3.789471 | 3.194014 |
| H | -3.875879 | -4.466185 | 2.965356 |
| H | -3.449510 | -2.931483 | 3.721371 |
| H | -2.349637 | -4.306017 | 3.819118 |
| C | 2.382768 | -3.922328 | -3.877958 |
| H | 2.513190 | -3.175415 | -4.647949 |
| H | 1.417129 | -4.390092 | -3.994430 |
| H | 3.161219 | -4.665382 | -3.992395 |
| C | 4.776338 | -0.149265 | 3.743533 |
| H | 5.345548 | -1.019154 | 3.452989 |
| H | 4.072894 | -0.420637 | 4.521122 |
| H | 5.445126 | 0.599887 | 4.140435 |

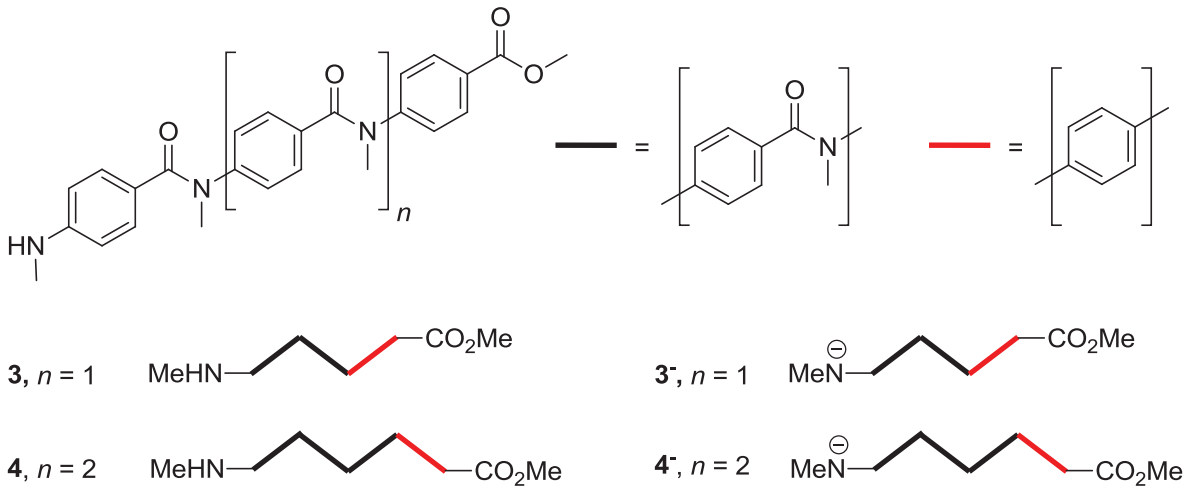
**cyclic hexamer:**

| | | | |
|---|---|---|---|
| H | 5.313835 | -0.930108 | 1.805587 |
| C | 4.766240 | -0.012691 | 1.699110 |
| C | 3.387081 | 2.377739 | 1.450421 |
| C | 5.088356 | 0.862091 | 0.675344 |
| C | 3.737276 | 0.291350 | 2.570358 |
| C | 3.018448 | 1.475316 | 2.440430 |
| C | 4.410464 | 2.068707 | 0.572144 |
| H | 3.483261 | -0.384711 | 3.362831 |
| H | 4.680729 | 2.766776 | -0.199746 |
| H | 2.885798 | 3.319606 | 1.349167 |
| N | 6.145057 | 0.558401 | -0.244980 |
| C | 5.839678 | 0.231266 | -1.548564 |
| O | 6.510160 | 0.601116 | -2.469149 |
| C | 4.668916 | -0.683050 | -1.782371 |
| C | 2.633927 | -2.479510 | -2.432056 |
| C | 3.743882 | -0.370184 | -2.770172 |
| C | 4.567341 | -1.900458 | -1.127458 |
| C | 3.573058 | -2.803849 | -1.464936 |
| C | 2.719517 | -1.246834 | -3.071526 |
| H | 3.829602 | 0.559242 | -3.302013 |
| H | 5.292186 | -2.170471 | -0.383046 |
| H | 3.538544 | -3.763555 | -0.983239 |
| H | 1.994581 | -0.990378 | -3.822632 |
| C | 1.922325 | 1.692836 | 3.450584 |
| O | 2.009958 | 1.159037 | 4.524881 |
| N | 1.640583 | -3.413186 | -2.851586 |
| H | -3.538544 | 3.763555 | -0.983239 |
| C | -3.573058 | 2.803849 | -1.464936 |
| C | -3.743882 | 0.370184 | -2.770172 |
| C | -2.633927 | 2.479510 | -2.432056 |
| C | -4.567341 | 1.900458 | -1.127458 |
| C | -4.668916 | 0.683050 | -1.782371 |
| C | -2.719517 | 1.246834 | -3.071526 |
| H | -5.292186 | 2.170471 | -0.383046 |
| H | -1.994581 | 0.990378 | -3.822632 |
| H | -3.829602 | -0.559242 | -3.302013 |
| N | -1.640583 | 3.413186 | -2.851586 |
| C | -0.921417 | 4.202637 | -1.984974 |
| O | -0.544047 | 5.292711 | -2.317393 |

| | | | |
|---|---|---|---|
| C | -0.534071 | 3.674534 | -0.632689 |
| C | 0.401524 | 2.877448 | 1.877271 |
| C | -0.230122 | 2.344636 | -0.384055 |
| C | -0.353729 | 4.605151 | 0.385877 |
| C | 0.099146 | 4.212167 | 1.629587 |
| C | 0.231303 | 1.950494 | 0.860742 |
| H | -0.339987 | 1.609627 | -1.158289 |
| H | -0.549859 | 5.641202 | 0.186742 |
| H | 0.242219 | 4.940730 | 2.406522 |
| H | 0.488839 | 0.925539 | 1.035132 |
| C | -5.839678 | -0.231266 | -1.548564 |
| O | -6.510160 | -0.601116 | -2.469149 |
| N | 0.845571 | 2.494210 | 3.173845 |
| H | -0.242219 | -4.940730 | 2.406522 |
| C | -0.099146 | -4.212167 | 1.629587 |
| C | 0.230122 | -2.344636 | -0.384055 |
| C | -0.401524 | -2.877448 | 1.877271 |
| C | 0.353729 | -4.605151 | 0.385877 |
| C | 0.534071 | -3.674534 | -0.632689 |
| C | -0.231303 | -1.950494 | 0.860742 |
| H | 0.549859 | -5.641202 | 0.186742 |
| H | -0.488839 | -0.925539 | 1.035132 |
| H | 0.339987 | -1.609627 | -1.158289 |
| N | -0.845571 | -2.494210 | 3.173845 |
| C | -1.922325 | -1.692836 | 3.450584 |
| O | -2.009958 | -1.159037 | 4.524881 |
| C | -3.018448 | -1.475316 | 2.440430 |
| C | -5.088356 | -0.862091 | 0.675344 |
| C | -3.387081 | -2.377739 | 1.450421 |
| C | -3.737276 | -0.291350 | 2.570358 |
| C | -4.766240 | 0.012691 | 1.699110 |
| C | -4.410464 | -2.068707 | 0.572144 |
| H | -2.885798 | -3.319606 | 1.349167 |
| H | -3.483261 | 0.384711 | 3.362831 |
| H | -5.313835 | 0.930108 | 1.805587 |
| H | -4.680729 | -2.766776 | -0.199746 |
| C | 0.921417 | -4.202637 | -1.984974 |
| O | 0.544047 | -5.292711 | -2.317393 |
| N | -6.145057 | -0.558401 | -0.244980 |
| C | 0.117332 | -2.632444 | 4.272888 |
| H | 0.609831 | -1.688980 | 4.475479 |
| H | 0.855234 | -3.369339 | 3.995550 |
| H | -0.391822 | -2.951918 | 5.168913 |
| C | -7.385494 | -1.302767 | -0.043887 |
| H | -7.628313 | -1.281260 | 1.009500 |
| H | -7.302101 | -2.334562 | -0.369002 |
| H | -8.177689 | -0.831733 | -0.604778 |
| C | -1.830997 | 3.981840 | -4.188389 |
| H | -2.538469 | 4.803492 | -4.169278 |
| H | -2.203557 | 3.211350 | -4.845907 |
| H | -0.888224 | 4.348667 | -4.561331 |
| C | -0.117332 | 2.632444 | 4.272888 |
| H | 0.391822 | 2.951918 | 5.168913 |
| H | -0.609831 | 1.688980 | 4.475479 |
| H | -0.855234 | 3.369339 | 3.995550 |
| C | 7.385494 | 1.302767 | -0.043887 |
| H | 7.302101 | 2.334562 | -0.369002 |
| H | 8.177689 | 0.831733 | -0.604778 |
| H | 7.628313 | 1.281260 | 1.009500 |
| C | 1.830997 | -3.981840 | -4.188389 |
| H | 2.203557 | -3.211350 | -4.845907 |
| H | 0.888224 | -4.348667 | -4.561331 |
| H | 2.538469 | -4.803492 | -4.169278 |

## Conformational analysis of 3, $3^-$, 4 and $4^-$

The conformational search of **3** and **4** (see Scheme SI1), where the presence of the hydrogen atom on the terminal nitrogen atom mimics a presence of a metal counterion, resulted in two libraries of conformers, from which 10 and 25 lowest-energy conformers, respectively, were selected, and their geometries were refined by M06-2X/6-31G(d) calculations. Inspection of the library of obtained conformers indicated that this approach failed to predict two low energy conformers of **3** (see below), and these were additionally included to the selection. Then, we also optimized the structures of conjugate bases of $\mathbf{3}^-$ and $\mathbf{4}^-$ which result after deprotonation of the amide group in **3** and **4** using the same level of theory. The energies and the corresponding equilibrium distributions (see Quantum Chemical Calculations description above) of conformers of **3** and **4**, and their conjugate bases $\mathbf{3}^-$ and $\mathbf{4}^-$, are collected in Tables SI3–SI6, respectively. A representative sample of the lowest energy conformers is shown in Figures SI22 and SI23.




**Scheme SI1**. The model structures used in calculations of distribution of conformers and the cyclization reactions and their cartoons.

*Table SI3.* Calculated relative energies of the conformers **3a-l** and **3**$^{-}$**a-l** and their distributions in solution.

| Conformer | Conformers of **3** | | Conformers of **3**$^{-}$ | |
|---|---|---|---|---|
| | Δ*E* (0K, kcal mol$^{-1}$) | Boltzmann distribution[a] (%) | Δ*E* (0K, kcal mol$^{-1}$) | Boltzmann distribution[a] (%) |
| **a** | 0.0 | 84.4 | 0.0 | 40.5 |
| **b** | 1.6 | 6.1 | 0.1 | 34.1 |
| **c** | 3.2 | 0.4 | 1.0 | 8.0 |
| **d** | 2.7 | 0.8 | 1.5 | 3.4 |
| **e** | 1.9 | 3.7 | –[b] | –[b] |
| **f** | 2.1 | 2.6 | 1.2 | 4.9 |
| **g** | 3.4 | 0.3 | 3.3 | 0.2 |
| **h** | 2.7 | 0.9 | 3.2 | 0.2 |
| **i** | 3.0 | 0.5 | 3.7 | 0.1 |
| **j** | 3.4 | 0.3 | 3.2 | 0.2 |
| **k** | 4.7 | 0 | 2.7 | 0.5 |
| **l** | 5.0 | 0 | 3.9 | 0.1 |

[a] Boltzmann distributions at 298.15 K were estimated using the calculated energies at 0 K, *i.e.* the effects of entropy and heat capacities were neglected and considered of equal importance for all the conformers; see the Quantum Chemical Calculations description above. [b] Deprotonation of conformers **3c** and **3e** results in a single indistinguishable conformer **3**$^{-}$**c**.

*Table SI4.* Calculated relative energies[a] of the conformers **3a-l** with various density functionals.

| Conformer | M06-2X | M06L | B97D |
|---|---|---|---|
| **a** | 0.0 | 0.0 | 0.0 |
| **b** | 1.6 | 2.1 | 0.8 |
| **c** | 3.2 | 3.4 | 3.3 |
| **d** | 2.7 | 3.1 | 2.5 |
| **e** | 1.9 | 3.0 | 2.5 |
| **f** | 2.1 | 2.4 | 2.3 |
| **g** | 3.4 | 4.1 | 4.2 |
| **h** | 2.7 | 3.4 | 3.5 |
| **i** | 3.0 | 3.8 | 3.8 |
| **j** | 3.4 | 4.1 | 4.2 |
| **k** | 4.7 | 5.4 | 6.5 |
| **l** | 5.0 | 5.6 | 6.7 |

[a] The calculated energies with respective density functional and 6-311+G(2d,p) basis set on M06-2X/6-31G(d) gas phase geometries at 0 K in kcal mol$^{-1}$ (see the Quantum Chemical Calculations description above).

*Table SI5.* Calculated relative energies of the conformers **4a-l** and **4**$^{-}$**a-l** and their distributions in solution.

| Conformer | Conformers of **4** | | Conformers of **4**$^{-}$ | |
|---|---|---|---|---|
| | Δ*E* (0K, kcal mol$^{-1}$) | Boltzmann distribution[a] (%) | Δ*E* (0K, kcal mol$^{-1}$) | Boltzmann distribution[a] (%) |
| **a** | 0.0 | 94.6 | 0.0 | 99.1 |
| **b** | 1.9 | 4.1 | 3.2 | 0.5 |
| **c** | 2.6 | 1.2 | 5.2 | 0.0 |
| **d** | 7.0 | 0.0 | 4.6 | 0.0 |
| **e** | 5.3 | 0.0 | 4.3 | 0.1 |
| **f** | 4.2 | 0.1 | 5.2 | 0.0 |
| **g** | 6.6 | 0.0 | 4.2 | 0.1 |
| **h** | 5.3 | 0.0 | 5.1 | 0.0 |
| **i** | 4.6 | 0.0 | 5.2 | 0.0 |
| **j** | 6.8 | 0.0 | 4.0 | 0.1 |
| **k** | 7.0 | 0.0 | 4.6 | 0.0 |
| **l** | 6.8 | 0.0 | 5.2 | 0.0 |

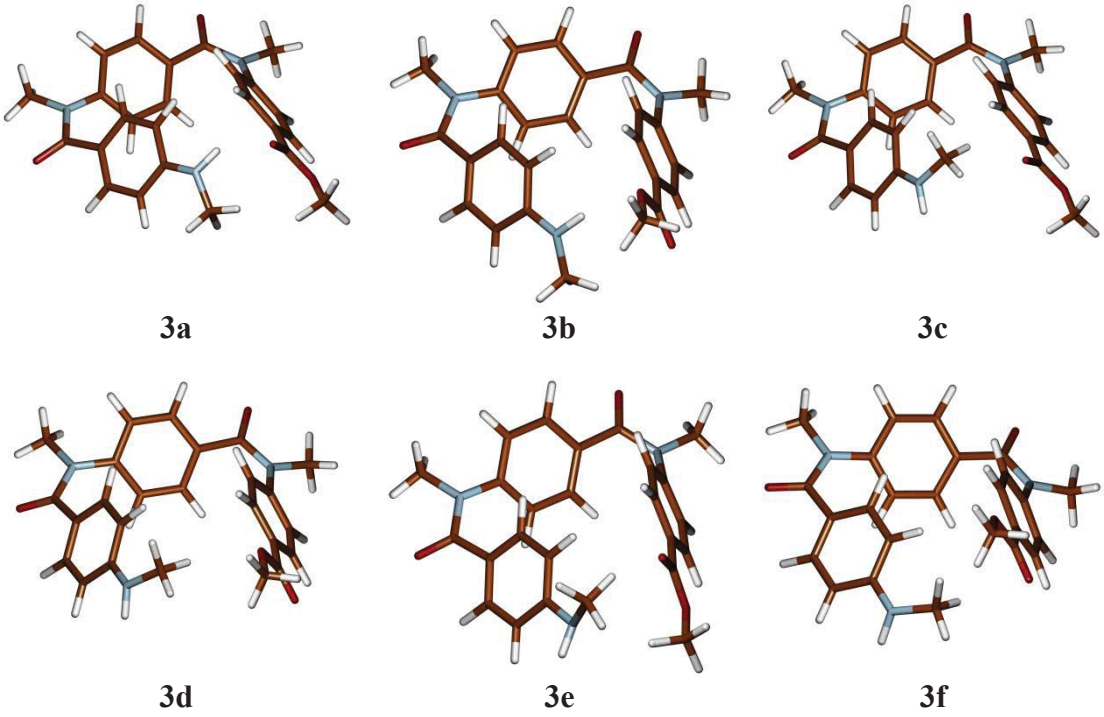
[a] Boltzmann distributions at 298.15 K were estimated using the calculated energies at 0 K, *i.e.* the effects of entropy and heat capacities were neglected and considered of equal importance for all the conformers; see the Quantum Chemical Calculations description above.

*Table SI6.* Calculated relative energies[a] of the conformers **4a-l** with various density functionals.

| Conformer | M06-2X | M06L | B97D |
|---|---|---|---|
| **a** | 0.0 | 0.0 | 0.0 |
| **b** | 1.9 | 1.4 | 3.1 |
| **c** | 2.6 | 1.0 | 3.4 |
| **d** | 7.0 | 7.0 | 10.3 |
| **e** | 5.3 | 4.5 | 7.9 |
| **f** | 4.2 | 3.7 | 5.6 |
| **g** | 6.6 | 6.1 | 8.4 |
| **h** | 5.3 | 6.0 | 7.6 |
| **i** | 4.6 | 3.9 | 5.9 |
| **j** | 6.8 | 6.3 | 8.6 |
| **k** | 7.0 | 7.0 | 10.3 |
| **l** | 6.8 | 6.8 | 10.1 |

[a] The calculated energies with respective density functional and 6-311+G(2d,p) basis set on M06-2X/6-31G(d) gas phase geometries at 0 K in kcal mol$^{-1}$ (see the Quantum Chemical Calculations description above).

*Neutral amides **3a-f***




*Conjugate bases **3⁻a-f***

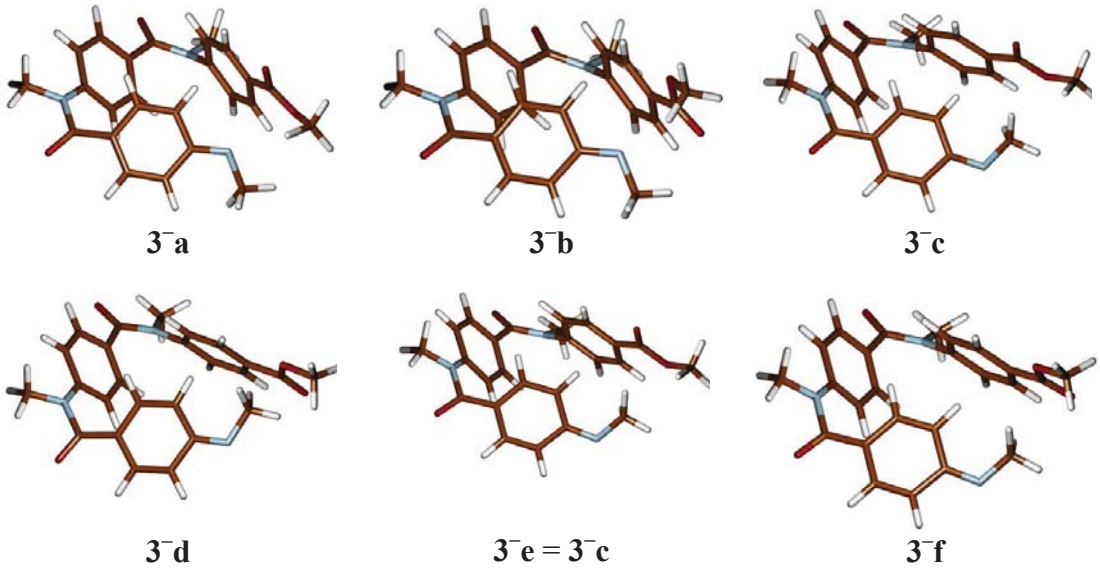
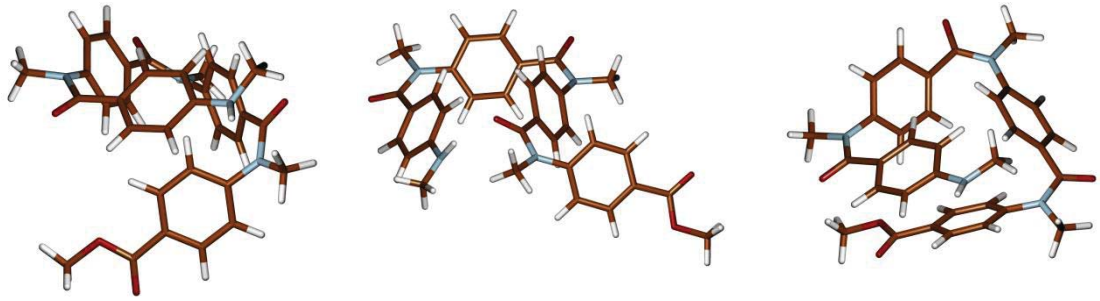


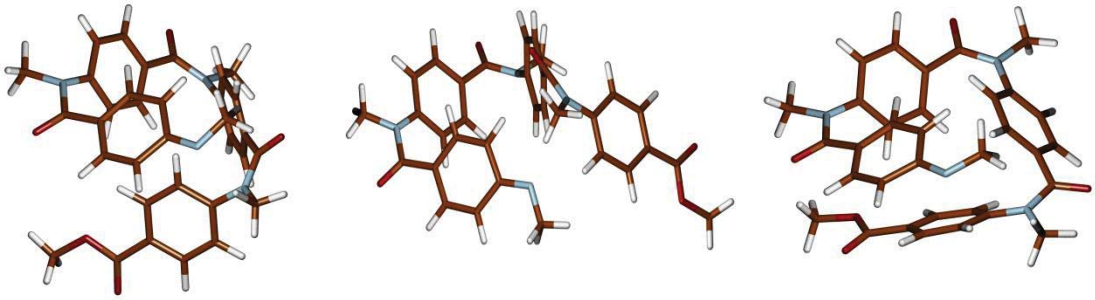

**Figure SI22.** Structures of the lowest energy conformers of neutral amides **3a-f** and their conjugate bases **3⁻a-f**.

*Neutral amides **4a-c***



**4a** **4b** **4c**

*Conjugate bases **4⁻a-c***

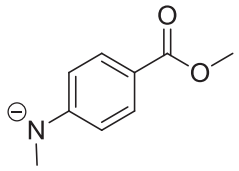


**4⁻a** **4⁻b** **4⁻c**

**Figure SI23.** Structures of the lowest energy conformers of neutral amides **4a-c** and their conjugate bases **4⁻a-c**.

## Solvation and Coordination of $Li^+$

The relative energies of coordination of a $Li^+$ counterion to the deprotonated nitrogen or the ester carbonyl oxygen atoms in the conjugate base of methyl *N*-methyl-4-aminobenzoate **8**$^-$ (Figure SI24) were computed. From the two coordination sites in the conjugate base of methyl *N*-methyl-4-aminobenzoate, the $Li^+$ ion prefers to be coordinated to the deprotonated nitrogen atom. The coordination to the ester oxygen atom is disfavored by 7.3 kcal mol$^{-1}$. The NBO (natural bond orbital) analysis suggests that $Li^+$ ion interaction with the amide nitrogen atom possesses little covalent character, but it is predominantly ionic.



**8**$^-$

**Figure SI24.** The structure of conjugate base of methyl *N*-methyl-4-aminobenzoate **8**$^-$.

We estimated the change in energy that accompanies desolvation of a $Li^+$ from its cluster with the THF solvent molecules, and its coordination to the nitrogen atom in **8**$^-$. We were, however, not able to converge the geometry optimization of a $Li^+\cdot(THF)_4$ cluster. Since only a single THF molecule is substituted by **8**$^-$, we estimated the corresponding energy via substitution of a THF molecule consecutively from a series of smaller $Li^+\cdot(THF)_x$ clusters, where x = 1–3. The results are summarized in Table SI7. The energy change corresponding to an energy change with a $Li^+\cdot(THF)_4$ cluster would thus be ca –16 kcal mol$^{-1}$.

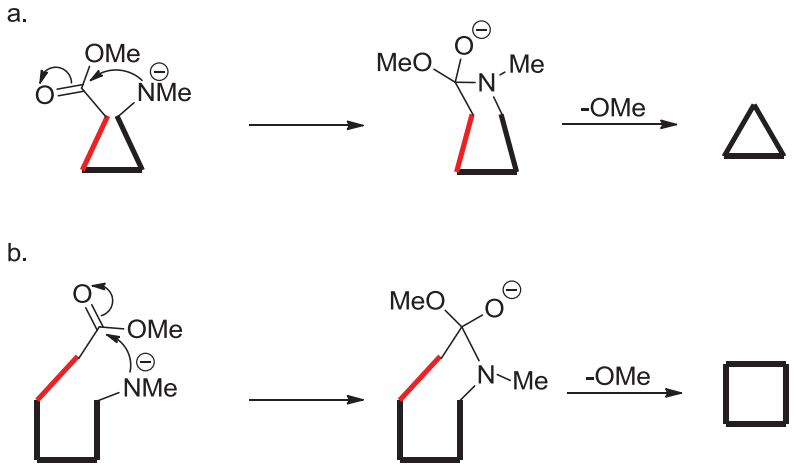
*Table SI7.*

| Reaction | $\Delta E$ (0K, kcal mol$^{-1}$)[a] |
|---|---|
| $Li^+\cdot(THF)_1 + \mathbf{3}^- \rightarrow Li^+\cdot\mathbf{3}^- + THF$ | –18.0 |
| $Li^+\cdot(THF)_2 + \mathbf{3}^- \rightarrow Li^+\cdot(THF)_1\cdot\mathbf{3}^- + THF$ | –17.5 |
| $Li^+\cdot(THF)_3 + \mathbf{3}^- \rightarrow Li^+\cdot(THF)_2\cdot\mathbf{3}^- + THF$ | –16.7 |

[a] M06-2X/6-311+G(2d,p)/PCM energies on M06-2X/6-31G(d)/PCM optimized geometries with non-scaled ZPVE corrections included; see the description of Quantum Chemical Calculations above for more details.

## Cyclization of the 3-membered oligomers in the absence of a $Li^+$ ion

The feasibility of the intramolecular nucleophilic attack of the deprotonated terminal *N*-methyl amino group on the ester group to form a tetrahedral intermediate (Scheme SI2), which, upon cleavage of the alkoxy group, results in the formation of the final cyclized product, has been first investigated in the absence of a lithium counter ion.
We located all four diastereomeric transition states, for which the subsequent IRC reaction path calculations provided the four reactants that appeared to correspond to the lowest-energy conformers **3**$^-$**a-f**. Energies of these transition states, the corresponding reactants and the tetrahedral intermediates are summarized in Table SI8. We repeated the calculations only for two diastereomeric transition states (out of four possible) for the cyclization producing a tetramer. The energies of the corresponding reactants **4**$^-$**m,n** found by IRC calculations from the located transition states, however, are 8.0 and 8.6 kcal mol$^{-1}$ higher in energy than the most stable conformer **4**$^-$**a** (Table SI8).




**Scheme SI2.**

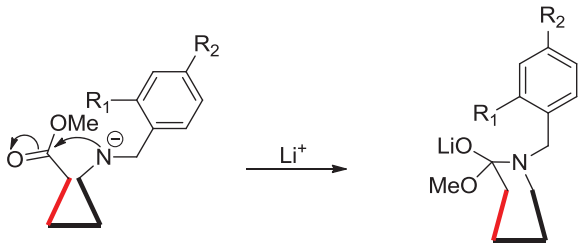
*Table SI8.* Energies of model chain-growth and cyclization reactions.[a]

| Reactant | Conformer | Reactant | TS | Tetrahedral Intermediate |
|---|---|---|---|---|
| Trimer[b] | **3**$^-$**a** | 0.4 | 6.9 | 5.3 |
| | **3**$^-$**b** | 0.0 | 5.1 | 1.8 |
| | **3**$^-$**c** | 0.1 | 11 | 9.3 |
| | **3**$^-$**d** | 2.2 | 9.4 | 6.3 |
| Tetramer[c] | **4**$^-$**m** | 0.0 (8.0[d]) | 5.8 | 0.8 |
| | **4**$^-$**n** | 0.6 (8.6[d]) | 4.2 | –1.0 |

[a] Energies in kcal mol$^{-1}$ computed at the M06-2X/6-311+G(2d,p)/PCM level of theory on M06-2X/6-31G(d)/PCM geometries; unscaled ZPVEs included (0K). [b] Energies relative to conformer **3**$^-$**b**; note that reoptimization of the conformers **3**$^-$**a-d** with a finer integration grid slightly affected their relative energies (compare with Table SI3). [c] Energies relative to conformer **4**$^-$**m**. [d] The number in parentheses is the energy of the corresponding conformer relative to **4**$^-$**a**.

## Cyclization of the 3-membered oligomers in the presence of a $Li^+$ ion and the necessity for an o-alkoxy coordinating group

In order to explain the requirement for an *o*-alkoxy group on the *N*-benzyl group (**5**, see Scheme SI3) when the $Li^+$ is present in the solution, we searched for the corresponding transition states with a simple *N*-benzyl protecting group, and a *N*-benzyl group that bears an *ortho* or a *para* methoxy group.




**5** **6**

**a,** $R_1$ = H, $R_2$ = H
**b**, $R_1$ = H, $R_2$ = OMe
**c**, $R_1$ = OMe, $R_2$ = H

**Scheme SI3**.

We focused on the case where the $Li^+$ ion is coordinated by both the carbonyl oxygen in the ester group and the amidic nitrogen atom as suggested by our calculations of solvation energies (see Table SI7 above). However, we first probed the effect of such coordination by considering two diastereomeric transition states only with a *N*-methyl group on the nucleophilic nitrogen, where the relative orientation of the *N*-methyl and the MeO group of the ester is such as was previously found for **3**$^-$**b** and **3**$^-$**d**, respectively (see Table SI8). We found that the barrier for the transition state which displayed the most favourite conformation for the cyclization in the absence of lithium (**3**$^-$**b**, see Table SI8) is now 20.5 kcal $mol^{-1}$, *i.e.* its energy is much higher than that of the corresponding transition state in the absence of $Li^+$. To our surprise, the energy of the diastereomeric transition state derived from that of cyclization of **3**$^-$**d** by adding a $Li^+$ has changed only slighly to 10.0 kcal $mol^{-1}$. The structures of these transition states and the corresponding minima from which these transition states are reached are summarized in Figure SI25. The energies of the two reactive conformations reached by IRC calculations are essentially identical.

We performed additional calculations to understand such behavior. Lithium ions were removed from the geometries obtained from both the transition state and the corresponding local energy minima geometry optimizations, and single point energy

calculations followed. We found that the high energy barrier of 21.0 kcal $mol^{-1}$ (no ZPVE included) previously found for the cyclization of $\mathbf{3^{-}b \cdot Li^{+}}$ decreased significantly to 11.8 kcal $mol^{-1}$ (no ZPVE included), whereas the barrier previously found for $\mathbf{3^{-}d \cdot Li^{+}}$ (9.6 kcal $mol^{-1}$; no ZPVE) decreased only slightly to 6.7 kcal $mol^{-1}$ (no ZPVE included). This suggests that the presence of $Li^{+}$ preferentially stabilizes the energy minimum from which the transition state is reached (the reactant) in the case of $\mathbf{3^{-}b \cdot Li^{+}}$, while its presence affects the relative energies of the reactant and the transition state to similar extents. In fact, a closer inspection of the optimized transition state geometries reveals that the distance of the *N*-alkyl and the ester alkoxy groups in the $\mathbf{3^{-}d \cdot Li^{+}}$ transition state is slightly longer by only 0.04 Å when compared to the transition state geometry in the absence of $Li^{+}$, while this distance diminishes from 3.884 Å to 3.285 Å in the case of $\mathbf{3^{-}b}$ transition states when the $Li^{+}$ is added.

Substitution of the *N*-methyl group for a simple *N*-benzyl group and that which bears an *ortho* or a *para* methoxy group was thus probed only for the lowest of the diastereomeric transition states (test calculations showed that energies of the other diastereomeric transition states remain high by this substitution and are in the range of ca 16-19 kcal $mol^{-1}$). The calculated energies and the structures of the transition states are summarized in Table SI9 and Figure SI26, respectively.

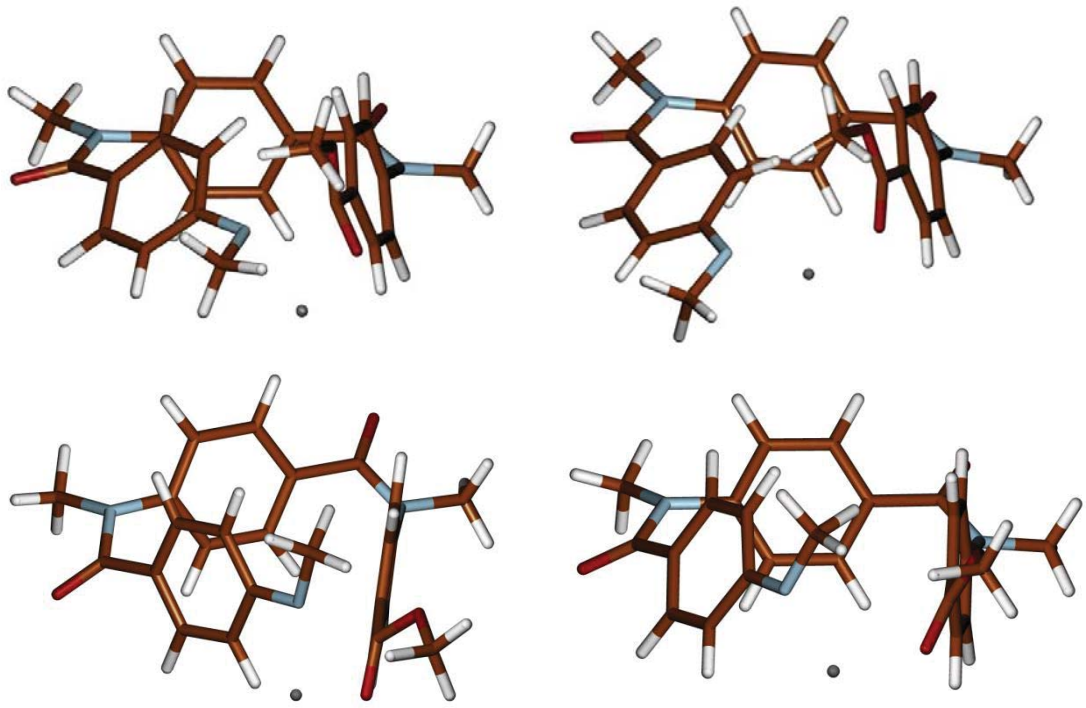
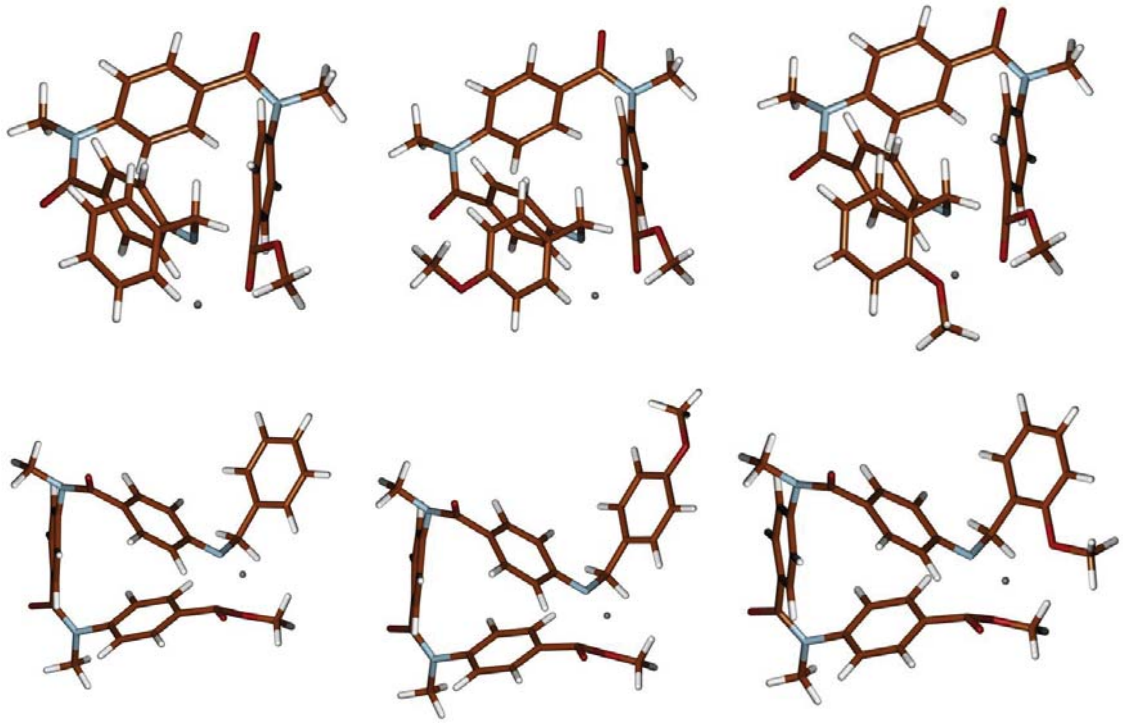


**Figure SI25.** The transition states (left) for cyclization of $\mathbf{3^{-}b}$ and $\mathbf{3^{-}d}$ with a $Li^{+}$ ion coordinated in between the amino nitrogen and the ester carbonyl oxygen atoms and the corresponding energy minima (right) from which these transition states are reached.

*Table SI9.* Energies calculated for the cyclization of **5** with the $Li^+$ ion fully coordinated in the reaction center.

| Compound | Coordination | **6**, $\Delta E$ (0K, kcal mol$^{-1}$)[a] | **5** → **6**, $\Delta E$ (0K, kcal mol$^{-1}$)[a] |
|---|---|---|---|
| **5a** | O···Li···N | 9.9 | 12.4 |
| **5b** | O···Li···N | 9.0 | 11.6 |
| **5c** | O···Li···N | 5.9 | 9.0 |

[a] M06-2X/6-311+G(2d,p)/PCM energies on M06-2X/6-31G(d)/PCM optimized geometries with non-scaled ZPVE corrections included; see Experimental section for more details.



**5a→6a** **5b→6b** **5c→6c**

**Figure SI26.** Transition states **5a-c→6a-c** with the $Li^+$ counterion coordinated between the nitrogen and the carbonyl oxygen atoms; side-view (top) and bottom view (bottom).

## Cartesian Coordinates

**3a** (M06-2X/6-31G(d) geometry, default G09 integration grid),

$E_{Tot}$ = -1432.32315389 Hartree

| | | | |
|---|---|---|---|
| 6 | 1.926051 | 2.945353 | -0.979872 |
| 6 | 0.854778 | 2.929661 | -0.077702 |
| 6 | 0.837744 | 1.973344 | 0.948097 |
| 6 | 1.852014 | 1.035343 | 1.038657 |
| 6 | 2.911704 | 1.043865 | 0.128323 |
| 6 | 2.945936 | 2.010052 | -0.877764 |
| 7 | -0.151223 | 3.913548 | -0.181729 |
| 6 | 0.271876 | 5.285508 | -0.461340 |
| 6 | 3.977376 | 0.022068 | 0.271159 |
| 8 | 4.949006 | 0.156692 | -0.640964 |
| 6 | -1.496775 | 3.714478 | 0.123299 |
| 8 | -2.225702 | 4.653952 | 0.386391 |
| 6 | -2.051909 | 2.326511 | 0.044200 |
| 6 | -1.612183 | 1.375914 | -0.882697 |
| 6 | -2.221100 | 0.134683 | -0.960858 |
| 6 | -3.265601 | -0.198929 | -0.087539 |
| 6 | -3.731995 | 0.766085 | 0.812228 |
| 6 | -3.136754 | 2.019552 | 0.865347 |
| 7 | -3.888756 | -1.463683 | -0.146337 |
| 6 | -5.348468 | -1.499865 | -0.115645 |
| 6 | -3.217069 | -2.654175 | -0.434793 |
| 8 | -3.811955 | -3.613463 | -0.894678 |
| 6 | -1.766846 | -2.737748 | -0.098806 |
| 6 | -0.963875 | -3.574979 | -0.873216 |
| 6 | 0.388831 | -3.728829 | -0.603507 |
| 6 | 0.971021 | -3.069210 | 0.492837 |
| 6 | 0.144001 | -2.265371 | 1.304441 |
| 6 | -1.192812 | -2.094722 | 1.006420 |
| 7 | 2.300576 | -3.208505 | 0.817770 |
| 6 | 3.238901 | -3.779948 | -0.120102 |
| 8 | 3.991204 | -0.849790 | 1.116396 |
| 1 | 2.685820 | -2.441803 | 1.356510 |
| 1 | -4.556635 | 0.527483 | 1.476315 |
| 1 | -3.504698 | 2.777724 | 1.549325 |
| 1 | -1.888160 | -0.589744 | -1.695972 |
| 1 | -0.803383 | 1.612516 | -1.567285 |
| 1 | -1.804026 | -1.466367 | 1.647731 |
| 1 | -1.420390 | -4.104386 | -1.704249 |
| 1 | 0.992665 | -4.366827 | -1.239251 |
| 1 | 0.573201 | -1.792750 | 2.184174 |
| 1 | 1.849107 | 0.295730 | 1.832265 |
| 1 | 3.768797 | 2.021714 | -1.583653 |
| 1 | 1.948992 | 3.686714 | -1.771924 |
| 1 | 0.028595 | 1.975653 | 1.670378 |
| 1 | 0.372102 | 5.457885 | -1.538474 |
| 1 | 1.231821 | 5.477143 | 0.022967 |
| 1 | -0.485340 | 5.957805 | -0.062332 |
| 1 | -5.667016 | -2.440295 | -0.561908 |
| 1 | -5.752119 | -0.662174 | -0.689994 |
| 1 | -5.725824 | -1.442920 | 0.911245 |
| 1 | 4.240904 | -3.683233 | 0.301307 |
| 1 | 3.218045 | -3.283855 | -1.103969 |
| 1 | 3.035841 | -4.845190 | -0.271931 |
| 6 | 5.993711 | -0.812049 | -0.568572 |
| 1 | 6.716086 | -0.524195 | -1.330685 |
| 1 | 6.451767 | -0.805038 | 0.422508 |
| 1 | 5.597897 | -1.809771 | -0.773762 |

**3b** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = - 1432.32024207 Hartree

| | | | |
|---|---|---|---|
| 6 | -1.098536 | -3.434734 | -1.081312 |
| 6 | -1.767073 | -2.714056 | -0.092884 |
| 6 | -1.017451 | -2.096415 | 0.915528 |
| 6 | 0.361101 | -2.168448 | 0.909963 |
| 6 | 1.042784 | -2.830358 | -0.130219 |
| 6 | 0.288746 | -3.478669 | -1.122024 |
| 6 | -3.256180 | -2.654731 | -0.143929 |
| 8 | -3.919217 | -3.627630 | -0.456812 |
| 7 | 2.420181 | -2.837132 | -0.136859 |
| 1 | 2.833467 | -2.164628 | 0.493959 |
| 7 | -3.865877 | -1.451505 | 0.221924 |
| 6 | -5.298900 | -1.480951 | 0.501882 |
| 6 | -3.234504 | -0.189889 | 0.152557 |
| 6 | -2.304821 | 0.101471 | -0.856743 |
| 6 | -1.670246 | 1.330930 | -0.891079 |
| 6 | -1.988169 | 2.320666 | 0.042775 |
| 6 | -2.971805 | 2.062578 | 0.996101 |
| 6 | -3.577049 | 0.813741 | 1.065864 |
| 6 | -1.403546 | 3.696305 | -0.015497 |
| 8 | -2.085051 | 4.673063 | 0.236273 |
| 7 | -0.082863 | 3.820292 | -0.444049 |
| 6 | 0.371837 | 5.148385 | -0.854303 |
| 6 | 0.900118 | 2.821347 | -0.268824 |
| 6 | 0.926982 | 2.028917 | 0.887070 |
| 6 | 1.936382 | 1.098208 | 1.073266 |
| 6 | 2.939366 | 0.943277 | 0.111900 |
| 6 | 2.917920 | 1.733648 | -1.038252 |
| 6 | 1.911036 | 2.669045 | -1.226492 |
| 6 | 4.061747 | -0.012145 | 0.280184 |
| 8 | 4.939078 | -0.203407 | -0.528212 |
| 8 | 4.004977 | -0.673359 | 1.460858 |
| 6 | 5.103476 | -1.552081 | 1.717211 |
| 6 | 3.160734 | -3.109108 | -1.351672 |
| 1 | -4.315553 | 0.613581 | 1.835395 |
| 1 | -3.250897 | 2.852021 | 1.687214 |
| 1 | -2.075321 | -0.646832 | -1.606442 |
| 1 | -0.940043 | 1.531341 | -1.669412 |
| 1 | -1.522843 | -1.548618 | 1.706277 |
| 1 | -1.684605 | -3.946293 | -1.839269 |
| 1 | 0.789135 | -4.018789 | -1.918388 |
| 1 | 0.939716 | -1.696667 | 1.700239 |
| 1 | 1.967134 | 0.510712 | 1.984114 |
| 1 | 3.702848 | 1.604577 | -1.776430 |
| 1 | 1.898823 | 3.282280 | -2.121903 |
| 1 | 0.163555 | 2.162855 | 1.645798 |
| 1 | 0.463056 | 5.216568 | -1.943315 |
| 1 | 1.341782 | 5.362471 | -0.399458 |
| 1 | -0.364134 | 5.873203 | -0.510053 |
| 1 | -5.690980 | -2.424787 | 0.127282 |
| 1 | -5.791971 | -0.647694 | -0.004716 |
| 1 | -5.495080 | -1.411672 | 1.577481 |
| 1 | 4.199424 | -2.806676 | -1.206600 |
| 1 | 2.760449 | -2.554853 | -2.212548 |
| 1 | 3.143305 | -4.177934 | -1.591042 |
| 1 | 4.954422 | -1.920546 | 2.730608 |
| 1 | 5.104587 | -2.384864 | 1.008387 |
| 1 | 6.047646 | -1.011272 | 1.632438 |

**3c** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1432.31721495 Hartree

| | | | |
|---|---|---|---|
| 6 | 1.873986 | -1.873629 | -0.843142 |
| 6 | 2.599134 | -2.193602 | 0.306848 |
| 6 | 2.157428 | -3.262679 | 1.096969 |
| 6 | 1.018509 | -3.968862 | 0.767683 |
| 6 | 0.289363 | -3.654360 | -0.397318 |
| 6 | 0.737193 | -2.586980 | -1.196460 |
| 6 | 3.905705 | -1.572901 | 0.668904 |
| 8 | 4.766101 | -2.226484 | 1.234773 |
| 7 | -0.799694 | -4.411990 | -0.747539 |
| 6 | -1.679986 | -4.046052 | -1.836280 |
| 7 | 4.152916 | -0.258104 | 0.272794 |
| 6 | 5.541671 | 0.197548 | 0.280534 |
| 6 | 3.153412 | 0.723317 | 0.103085 |
| 6 | 2.036696 | 0.778481 | 0.947911 |
| 6 | 1.088110 | 1.777213 | 0.791015 |
| 6 | 1.242340 | 2.756585 | -0.195909 |
| 6 | 2.376318 | 2.724148 | -1.008519 |
| 6 | 3.316891 | 1.713028 | -0.872419 |
| 6 | 0.338173 | 3.941428 | -0.348966 |
| 8 | 0.798576 | 5.012598 | -0.704129 |
| 7 | -1.005990 | 3.821621 | -0.010548 |
| 6 | -1.755984 | 5.065600 | 0.165650 |
| 6 | -1.734790 | 2.613144 | 0.024317 |
| 6 | -2.749620 | 2.457235 | 0.976254 |
| 6 | -3.519627 | 1.302882 | 1.001742 |
| 6 | -3.281862 | 0.283240 | 0.079997 |
| 6 | -2.270287 | 0.436293 | -0.871660 |
| 6 | -1.511678 | 1.594469 | -0.912827 |
| 6 | -4.086644 | -0.964645 | 0.058575 |
| 8 | -3.920412 | -1.877244 | -0.719461 |
| 8 | -5.042434 | -0.979115 | 1.002166 |
| 6 | -5.851660 | -2.153160 | 1.018734 |
| 1 | -1.200002 | -4.972064 | -0.010334 |
| 1 | 4.186462 | 1.689250 | -1.521302 |
| 1 | 2.512809 | 3.510397 | -1.743738 |
| 1 | 1.924455 | 0.040148 | 1.734454 |
| 1 | 0.239078 | 1.808438 | 1.466669 |
| 1 | 2.206732 | -1.065662 | -1.488555 |
| 1 | 2.741575 | -3.536279 | 1.970001 |
| 1 | 0.690520 | -4.797986 | 1.389707 |
| 1 | 0.203275 | -2.324694 | -2.102986 |
| 1 | -2.104058 | -0.358094 | -1.592190 |
| 1 | -4.303517 | 1.186089 | 1.741620 |
| 1 | -2.926982 | 3.243048 | 1.703230 |
| 1 | -0.746692 | 1.721159 | -1.671074 |
| 1 | -1.837737 | 5.333215 | 1.224774 |
| 1 | -2.757099 | 4.947478 | -0.253526 |
| 1 | -1.224599 | 5.856999 | -0.359319 |
| 1 | 6.129748 | -0.537469 | 0.827000 |
| 1 | 5.610364 | 1.168683 | 0.777045 |
| 1 | 5.934793 | 0.288949 | -0.737657 |
| 1 | -2.488937 | -4.776285 | -1.888824 |
| 1 | -1.136732 | -4.079830 | -2.787069 |
| 1 | -2.125603 | -3.052127 | -1.708014 |
| 1 | -6.588327 | -1.994769 | 1.804558 |
| 1 | -6.340553 | -2.291179 | 0.052080 |
| 1 | -5.240984 | -3.032607 | 1.235398 |

**3d** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1432.31569350 Hartree

| | | | |
|---|---|---|---|
| 6 | -2.779063 | 2.313254 | 1.265786 |
| 6 | -1.837317 | 2.565378 | 0.259732 |
| 6 | -1.696006 | 1.647415 | -0.790417 |
| 6 | -2.479196 | 0.503810 | -0.827392 |
| 6 | -3.427364 | 0.264247 | 0.170666 |
| 6 | -3.567167 | 1.173549 | 1.218764 |
| 7 | -1.118041 | 3.780054 | 0.283049 |
| 6 | -1.862255 | 4.989327 | 0.636583 |
| 6 | -4.335053 | -0.911113 | 0.146072 |
| 8 | -4.159293 | -1.676639 | -0.949841 |
| 6 | -5.026772 | -2.804612 | -1.034567 |
| 6 | 0.167732 | 3.952250 | -0.221643 |
| 8 | 0.561249 | 5.046773 | -0.584119 |
| 6 | 1.106945 | 2.785737 | -0.219833 |
| 6 | 1.094592 | 1.786600 | 0.758353 |
| 6 | 2.094820 | 0.827348 | 0.801348 |
| 6 | 3.114947 | 0.824049 | -0.160838 |
| 6 | 3.123411 | 1.823338 | -1.141300 |
| 6 | 2.140377 | 2.801834 | -1.155911 |
| 7 | 4.180510 | -0.101095 | -0.113481 |
| 6 | 5.525328 | 0.418818 | -0.357819 |
| 6 | 4.083971 | -1.412304 | 0.352461 |
| 8 | 5.068607 | -2.001232 | 0.765822 |
| 6 | 2.771303 | -2.115826 | 0.266355 |
| 6 | 2.542009 | -3.144315 | 1.188560 |
| 6 | 1.393817 | -3.908046 | 1.130855 |
| 6 | 0.438800 | -3.689592 | 0.119350 |
| 6 | 0.677603 | -2.671244 | -0.819515 |
| 6 | 1.829100 | -1.899765 | -0.740322 |
| 7 | -0.677616 | -4.493283 | 0.049161 |
| 6 | -1.795896 | -4.159641 | -0.803775 |
| 8 | -5.154025 | -1.165176 | 0.997128 |
| 1 | -0.900844 | -4.991535 | 0.898098 |
| 1 | 3.913447 | 1.839300 | -1.884751 |
| 1 | 2.169202 | 3.603234 | -1.887212 |
| 1 | 2.099813 | 0.084101 | 1.590842 |
| 1 | 0.321029 | 1.779084 | 1.520512 |
| 1 | 1.995966 | -1.125809 | -1.483841 |
| 1 | 3.294375 | -3.335169 | 1.947257 |
| 1 | 1.226961 | -4.700183 | 1.856391 |
| 1 | -0.033489 | -2.487303 | -1.617055 |
| 1 | -2.379656 | -0.194676 | -1.651147 |
| 1 | -4.305821 | 0.974693 | 1.988591 |
| 1 | -2.893080 | 3.017852 | 2.082794 |
| 1 | -0.986499 | 1.846522 | -1.586249 |
| 1 | -1.915187 | 5.116055 | 1.722973 |
| 1 | -2.875974 | 4.928291 | 0.233993 |
| 1 | -1.342988 | 5.840890 | 0.201545 |
| 1 | 6.235397 | -0.261298 | 0.108188 |
| 1 | 5.622150 | 1.414340 | 0.082009 |
| 1 | 5.737619 | 0.479971 | -1.430650 |
| 1 | -2.599124 | -4.876336 | -0.621939 |
| 1 | -1.510193 | -4.242913 | -1.858349 |
| 1 | -2.178705 | -3.143418 | -0.631079 |
| 1 | -4.746628 | -3.326364 | -1.949258 |
| 1 | -4.897515 | -3.452333 | -0.163988 |
| 1 | -6.068530 | -2.479509 | -1.080028 |

**3e** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1432.31946972 Hartree

| | | | |
|---|---|---|---|
| 6 | 1.373595 | 2.147949 | -1.029413 |
| 6 | 2.002057 | 2.533829 | 0.157485 |
| 6 | 1.248550 | 3.088868 | 1.195070 |
| 6 | -0.129501 | 3.202254 | 1.070782 |
| 6 | -0.759259 | 2.768770 | -0.097540 |
| 6 | -0.002368 | 2.255908 | -1.150573 |
| 6 | -2.234729 | 2.812497 | -0.273443 |
| 8 | -2.879002 | 3.230043 | 0.821690 |
| 7 | 3.400819 | 2.339678 | 0.322638 |
| 6 | 4.252154 | 3.522128 | 0.426694 |
| 8 | -2.798242 | 2.501012 | -1.299753 |
| 6 | 4.024939 | 1.168636 | -0.081018 |
| 8 | 5.201225 | 1.159562 | -0.398502 |
| 6 | 3.207651 | -0.086926 | -0.051554 |
| 6 | 2.230508 | -0.330738 | 0.918767 |
| 6 | 1.524691 | -1.522152 | 0.929824 |
| 6 | 1.756362 | -2.487532 | -0.059675 |
| 6 | 2.750001 | -2.252794 | -1.017736 |
| 6 | 3.478462 | -1.070057 | -1.000307 |
| 7 | 1.076968 | -3.724292 | -0.052886 |
| 6 | 1.872630 | -4.922505 | -0.316400 |
| 6 | -0.218727 | -3.914397 | 0.425185 |
| 6 | -1.214669 | -2.802657 | 0.317798 |
| 6 | -2.303553 | -2.850929 | 1.195439 |
| 6 | -3.368089 | -1.981613 | 1.054988 |
| 6 | -3.402318 | -1.053966 | -0.000018 |
| 6 | -2.301853 | -0.986481 | -0.869520 |
| 6 | -1.224087 | -1.849237 | -0.704044 |
| 7 | -4.517960 | -0.235903 | -0.155642 |
| 6 | -4.910560 | 0.180902 | -1.497894 |
| 8 | -0.573445 | -5.002343 | 0.847258 |
| 1 | 2.950902 | -3.000349 | -1.777966 |
| 1 | 4.262934 | -0.893160 | -1.729698 |
| 1 | 0.793431 | -1.714000 | 1.707337 |
| 1 | 2.036426 | 0.408438 | 1.689534 |
| 1 | -2.313201 | -3.612566 | 1.968674 |
| 1 | -0.394593 | -1.795292 | -1.403683 |
| 1 | -2.298592 | -0.262602 | -1.678274 |
| 1 | -4.211502 | -2.039905 | 1.739102 |
| 1 | -0.511999 | 1.947632 | -2.057604 |
| 1 | -0.724499 | 3.602000 | 1.884457 |
| 1 | 1.747235 | 3.384367 | 2.113893 |
| 1 | 1.970216 | 1.738864 | -1.838879 |
| 1 | 3.721478 | 4.291323 | 0.989469 |
| 1 | 4.509716 | 3.912054 | -0.564497 |
| 1 | 5.174352 | 3.252532 | 0.941314 |
| 1 | 1.352369 | -5.772800 | 0.119440 |
| 1 | 2.859789 | -4.818867 | 0.140883 |
| 1 | 1.993516 | -5.085671 | -1.392669 |
| 1 | -5.900913 | 0.637977 | -1.436929 |
| 1 | -4.950716 | -0.663271 | -2.200787 |
| 1 | -4.220967 | 0.936440 | -1.874719 |
| 6 | -4.304627 | 3.216416 | 0.721661 |
| 1 | -5.302432 | -0.579234 | 0.385406 |
| 1 | -4.669051 | 3.619027 | 1.665630 |
| 1 | -4.630887 | 3.838175 | -0.114926 |
| 1 | -4.649613 | 2.189291 | 0.573835 |

**3f** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1432.31820042 Hartree

| | | | |
|---|---|---|---|
| 6 | 1.128081 | 1.988619 | 0.869427 |
| 6 | 1.276390 | 2.661398 | -0.352600 |
| 6 | 2.313294 | 2.284631 | -1.215130 |
| 6 | 3.177964 | 1.257796 | -0.863464 |
| 6 | 3.019328 | 0.583997 | 0.347740 |
| 6 | 1.982811 | 0.952804 | 1.209401 |
| 6 | 4.002750 | -0.475115 | 0.691965 |
| 8 | 3.712006 | -1.091540 | 1.852705 |
| 7 | 0.456588 | 3.764976 | -0.683227 |
| 6 | 1.113920 | 4.958349 | -1.213083 |
| 8 | 4.960181 | -0.770431 | 0.014010 |
| 6 | -0.868153 | 3.889339 | -0.266508 |
| 8 | -1.398291 | 4.974909 | -0.123291 |
| 6 | -1.637331 | 2.621723 | -0.072744 |
| 6 | -1.568474 | 1.570798 | -0.990319 |
| 6 | -2.336941 | 0.431423 | -0.816886 |
| 6 | -3.126754 | 0.280048 | 0.333017 |
| 6 | -3.215177 | 1.349043 | 1.234932 |
| 6 | -2.501007 | 2.519557 | 1.014350 |
| 7 | -3.880962 | -0.888339 | 0.573378 |
| 6 | -5.197969 | -0.723587 | 1.187417 |
| 6 | -3.536187 | -2.183846 | 0.181671 |
| 6 | -2.121393 | -2.503565 | -0.173222 |
| 6 | -1.932867 | -3.498031 | -1.140742 |
| 6 | -0.664534 | -3.872918 | -1.537838 |
| 6 | 0.471885 | -3.277894 | -0.959839 |
| 6 | 0.285950 | -2.311428 | 0.045453 |
| 6 | -0.995131 | -1.937287 | 0.427807 |
| 7 | 1.729111 | -3.672062 | -1.366261 |
| 6 | 2.892185 | -2.871934 | -1.054529 |
| 8 | -4.382438 | -3.061910 | 0.153471 |
| 1 | -3.843178 | 1.262062 | 2.114900 |
| 1 | -2.587850 | 3.355820 | 1.701731 |
| 1 | -2.309418 | -0.356919 | -1.559583 |
| 1 | -0.926033 | 1.656280 | -1.862220 |
| 1 | -2.808274 | -3.966920 | -1.578716 |
| 1 | -1.111668 | -1.179708 | 1.197990 |
| 1 | 1.142192 | -1.847754 | 0.524826 |
| 1 | -0.533855 | -4.636335 | -2.300688 |
| 1 | 1.870247 | 0.448036 | 2.163046 |
| 1 | 3.992994 | 0.966366 | -1.518534 |
| 1 | 2.440858 | 2.800350 | -2.161262 |
| 1 | 0.353549 | 2.297049 | 1.562190 |
| 1 | 1.319670 | 4.850609 | -2.282734 |
| 1 | 2.054095 | 5.134605 | -0.684012 |
| 1 | 0.442929 | 5.801733 | -1.059109 |
| 1 | -5.804879 | -1.583956 | 0.914882 |
| 1 | -5.660392 | 0.193092 | 0.814957 |
| 1 | -5.124322 | -0.670570 | 2.279441 |
| 1 | 3.770485 | -3.307134 | -1.533413 |
| 1 | 3.067749 | -2.872912 | 0.025821 |
| 1 | 2.792759 | -1.826837 | -1.383306 |
| 6 | 4.664346 | -2.071614 | 2.265665 |
| 1 | 1.752310 | -4.147441 | -2.257067 |
| 1 | 4.284459 | -2.476962 | 3.201735 |
| 1 | 4.756267 | -2.858110 | 1.513065 |
| 1 | 5.642558 | -1.608528 | 2.412014 |

**3**$^{-}$**a** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1431.74926237 Hartree

| | | | |
|---|---|---|---|
| 6 | 0.556624 | 2.371350 | 1.029645 |
| 6 | 0.511573 | 2.823603 | -0.289749 |
| 6 | 1.504107 | 2.429093 | -1.190288 |
| 6 | 2.525609 | 1.580018 | -0.780176 |
| 6 | 2.563875 | 1.124783 | 0.537365 |
| 6 | 1.573376 | 1.519542 | 1.434890 |
| 6 | 3.637502 | 0.226089 | 1.052480 |
| 8 | 4.667349 | 0.094303 | 0.202134 |
| 7 | -0.534799 | 3.701744 | -0.716165 |
| 6 | -0.150658 | 5.086529 | -0.958383 |
| 8 | 3.627580 | -0.249985 | 2.164438 |
| 6 | -1.856500 | 3.496070 | -0.330252 |
| 8 | -2.613808 | 4.441456 | -0.162418 |
| 6 | -2.293480 | 2.080807 | -0.188768 |
| 6 | -1.773807 | 1.054863 | -0.988009 |
| 6 | -2.172767 | -0.253792 | -0.820424 |
| 6 | -3.085755 | -0.604615 | 0.196659 |
| 6 | -3.657049 | 0.436915 | 0.949404 |
| 6 | -3.269346 | 1.757368 | 0.750217 |
| 7 | -3.461795 | -1.930062 | 0.424211 |
| 6 | -4.801313 | -2.187027 | 0.920973 |
| 6 | -2.722340 | -3.059234 | -0.073369 |
| 6 | -1.279542 | -2.942334 | -0.034922 |
| 6 | -0.577734 | -2.133611 | 0.900921 |
| 6 | 0.765529 | -1.920186 | 0.799099 |
| 6 | 1.540068 | -2.407272 | -0.324040 |
| 6 | 0.823639 | -3.300515 | -1.212941 |
| 6 | -0.517356 | -3.557859 | -1.049359 |
| 7 | 2.785289 | -2.001286 | -0.454106 |
| 6 | 3.469747 | -2.438444 | -1.643637 |
| 8 | -3.348327 | -4.031907 | -0.483833 |
| 1 | -4.387726 | 0.209179 | 1.718105 |
| 1 | -3.707818 | 2.554223 | 1.344652 |
| 1 | -1.753169 | -1.022800 | -1.455869 |
| 1 | -1.049561 | 1.287697 | -1.762365 |
| 1 | -1.129252 | -1.687462 | 1.727172 |
| 1 | -1.037850 | -4.213673 | -1.745268 |
| 1 | 1.355857 | -3.774171 | -2.031870 |
| 1 | 1.300962 | -1.338751 | 1.544421 |
| 1 | 1.620749 | 1.144669 | 2.452163 |
| 1 | 3.281594 | 1.239403 | -1.479239 |
| 1 | 1.444662 | 2.767091 | -2.221649 |
| 1 | -0.221533 | 2.676184 | 1.723389 |
| 1 | 0.773326 | 5.101345 | -1.539642 |
| 1 | 0.009900 | 5.628483 | -0.017365 |
| 1 | -0.948542 | 5.584232 | -1.509377 |
| 1 | -5.026470 | -3.232635 | 0.716434 |
| 1 | -5.535430 | -1.553599 | 0.409650 |
| 1 | -4.875289 | -2.001042 | 2.000408 |
| 1 | 4.438250 | -1.925243 | -1.716337 |
| 1 | 2.916864 | -2.216223 | -2.575657 |
| 1 | 3.677550 | -3.525847 | -1.664987 |
| 6 | 5.569775 | -0.940507 | 0.575757 |
| 1 | 6.309705 | -0.995576 | -0.223913 |
| 1 | 6.051881 | -0.705295 | 1.528842 |
| 1 | 5.005460 | -1.873682 | 0.659595 |

**3**$^{-}$**b** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1431.75176201 Hartree

| | | | |
|---|---|---|---|
| 6 | 0.633011 | 2.248646 | 0.933865 |
| 6 | 0.512979 | 2.886276 | -0.301814 |
| 6 | 1.489106 | 2.678058 | -1.281030 |
| 6 | 2.565972 | 1.839834 | -1.025638 |
| 6 | 2.677487 | 1.190737 | 0.203717 |
| 6 | 1.702059 | 1.396556 | 1.179198 |
| 6 | 3.874584 | 0.330274 | 0.444199 |
| 8 | 3.873245 | -0.193729 | 1.680118 |
| 7 | -0.580128 | 3.766894 | -0.569142 |
| 6 | -0.252636 | 5.176506 | -0.748866 |
| 8 | 4.793362 | 0.222657 | -0.335931 |
| 6 | -1.879506 | 3.502649 | -0.150831 |
| 8 | -2.646248 | 4.422417 | 0.101486 |
| 6 | -2.298405 | 2.076665 | -0.077671 |
| 6 | -1.777057 | 1.085899 | -0.920087 |
| 6 | -2.175957 | -0.229002 | -0.807745 |
| 6 | -3.093365 | -0.622316 | 0.189696 |
| 6 | -3.666373 | 0.385320 | 0.985320 |
| 6 | -3.275882 | 1.712046 | 0.845007 |
| 7 | -3.468593 | -1.956016 | 0.359545 |
| 6 | -4.810854 | -2.236867 | 0.835210 |
| 6 | -2.714016 | -3.064724 | -0.160110 |
| 6 | -1.273146 | -2.944570 | -0.091209 |
| 6 | -0.592160 | -2.145598 | 0.867817 |
| 6 | 0.755032 | -1.944707 | 0.802983 |
| 6 | 1.562632 | -2.450477 | -0.287947 |
| 6 | 0.862151 | -3.326633 | -1.206076 |
| 6 | -0.486481 | -3.562502 | -1.087008 |
| 7 | 2.821595 | -2.080928 | -0.358592 |
| 6 | 3.573480 | -2.549301 | -1.494802 |
| 8 | -3.327239 | -4.028202 | -0.610141 |
| 1 | -4.399180 | 0.124394 | 1.741474 |
| 1 | -3.714204 | 2.483546 | 1.471702 |
| 1 | -1.753613 | -0.973162 | -1.470926 |
| 1 | -1.051443 | 1.349546 | -1.683286 |
| 1 | -1.162680 | -1.696627 | 1.679347 |
| 1 | -0.994443 | -4.207859 | -1.801488 |
| 1 | 1.414829 | -3.801646 | -2.010475 |
| 1 | 1.276887 | -1.363266 | 1.558132 |
| 1 | 1.793054 | 0.895562 | 2.135975 |
| 1 | 3.330579 | 1.659377 | -1.774187 |
| 1 | 1.380163 | 3.160827 | -2.248701 |
| 1 | -0.126907 | 2.409056 | 1.692591 |
| 1 | 0.671690 | 5.253971 | -1.323245 |
| 1 | -0.119232 | 5.680866 | 0.216371 |
| 1 | -1.067258 | 5.667818 | -1.281043 |
| 1 | -5.033711 | -3.272224 | 0.581443 |
| 1 | -5.541689 | -1.580509 | 0.349100 |
| 1 | -4.892780 | -2.101590 | 1.921779 |
| 1 | 4.560829 | -2.072514 | -1.484762 |
| 1 | 3.099326 | -2.305368 | -2.463459 |
| 1 | 3.729209 | -3.645088 | -1.496937 |
| 6 | 4.834689 | -1.222754 | 1.881422 |
| 1 | 4.755909 | -1.501350 | 2.933188 |
| 1 | 4.564842 | -2.058779 | 1.229747 |
| 1 | 5.840684 | -0.859872 | 1.655145 |

**3**$^{-}$**c** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = - 1431.74154522 Hartree

| | | | |
|---|---|---|---|
| 6 | 0.810315 | -2.158639 | -0.451843 |
| 6 | 1.889832 | -2.811421 | 0.199020 |
| 6 | 1.550385 | -3.863529 | 1.102897 |
| 6 | 0.258513 | -4.186217 | 1.379435 |
| 6 | -0.866657 | -3.484752 | 0.784121 |
| 6 | -0.497967 | -2.465192 | -0.189343 |
| 6 | 3.278526 | -2.504829 | 0.011261 |
| 8 | 4.215337 | -3.239026 | 0.321027 |
| 7 | -2.076294 | -3.813200 | 1.157499 |
| 6 | -3.145774 | -3.049065 | 0.567597 |
| 7 | 3.624027 | -1.249867 | -0.645926 |
| 6 | 4.825783 | -1.290718 | -1.460453 |
| 6 | 3.096299 | -0.012114 | -0.328334 |
| 6 | 2.206114 | 0.182342 | 0.755750 |
| 6 | 1.630567 | 1.413803 | 0.983451 |
| 6 | 1.955671 | 2.528522 | 0.197676 |
| 6 | 2.917607 | 2.375180 | -0.797300 |
| 6 | 3.468306 | 1.131111 | -1.071022 |
| 6 | 1.313411 | 3.851600 | 0.385753 |
| 8 | 1.936268 | 4.899585 | 0.313805 |
| 7 | -0.053750 | 3.847992 | 0.694242 |
| 6 | -0.627319 | 5.078534 | 1.223617 |
| 6 | -0.951868 | 2.830260 | 0.292134 |
| 6 | -2.079300 | 2.552844 | 1.073534 |
| 6 | -3.002831 | 1.597184 | 0.667321 |
| 6 | -2.813633 | 0.901938 | -0.525692 |
| 6 | -1.689151 | 1.175315 | -1.307867 |
| 6 | -0.775408 | 2.136738 | -0.915406 |
| 6 | -3.785514 | -0.103377 | -1.027858 |
| 8 | -3.661085 | -0.721901 | -2.059403 |
| 8 | -4.854152 | -0.236954 | -0.219515 |
| 6 | -5.795529 | -1.219532 | -0.639040 |
| 1 | 4.177385 | 1.042522 | -1.884771 |
| 1 | 3.207190 | 3.241809 | -1.385500 |
| 1 | 1.944570 | -0.655899 | 1.387269 |
| 1 | 0.913986 | 1.516936 | 1.794044 |
| 1 | 1.027085 | -1.390425 | -1.192675 |
| 1 | 2.369685 | -4.394179 | 1.581460 |
| 1 | 0.010877 | -4.976159 | 2.083583 |
| 1 | -1.281044 | -1.943981 | -0.733488 |
| 1 | -1.556294 | 0.630603 | -2.237192 |
| 1 | -3.870117 | 1.379885 | 1.280959 |
| 1 | -2.224796 | 3.077660 | 2.012337 |
| 1 | 0.085559 | 2.352989 | -1.537202 |
| 1 | -0.882059 | 4.976374 | 2.284731 |
| 1 | -1.532296 | 5.339845 | 0.667777 |
| 1 | 0.116562 | 5.865064 | 1.107723 |
| 1 | 5.221828 | -2.302152 | -1.405425 |
| 1 | 5.586218 | -0.594483 | -1.085653 |
| 1 | 4.605282 | -1.035444 | -2.504821 |
| 1 | -4.106909 | -3.403182 | 0.964364 |
| 1 | -3.197368 | -3.126398 | -0.535780 |
| 1 | -3.083051 | -1.966446 | 0.793831 |
| 1 | -6.544784 | -1.267858 | 0.150765 |
| 1 | -6.254067 | -0.924789 | -1.587093 |
| 1 | -5.304534 | -2.186315 | -0.763708 |

**3**$^{-}$**d** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1431.74244177 Hartree

| | | | |
|---|---|---|---|
| 6 | -3.166783 | 2.060133 | 1.133762 |
| 6 | -2.179058 | 2.387097 | 0.194632 |
| 6 | -1.827726 | 1.440055 | -0.778791 |
| 6 | -2.429600 | 0.191153 | -0.789678 |
| 6 | -3.418746 | -0.125446 | 0.145613 |
| 6 | -3.780327 | 0.817117 | 1.105611 |
| 7 | -1.619812 | 3.683861 | 0.215326 |
| 6 | -2.522243 | 4.789850 | 0.519939 |
| 6 | -4.121168 | -1.435035 | 0.161331 |
| 8 | -3.759532 | -2.225067 | -0.861116 |
| 6 | -4.346140 | -3.523698 | -0.856234 |
| 6 | -0.321976 | 4.025833 | -0.184803 |
| 8 | -0.069798 | 5.179732 | -0.502696 |
| 6 | 0.745296 | 2.993795 | -0.159002 |
| 6 | 0.794273 | 1.910009 | 0.732736 |
| 6 | 1.857665 | 1.030908 | 0.735120 |
| 6 | 2.934178 | 1.187741 | -0.170621 |
| 6 | 2.894968 | 2.298878 | -1.039381 |
| 6 | 1.825671 | 3.179609 | -1.022010 |
| 7 | 4.020135 | 0.335434 | -0.181129 |
| 6 | 5.285546 | 0.833932 | -0.689005 |
| 6 | 4.081557 | -0.927401 | 0.539750 |
| 8 | 5.097030 | -1.148520 | 1.195970 |
| 6 | 2.984304 | -1.835898 | 0.368566 |
| 6 | 2.882385 | -2.960777 | 1.242291 |
| 6 | 1.887255 | -3.880277 | 1.118026 |
| 6 | 0.872124 | -3.799976 | 0.080539 |
| 6 | 1.018203 | -2.664682 | -0.818143 |
| 6 | 2.018952 | -1.742643 | -0.665743 |
| 7 | -0.051550 | -4.725021 | 0.029901 |
| 6 | -1.023899 | -4.581932 | -1.024414 |
| 8 | -4.942884 | -1.760726 | 0.988774 |
| 1 | 3.702587 | 2.464023 | -1.742888 |
| 1 | 1.812744 | 4.036516 | -1.688678 |
| 1 | 1.873040 | 0.206646 | 1.437217 |
| 1 | -0.002853 | 1.761380 | 1.455244 |
| 1 | 2.089196 | -0.926109 | -1.382181 |
| 1 | 3.632035 | -3.057547 | 2.023929 |
| 1 | 1.812112 | -4.726270 | 1.796011 |
| 1 | 0.328176 | -2.555599 | -1.648879 |
| 1 | -2.136101 | -0.545018 | -1.530134 |
| 1 | -4.543011 | 0.553968 | 1.831615 |
| 1 | -3.443213 | 2.781580 | 1.895499 |
| 1 | -1.072916 | 1.683871 | -1.517586 |
| 1 | -2.625623 | 4.937487 | 1.601479 |
| 1 | -3.508887 | 4.586846 | 0.095784 |
| 1 | -2.105653 | 5.692076 | 0.076887 |
| 1 | 6.063918 | 0.162707 | -0.330380 |
| 1 | 5.488834 | 1.844947 | -0.316330 |
| 1 | 5.298264 | 0.858547 | -1.786627 |
| 1 | -1.773315 | -5.380441 | -0.940083 |
| 1 | -0.588503 | -4.656051 | -2.039245 |
| 1 | -1.565133 | -3.617251 | -0.996296 |
| 1 | -3.957187 | -4.025788 | -1.740848 |
| 1 | -4.050967 | -4.067555 | 0.043705 |
| 1 | -5.435736 | -3.446315 | -0.893918 |

**3**$^{-}$**e** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1431.74154425 Hartree

| | | | |
|---|---|---|---|
| 6 | -0.774722 | 2.136658 | -0.915279 |
| 6 | -0.951052 | 2.830502 | 0.292104 |
| 6 | -2.078637 | 2.553601 | 1.073463 |
| 6 | -3.002457 | 1.598173 | 0.667358 |
| 6 | -2.813415 | 0.902640 | -0.525511 |
| 6 | -1.688764 | 1.175478 | -1.307627 |
| 6 | -3.785589 | -0.102420 | -1.027594 |
| 8 | -4.854378 | -0.235478 | -0.219361 |
| 7 | -0.052690 | 3.848059 | 0.694067 |
| 6 | -0.625948 | 5.078687 | 1.223611 |
| 8 | -3.661274 | -0.721196 | -2.059000 |
| 6 | 1.314471 | 3.851381 | 0.385582 |
| 8 | 1.937501 | 4.899256 | 0.313524 |
| 6 | 1.956471 | 2.528164 | 0.197625 |
| 6 | 1.631045 | 1.413563 | 0.983418 |
| 6 | 2.206200 | 0.181911 | 0.755740 |
| 6 | 3.096311 | -0.012832 | -0.328346 |
| 6 | 3.468670 | 1.130278 | -1.071057 |
| 6 | 2.918359 | 2.374516 | -0.797364 |
| 7 | 3.623588 | -1.250750 | -0.645991 |
| 6 | 4.825416 | -1.292000 | -1.460399 |
| 6 | 3.277819 | -2.505548 | 0.011465 |
| 6 | 1.889074 | -2.811872 | 0.199109 |
| 6 | 1.549362 | -3.863947 | 1.102926 |
| 6 | 0.257415 | -4.186432 | 1.379310 |
| 6 | -0.867578 | -3.484773 | 0.783881 |
| 6 | -0.498624 | -2.465168 | -0.189450 |
| 6 | 0.809730 | -2.158833 | -0.451806 |
| 7 | -2.077282 | -3.813107 | 1.157075 |
| 6 | -3.146605 | -3.048818 | 0.567078 |
| 8 | 4.214493 | -3.239813 | 0.321482 |
| 1 | 4.177711 | 1.041432 | -1.884813 |
| 1 | 3.208195 | 3.241036 | -1.385599 |
| 1 | 1.944368 | -0.656245 | 1.387253 |
| 1 | 0.914482 | 1.516935 | 1.793999 |
| 1 | 2.368538 | -4.394723 | 1.581560 |
| 1 | 1.026736 | -1.390572 | -1.192522 |
| 1 | -1.281590 | -1.943766 | -0.733573 |
| 1 | 0.009558 | -4.976346 | 2.083410 |
| 1 | -1.555984 | 0.630539 | -2.236828 |
| 1 | -3.869863 | 1.381307 | 1.280979 |
| 1 | -2.224056 | 3.078630 | 2.012157 |
| 1 | 0.086373 | 2.352468 | -1.537050 |
| 1 | -0.880372 | 4.976549 | 2.284803 |
| 1 | -1.531058 | 5.340081 | 0.668034 |
| 1 | 0.118010 | 5.865105 | 1.107482 |
| 1 | 5.221138 | -2.303557 | -1.405292 |
| 1 | 5.586033 | -0.595995 | -1.085540 |
| 1 | 4.605098 | -1.036695 | -2.504796 |
| 1 | -4.107808 | -3.402831 | 0.963764 |
| 1 | -3.198129 | -3.126111 | -0.536304 |
| 1 | -3.083755 | -1.966211 | 0.793320 |
| 6 | -5.796041 | -1.217768 | -0.638900 |
| 1 | -6.545717 | -1.265335 | 0.150552 |
| 1 | -6.253951 | -0.923226 | -1.587322 |
| 1 | -5.305484 | -2.184861 | -0.762909 |

**3**$^{-}$**f** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1431.74257375 Hartree

| | | | |
|---|---|---|---|
| 6 | 1.445666 | 1.790709 | 0.782889 |
| 6 | 1.745888 | 2.586796 | -0.333864 |
| 6 | 2.796390 | 2.199129 | -1.176098 |
| 6 | 3.519564 | 1.044429 | -0.913622 |
| 6 | 3.204289 | 0.247488 | 0.184765 |
| 6 | 2.154814 | 0.625756 | 1.025697 |
| 6 | 4.032580 | -0.961286 | 0.427521 |
| 8 | 3.616647 | -1.669587 | 1.491078 |
| 7 | 1.072117 | 3.803863 | -0.584678 |
| 6 | 1.873441 | 4.925159 | -1.061916 |
| 8 | 4.993465 | -1.275883 | -0.238128 |
| 6 | -0.245714 | 4.083573 | -0.197465 |
| 8 | -0.607197 | 5.236991 | -0.019825 |
| 6 | -1.181784 | 2.942385 | -0.055636 |
| 6 | -1.160002 | 1.813417 | -0.887611 |
| 6 | -2.046945 | 0.772764 | -0.707993 |
| 6 | -2.977944 | 0.787357 | 0.359708 |
| 6 | -3.025752 | 1.951195 | 1.159238 |
| 6 | -2.153536 | 3.006927 | 0.940340 |
| 7 | -3.842893 | -0.261021 | 0.606817 |
| 6 | -5.026244 | 0.004106 | 1.406108 |
| 6 | -3.858414 | -1.525419 | -0.120955 |
| 6 | -2.618801 | -2.229660 | -0.277733 |
| 6 | -2.574637 | -3.322731 | -1.196336 |
| 6 | -1.438514 | -4.039297 | -1.408413 |
| 6 | -0.192120 | -3.752700 | -0.718038 |
| 6 | -0.269530 | -2.658375 | 0.240226 |
| 6 | -1.425824 | -1.952102 | 0.438403 |
| 7 | 0.858747 | -4.479314 | -0.996950 |
| 6 | 2.065496 | -4.135768 | -0.291156 |
| 8 | -4.955838 | -1.926057 | -0.503806 |
| 1 | -3.740437 | 2.024630 | 1.969596 |
| 1 | -2.202321 | 3.894609 | 1.564806 |
| 1 | -2.014704 | -0.080093 | -1.373130 |
| 1 | -0.438285 | 1.753130 | -1.697943 |
| 1 | -3.489053 | -3.561135 | -1.733657 |
| 1 | -1.430157 | -1.154798 | 1.179974 |
| 1 | 0.611917 | -2.399656 | 0.820023 |
| 1 | -1.412114 | -4.861877 | -2.118130 |
| 1 | 1.906822 | 0.011243 | 1.884045 |
| 1 | 4.335525 | 0.738624 | -1.560411 |
| 1 | 3.041020 | 2.801615 | -2.044588 |
| 1 | 0.649387 | 2.085467 | 1.456034 |
| 1 | 2.014898 | 4.881629 | -2.147957 |
| 1 | 2.854154 | 4.914331 | -0.578314 |
| 1 | 1.345458 | 5.841838 | -0.806011 |
| 1 | -5.693580 | -0.847912 | 1.295701 |
| 1 | -5.547701 | 0.905765 | 1.061448 |
| 1 | -4.767821 | 0.135905 | 2.464641 |
| 1 | 2.872521 | -4.815887 | -0.594269 |
| 1 | 1.973003 | -4.210257 | 0.810263 |
| 1 | 2.415408 | -3.105075 | -0.495581 |
| 6 | 4.370559 | -2.851461 | 1.745925 |
| 1 | 3.864335 | -3.353632 | 2.568983 |
| 1 | 4.384671 | -3.488903 | 0.859959 |
| 1 | 5.397089 | -2.592317 | 2.019721 |

**4a** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1871.20812862 Hartree

| | | | |
|---|---|---|---|
| 6 | 1.914365 | 0.840824 | 1.226511 |
| 6 | 2.768630 | 0.907032 | 2.327631 |
| 6 | 3.485886 | -0.225086 | 2.717436 |
| 6 | 3.352878 | -1.409296 | 2.008543 |
| 6 | 2.501921 | -1.474934 | 0.899374 |
| 6 | 1.777367 | -0.342969 | 0.513375 |
| 7 | 2.426510 | -2.688132 | 0.159121 |
| 6 | 3.658266 | -3.203296 | -0.442920 |
| 6 | 2.960671 | 2.157539 | 3.112608 |
| 8 | 2.224385 | 3.176867 | 2.641477 |
| 6 | 2.381197 | 4.406589 | 3.347449 |
| 6 | 1.263251 | -3.184089 | -0.385014 |
| 8 | 1.292927 | -3.950901 | -1.336746 |
| 6 | -0.040268 | -2.829031 | 0.262588 |
| 6 | -0.193235 | -2.683073 | 1.643517 |
| 6 | -1.435701 | -2.368745 | 2.177291 |
| 6 | -2.531077 | -2.179512 | 1.331936 |
| 6 | -2.393241 | -2.393017 | -0.040540 |
| 6 | -1.153063 | -2.718438 | -0.569341 |
| 7 | -3.771744 | -1.729903 | 1.866065 |
| 6 | -4.528082 | -2.635994 | 2.726009 |
| 6 | -4.484526 | -0.701181 | 1.277816 |
| 8 | -5.690186 | -0.600890 | 1.424778 |
| 6 | -3.706469 | 0.315388 | 0.492980 |
| 6 | -4.326154 | 0.891943 | -0.615829 |
| 6 | -3.651716 | 1.826330 | -1.390940 |
| 6 | -2.358665 | 2.226028 | -1.041479 |
| 6 | -1.762068 | 1.694217 | 0.104293 |
| 6 | -2.423783 | 0.734407 | 0.855051 |
| 7 | -1.686058 | 3.199305 | -1.825962 |
| 6 | -2.290105 | 4.531275 | -1.884803 |
| 6 | -0.321116 | 3.163812 | -2.081041 |
| 8 | 0.292417 | 4.207538 | -2.239360 |
| 6 | 0.365917 | 1.847294 | -2.280050 |
| 6 | -0.266493 | 0.659118 | -2.657697 |
| 6 | 0.470797 | -0.466051 | -3.014527 |
| 6 | 1.875556 | -0.433347 | -2.996284 |
| 6 | 2.509866 | 0.757409 | -2.594037 |
| 6 | 1.768109 | 1.872137 | -2.258595 |
| 7 | 2.639846 | -1.531165 | -3.340866 |
| 6 | 2.067046 | -2.631012 | -4.097703 |
| 8 | 3.695557 | 2.256359 | 4.066961 |
| 1 | -1.349792 | 0.606902 | -2.710845 |
| 1 | -0.046295 | -1.363138 | -3.337059 |
| 1 | 2.261630 | 2.802491 | -1.996431 |
| 1 | 3.596004 | 0.795283 | -2.562260 |
| 1 | 2.868982 | -3.325740 | -4.353155 |
| 1 | 1.350849 | -3.177620 | -3.480579 |
| 1 | 1.578474 | -2.292789 | -5.022812 |
| 1 | -0.779427 | 2.043319 | 0.404131 |
| 1 | -4.115437 | 2.243314 | -2.280145 |
| 1 | -5.336990 | 0.586211 | -0.867433 |
| 1 | -1.940747 | 0.321116 | 1.734783 |
| 1 | -1.955737 | 5.035835 | -2.790988 |
| 1 | -1.992070 | 5.137476 | -1.022288 |
| 1 | -3.374990 | 4.425796 | -1.894283 |
| 1 | -3.257302 | -2.273389 | -0.687426 |
| 1 | -1.555105 | -2.215547 | 3.246231 |
| 1 | 0.664414 | -2.792610 | 2.300617 |
| 1 | -1.028225 | -2.893184 | -1.632860 |
| 1 | -5.182289 | -2.049978 | 3.371510 |
| 1 | -3.828259 | -3.216081 | 3.329241 |
| 1 | -5.147174 | -3.318268 | 2.132893 |
| 1 | 4.509504 | -2.854736 | 0.140978 |
| 1 | 3.740993 | -2.847242 | -1.475240 |
| 1 | 3.629898 | -4.293700 | -0.448090 |
| 1 | 1.119746 | -0.385537 | -0.350266 |
| 1 | 3.900176 | -2.296761 | 2.312934 |
| 1 | 4.139899 | -0.157450 | 3.580716 |
| 1 | 1.383770 | 1.730432 | 0.904950 |
| 1 | 3.422792 | 4.733265 | 3.313414 |
| 1 | 2.082159 | 4.285915 | 4.391044 |
| 1 | 1.736006 | 5.122626 | 2.841011 |
| 1 | 3.588098 | -1.292387 | -3.599338 |

**4b** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1871.20584582 Hartree

| | | | |
|---|---|---|---|
| 1 | 0.728632 | 1.094701 | -1.531844 |
| 6 | 1.440811 | 0.284948 | -1.610709 |
| 6 | 3.197355 | -1.834731 | -1.969278 |
| 6 | 2.757343 | 0.415306 | -1.152201 |
| 6 | 0.995056 | -0.892622 | -2.201822 |
| 6 | 1.856731 | -1.985433 | -2.365411 |
| 6 | 3.625487 | -0.670659 | -1.366768 |
| 1 | -0.029880 | -0.948318 | -2.552976 |
| 1 | 4.651157 | -0.574862 | -1.030433 |
| 1 | 3.888567 | -2.664684 | -2.097675 |
| 7 | 1.415341 | -3.204516 | -2.839611 |
| 1 | 2.128095 | -3.788550 | -3.253175 |
| 6 | 0.075690 | -3.372375 | -3.353026 |
| 1 | -0.042299 | -4.399724 | -3.701759 |
| 1 | -0.653804 | -3.204208 | -2.550359 |
| 1 | -0.161356 | -2.690580 | -4.182591 |
| 6 | 3.411353 | 1.602094 | -0.497732 |
| 8 | 4.617621 | 1.576030 | -0.270960 |
| 7 | 2.717198 | 2.747334 | -0.178675 |
| 6 | 1.305209 | 2.920061 | -0.190007 |
| 6 | -1.460753 | 3.259808 | -0.267971 |
| 6 | 0.500532 | 2.286442 | 0.757188 |
| 6 | 0.734025 | 3.761183 | -1.144806 |
| 6 | -0.641178 | 3.938980 | -1.173115 |
| 6 | -0.881604 | 2.444394 | 0.709256 |
| 1 | 0.975846 | 1.652537 | 1.500503 |
| 1 | 1.377058 | 4.254188 | -1.868020 |
| 1 | -1.102832 | 4.604303 | -1.894950 |
| 1 | -1.505243 | 1.931325 | 1.435888 |
| 6 | 3.516681 | 3.857240 | 0.338943 |
| 1 | 4.413513 | 3.979666 | -0.269680 |
| 1 | 3.829238 | 3.668685 | 1.371947 |
| 1 | 2.910037 | 4.763166 | 0.307754 |
| 6 | -2.928358 | 3.575929 | -0.373334 |
| 8 | -3.266823 | 4.713373 | -0.656407 |
| 7 | -3.882579 | 2.603367 | -0.138614 |
| 6 | -3.653850 | 1.215276 | 0.017876 |
| 6 | -3.284615 | -1.536791 | 0.366478 |
| 6 | -2.731982 | 0.520121 | -0.775230 |
| 6 | -4.419727 | 0.508304 | 0.951357 |
| 6 | -4.258939 | -0.862550 | 1.097996 |
| 6 | -2.524519 | -0.836206 | -0.571080 |
| 1 | -2.173927 | 1.047705 | -1.541350 |
| 1 | -5.144661 | 1.037711 | 1.561326 |
| 1 | -4.873153 | -1.421254 | 1.797287 |
| 1 | -1.768965 | -1.357782 | -1.151787 |
| 6 | -5.268438 | 3.076634 | -0.100610 |
| 1 | -5.380449 | 3.878436 | -0.828895 |
| 1 | -5.528766 | 3.468816 | 0.888351 |
| 1 | -5.930137 | 2.247355 | -0.351029 |
| 6 | -3.156918 | -3.015121 | 0.572248 |
| 8 | -4.158602 | -3.703283 | 0.659532 |
| 7 | -1.883962 | -3.567123 | 0.605002 |
| 6 | -1.791969 | -5.023471 | 0.509038 |
| 1 | -1.435118 | -5.331183 | -0.479851 |
| 1 | -2.785912 | -5.434347 | 0.673791 |
| 1 | -1.102345 | -5.398536 | 1.268460 |
| 6 | -0.699046 | -2.857033 | 0.924411 |
| 6 | 1.689992 | -1.546876 | 1.577304 |
| 6 | 0.522768 | -3.316564 | 0.422330 |
| 6 | -0.705947 | -1.760100 | 1.799872 |
| 6 | 0.473430 | -1.097080 | 2.097136 |
| 6 | 1.707198 | -2.679495 | 0.768050 |
| 1 | 0.552033 | -4.167226 | -0.250584 |
| 1 | -1.633666 | -1.433325 | 2.254324 |
| 1 | 0.459511 | -0.250884 | 2.776265 |
| 1 | 2.659444 | -3.040166 | 0.396534 |
| 6 | 2.985851 | -0.889951 | 1.896141 |
| 8 | 4.070377 | -1.375888 | 1.682043 |
| 8 | 2.817962 | 0.318499 | 2.466396 |
| 6 | 4.032448 | 0.972800 | 2.851931 |
| 1 | 4.643592 | 1.174425 | 1.969826 |
| 1 | 4.588121 | 0.345058 | 3.552277 |
| 1 | 3.720689 | 1.899506 | 3.334156 |

**4c** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1871.20575560 Hartree

| | | | |
|---|---|---|---|
| 1 | -5.014147 | -3.087810 | -2.031577 |
| 6 | -4.283512 | -2.810794 | -1.278109 |
| 6 | -2.478676 | -2.110795 | 0.709297 |
| 6 | -4.531072 | -1.677419 | -0.501995 |
| 6 | -3.144086 | -3.580709 | -1.094264 |
| 6 | -2.213807 | -3.236725 | -0.098645 |
| 6 | -3.614516 | -1.351723 | 0.509747 |
| 1 | -2.978685 | -4.450383 | -1.720830 |
| 1 | -3.795530 | -0.499869 | 1.158496 |
| 1 | -1.773175 | -1.859050 | 1.495917 |
| 7 | -1.060959 | -3.959590 | 0.102666 |
| 1 | -0.562079 | -3.739734 | 0.956607 |
| 6 | -0.913205 | -5.294101 | -0.428061 |
| 1 | -0.004836 | -5.738857 | -0.016533 |
| 1 | -1.763085 | -5.945260 | -0.176938 |
| 1 | -0.811713 | -5.275846 | -1.519360 |
| 6 | -5.819131 | -0.963994 | -0.745534 |
| 8 | -6.793316 | -1.571959 | -1.158572 |
| 7 | -5.918829 | 0.396421 | -0.445401 |
| 6 | -4.832722 | 1.287361 | -0.325893 |
| 6 | -2.687930 | 3.069386 | -0.039867 |
| 6 | -3.707643 | 1.182586 | -1.156163 |
| 6 | -4.896632 | 2.334187 | 0.602045 |
| 6 | -3.840000 | 3.226608 | 0.728012 |
| 6 | -2.638005 | 2.046538 | -0.992117 |
| 1 | -3.673591 | 0.409328 | -1.915127 |
| 1 | -5.772742 | 2.438925 | 1.233611 |
| 1 | -3.891010 | 4.050033 | 1.433660 |
| 1 | -1.765257 | 1.942683 | -1.629429 |
| 6 | -7.265806 | 0.958190 | -0.369037 |
| 1 | -7.931581 | 0.313845 | -0.939705 |
| 1 | -7.263850 | 1.963718 | -0.794825 |
| 1 | -7.620565 | 1.007965 | 0.666648 |
| 6 | -1.584189 | 4.062816 | 0.132893 |
| 8 | -1.808398 | 5.232782 | 0.387369 |
| 7 | -0.287249 | 3.611036 | -0.075838 |
| 6 | 0.113512 | 2.288876 | 0.263469 |
| 6 | 0.989149 | -0.282573 | 0.935614 |
| 6 | 0.970507 | 1.589256 | -0.590574 |
| 6 | -0.312205 | 1.689429 | 1.451862 |
| 6 | 0.110922 | 0.407197 | 1.773781 |
| 6 | 1.406559 | 0.314987 | -0.258054 |
| 1 | 1.272735 | 2.046595 | -1.528116 |
| 1 | -0.978150 | 2.232351 | 2.115474 |
| 1 | -0.225514 | -0.073244 | 2.687185 |
| 1 | 2.056477 | -0.220441 | -0.942127 |
| 6 | 0.752218 | 4.639694 | -0.061126 |
| 1 | 0.411022 | 5.494431 | -0.644192 |
| 1 | 1.663534 | 4.229393 | -0.497941 |
| 1 | 0.960139 | 4.977423 | 0.960461 |
| 6 | 1.353522 | -1.679484 | 1.331415 |
| 8 | 0.573020 | -2.364103 | 1.986776 |
| 7 | 2.543965 | -2.220303 | 0.905227 |
| 6 | 2.700000 | -3.656077 | 1.146541 |
| 1 | 1.916835 | -4.205894 | 0.618517 |
| 1 | 2.617197 | -3.872385 | 2.214925 |
| 1 | 3.677755 | -3.968748 | 0.783214 |
| 6 | 3.693567 | -1.463773 | 0.549520 |
| 6 | 5.967110 | -0.020110 | -0.167329 |
| 6 | 4.101505 | -0.373088 | 1.322957 |
| 6 | 4.437075 | -1.836942 | -0.574053 |
| 6 | 5.572618 | -1.121241 | -0.929078 |
| 6 | 5.226610 | 0.350516 | 0.956088 |
| 1 | 3.530613 | -0.098853 | 2.204259 |
| 1 | 4.106605 | -2.678063 | -1.176250 |
| 1 | 6.148931 | -1.404420 | -1.802563 |
| 1 | 5.558554 | 1.202494 | 1.540191 |
| 6 | 7.170461 | 0.791392 | -0.503966 |
| 8 | 7.538697 | 1.754160 | 0.125818 |
| 8 | 7.809156 | 0.335332 | -1.593494 |
| 6 | 8.970882 | 1.079816 | -1.958642 |
| 1 | 9.701602 | 1.063480 | -1.147400 |
| 1 | 8.704446 | 2.116630 | -2.174114 |
| 1 | 9.368820 | 0.591205 | -2.846302 |

**4**$^{-}$**a** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1870.63840363 Hartree

| | | | |
|---|---|---|---|
| 1 | -1.207504 | 1.019656 | -2.846526 |
| 6 | -0.137450 | 1.096491 | -2.662558 |
| 6 | 2.611131 | 1.319788 | -2.280376 |
| 6 | 0.369830 | 2.248751 | -2.019407 |
| 6 | 0.677395 | 0.080150 | -3.105722 |
| 6 | 2.118326 | 0.111939 | -2.917992 |
| 6 | 1.785607 | 2.325417 | -1.872067 |
| 1 | 0.228445 | -0.760293 | -3.625444 |
| 1 | 2.194349 | 3.222996 | -1.413474 |
| 1 | 3.687339 | 1.384168 | -2.141798 |
| 7 | 2.976319 | -0.818567 | -3.264728 |
| 6 | 2.423679 | -1.962070 | -3.954002 |
| 1 | 3.218347 | -2.694322 | -4.140562 |
| 1 | 1.637945 | -2.492007 | -3.389303 |
| 1 | 1.983764 | -1.696878 | -4.933320 |
| 6 | -0.425970 | 3.401939 | -1.643634 |
| 8 | 0.032495 | 4.520756 | -1.419480 |
| 7 | -1.849901 | 3.251531 | -1.611607 |
| 6 | -2.459180 | 2.170997 | -0.945530 |
| 6 | -3.690222 | -0.000679 | 0.358353 |
| 6 | -1.832618 | 1.531587 | 0.134479 |
| 6 | -3.734039 | 1.731234 | -1.330159 |
| 6 | -4.344757 | 0.670432 | -0.675627 |
| 6 | -2.430620 | 0.454552 | 0.764540 |
| 1 | -0.866630 | 1.889792 | 0.469671 |
| 1 | -4.229626 | 2.211004 | -2.168780 |
| 1 | -5.333048 | 0.331447 | -0.971539 |
| 1 | -1.913909 | -0.026548 | 1.589290 |
| 6 | -2.581628 | 4.513311 | -1.594863 |
| 1 | -2.162108 | 5.175880 | -2.351808 |
| 1 | -2.498818 | 5.016036 | -0.622831 |
| 1 | -3.634736 | 4.327839 | -1.813518 |
| 6 | -4.396323 | -1.149867 | 1.000977 |
| 8 | -5.614408 | -1.181588 | 1.104865 |
| 7 | -3.620096 | -2.173894 | 1.520145 |
| 6 | -2.328806 | -2.491752 | 1.002271 |
| 6 | 0.233293 | -2.972781 | 0.009125 |
| 6 | -2.113117 | -2.558207 | -0.374348 |
| 6 | -1.268285 | -2.718454 | 1.881455 |
| 6 | 0.008892 | -2.949374 | 1.386500 |
| 6 | -0.837666 | -2.799965 | -0.866487 |
| 1 | -2.943398 | -2.385586 | -1.052685 |
| 1 | -1.445090 | -2.663149 | 2.952282 |
| 1 | 0.838654 | -3.085675 | 2.074106 |
| 1 | -0.651000 | -2.841541 | -1.934934 |
| 6 | -4.338313 | -3.226403 | 2.228015 |
| 1 | -5.067672 | -2.774088 | 2.900476 |
| 1 | -3.620826 | -3.819623 | 2.797322 |
| 1 | -4.874186 | -3.881741 | 1.530476 |
| 6 | 1.578436 | -3.241201 | -0.605340 |
| 8 | 1.677103 | -4.052448 | -1.513802 |
| 7 | 2.664812 | -2.579998 | -0.091807 |
| 6 | 3.945431 | -2.767214 | -0.785621 |
| 1 | 4.757950 | -2.602806 | -0.074112 |
| 1 | 4.011444 | -2.051309 | -1.618303 |
| 1 | 3.981536 | -3.787338 | -1.165957 |
| 6 | 2.569145 | -1.431125 | 0.747436 |
| 6 | 2.511801 | 0.808865 | 2.400280 |
| 6 | 1.795709 | -0.326742 | 0.389445 |
| 6 | 3.317040 | -1.410189 | 1.931255 |
| 6 | 3.284733 | -0.299123 | 2.758600 |
| 6 | 1.778366 | 0.792897 | 1.213754 |
| 1 | 1.232170 | -0.328020 | -0.539887 |
| 1 | 3.911628 | -2.281050 | 2.193317 |
| 1 | 3.850016 | -0.267093 | 3.684505 |
| 1 | 1.228465 | 1.673948 | 0.902648 |
| 6 | 2.511168 | 1.985013 | 3.308046 |
| 8 | 3.133967 | 2.061380 | 4.344218 |
| 8 | 1.727370 | 2.978626 | 2.855583 |
| 6 | 1.696850 | 4.145082 | 3.667411 |
| 1 | 2.702036 | 4.557840 | 3.781777 |
| 1 | 1.297594 | 3.912076 | 4.658069 |
| 1 | 1.049672 | 4.849284 | 3.146487 |

**4**$^{-}$**b** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1870.63777708 Hartree

| | | | |
|---|---|---|---|
| 6 | 1.648080 | -2.684250 | 0.914373 |
| 6 | 1.614108 | -1.548450 | 1.717344 |
| 6 | 0.382644 | -1.070622 | 2.175451 |
| 6 | -0.792929 | -1.714365 | 1.823112 |
| 6 | -0.761706 | -2.803310 | 0.936198 |
| 6 | 0.470272 | -3.292152 | 0.498242 |
| 7 | -1.947959 | -3.478542 | 0.539333 |
| 6 | -1.858909 | -4.919623 | 0.318795 |
| 6 | 2.906177 | -0.895518 | 2.052266 |
| 8 | 2.736314 | 0.359616 | 2.520661 |
| 6 | 3.948483 | 1.075060 | 2.766404 |
| 6 | -3.198382 | -2.903807 | 0.432559 |
| 8 | -4.222865 | -3.571242 | 0.428023 |
| 6 | -3.284572 | -1.416437 | 0.272125 |
| 6 | -4.259586 | -0.739655 | 0.999139 |
| 6 | -4.367953 | 0.640910 | 0.903668 |
| 6 | -3.555012 | 1.355155 | 0.016333 |
| 6 | -2.644098 | 0.657324 | -0.785882 |
| 6 | -2.476056 | -0.710524 | -0.620518 |
| 7 | -3.722167 | 2.762128 | -0.068946 |
| 6 | -5.086082 | 3.284267 | -0.011319 |
| 6 | -2.729274 | 3.722410 | -0.180658 |
| 8 | -3.047250 | 4.896594 | -0.317097 |
| 6 | -1.278734 | 3.346529 | -0.169190 |
| 6 | -0.469756 | 4.111613 | -1.013535 |
| 6 | 0.887013 | 3.852481 | -1.121753 |
| 6 | 1.475380 | 2.831786 | -0.366791 |
| 6 | 0.681049 | 2.109549 | 0.533507 |
| 6 | -0.681449 | 2.358685 | 0.624532 |
| 7 | 2.852639 | 2.575125 | -0.505203 |
| 6 | 3.774030 | 3.670614 | -0.226421 |
| 6 | 3.469607 | 1.313402 | -0.667305 |
| 8 | 4.673625 | 1.272537 | -0.385062 |
| 6 | 2.751735 | 0.166655 | -1.208965 |
| 6 | 1.459812 | 0.140904 | -1.788025 |
| 6 | 0.905584 | -1.008951 | -2.303099 |
| 6 | 1.607430 | -2.278563 | -2.295919 |
| 6 | 2.976146 | -2.187662 | -1.831747 |
| 6 | 3.497013 | -1.047290 | -1.295358 |
| 7 | 1.126869 | -3.452487 | -2.639144 |
| 6 | -0.258475 | -3.469315 | -3.032645 |
| 8 | 3.992107 | -1.409155 | 1.930550 |
| 1 | 0.876170 | 1.053418 | -1.866030 |
| 1 | -0.077264 | -0.948925 | -2.762976 |
| 1 | 4.511276 | -1.035457 | -0.908012 |
| 1 | 3.561116 | -3.103856 | -1.872671 |
| 1 | -0.557482 | -4.496453 | -3.278758 |
| 1 | -0.947785 | -3.115536 | -2.235089 |
| 1 | -0.486625 | -2.849718 | -3.920475 |
| 1 | 1.150259 | 1.335753 | 1.132527 |
| 1 | 1.499594 | 4.413874 | -1.821176 |
| 1 | -0.932416 | 4.899863 | -1.598339 |
| 1 | -1.279040 | 1.769924 | 1.314827 |
| 1 | 4.573748 | 3.691652 | -0.969742 |
| 1 | 4.242479 | 3.551180 | 0.757517 |
| 1 | 3.221048 | 4.611005 | -0.245491 |
| 1 | -2.036607 | 1.190152 | -1.509084 |
| 1 | -5.083740 | 1.173023 | 1.522482 |
| 1 | -4.908793 | -1.303587 | 1.662087 |
| 1 | -1.702330 | -1.225587 | -1.185034 |
| 1 | -5.159356 | 4.140342 | -0.680688 |
| 1 | -5.349536 | 3.618354 | 0.999120 |
| 1 | -5.775144 | 2.499945 | -0.325912 |
| 1 | -1.433462 | -5.131396 | -0.668073 |
| 1 | -2.864212 | -5.331160 | 0.380917 |
| 1 | -1.221153 | -5.367241 | 1.084802 |
| 1 | 0.529078 | -4.099571 | -0.223846 |
| 1 | -1.736369 | -1.366307 | 2.227323 |
| 1 | 0.351169 | -0.209710 | 2.836626 |
| 1 | 2.605066 | -3.056001 | 0.572284 |
| 1 | 4.541149 | 1.127854 | 1.849564 |
| 1 | 4.522860 | 0.582745 | 3.556165 |
| 1 | 3.635652 | 2.069960 | 3.086761 |

**4**$^{-}$**c** (M06-2X/6-31G(d) geometry, default G09 integration grid)

$E_{Tot}$ = -1870.63581869 Hartree

| | | | |
|---|---|---|---|
| 6 | -4.708289 | 1.057294 | -0.713217 |
| 6 | -5.276756 | 0.130289 | 0.164964 |
| 6 | -4.758164 | -1.166513 | 0.224473 |
| 6 | -3.687051 | -1.533507 | -0.575643 |
| 6 | -3.112539 | -0.601466 | -1.449364 |
| 6 | -3.645663 | 0.695117 | -1.522839 |
| 7 | -2.059249 | -0.991590 | -2.289761 |
| 6 | -2.040209 | -2.367023 | -2.790422 |
| 6 | -6.416820 | 0.571846 | 0.998899 |
| 8 | -6.879922 | -0.405015 | 1.809036 |
| 6 | -7.963810 | -0.016974 | 2.641870 |
| 6 | -1.022937 | -0.153401 | -2.668922 |
| 8 | -0.394377 | -0.334347 | -3.698467 |
| 6 | -0.591998 | 0.915280 | -1.705405 |
| 6 | 0.060054 | 2.030404 | -2.229839 |
| 6 | 0.640603 | 2.960129 | -1.378244 |
| 6 | 0.579281 | 2.772799 | 0.003239 |
| 6 | -0.087211 | 1.667826 | 0.527622 |
| 6 | -0.654501 | 0.723748 | -0.321554 |
| 7 | 1.235315 | 3.725487 | 0.862290 |
| 6 | 0.533459 | 4.991823 | 1.027447 |
| 6 | 2.627661 | 3.810004 | 0.798878 |
| 8 | 3.203597 | 4.883794 | 0.864151 |
| 6 | 3.334479 | 2.502990 | 0.691977 |
| 6 | 4.419408 | 2.354383 | -0.166167 |
| 6 | 5.037577 | 1.117623 | -0.321596 |
| 6 | 4.595060 | -0.006045 | 0.397696 |
| 6 | 3.560411 | 0.178664 | 1.336947 |
| 6 | 2.934788 | 1.401969 | 1.458039 |
| 7 | 5.213735 | -1.246929 | 0.223798 |
| 6 | 6.618174 | -1.261923 | -0.147434 |
| 6 | 4.647315 | -2.488245 | 0.667377 |
| 8 | 5.397286 | -3.337936 | 1.135996 |
| 6 | 3.214748 | -2.658789 | 0.494321 |
| 6 | 2.521689 | -3.523845 | 1.362951 |
| 6 | 1.152165 | -3.657409 | 1.328554 |
| 6 | 0.341311 | -2.937143 | 0.371759 |
| 6 | 1.094111 | -2.149679 | -0.578088 |
| 6 | 2.448556 | -1.989733 | -0.495698 |
| 7 | -0.980616 | -2.939262 | 0.302868 |
| 6 | -1.644252 | -3.728131 | 1.312139 |
| 8 | -6.905675 | 1.679899 | 0.982488 |
| 1 | 3.104427 | -4.073340 | 2.099646 |
| 1 | 0.673122 | -4.319860 | 2.041745 |
| 1 | 2.952886 | -1.353443 | -1.220233 |
| 1 | 0.537792 | -1.665479 | -1.375052 |
| 1 | -2.733590 | -3.616973 | 1.218531 |
| 1 | -1.427882 | -4.811003 | 1.242683 |
| 1 | -1.383891 | -3.431212 | 2.344909 |
| 1 | 3.237049 | -0.654492 | 1.948059 |
| 1 | 5.850881 | 1.016572 | -1.031805 |
| 1 | 4.761541 | 3.212070 | -0.738841 |
| 1 | 2.133739 | 1.519464 | 2.180435 |
| 1 | 7.009313 | -2.247573 | 0.099246 |
| 1 | 7.175757 | -0.501990 | 0.411707 |
| 1 | 6.753151 | -1.072856 | -1.220102 |
| 1 | -0.110828 | 1.522820 | 1.602773 |
| 1 | 1.177796 | 3.819402 | -1.772896 |
| 1 | 0.142055 | 2.128690 | -3.307827 |
| 1 | -1.082497 | -0.193512 | 0.082801 |
| 1 | 1.018225 | 5.562845 | 1.819911 |
| 1 | -0.503503 | 4.780907 | 1.297440 |
| 1 | 0.551386 | 5.594814 | 0.109702 |
| 1 | -1.679226 | -3.025871 | -1.991749 |
| 1 | -1.367577 | -2.395816 | -3.645866 |
| 1 | -3.047661 | -2.654207 | -3.105347 |
| 1 | -3.223382 | 1.408770 | -2.222799 |
| 1 | -3.233365 | -2.513532 | -0.492999 |
| 1 | -5.186049 | -1.884586 | 0.915864 |
| 1 | -5.128786 | 2.056743 | -0.761535 |
| 1 | -8.818717 | 0.299089 | 2.038716 |
| 1 | -7.671345 | 0.811303 | 3.292038 |
| 1 | -8.216294 | -0.897010 | 3.232534 |

**3⁻d···Li⁺** reactant (M06-2X/6-31G(d)/PCM geometry, Ultrafine integration grid)

$E_{Tot}$ = -1439.32424157 Hartree

| | | | |
|---|---|---|---|
| 6 | 1.488111 | -1.246733 | 0.479272 |
| 6 | 1.784034 | -2.504077 | -0.091276 |
| 6 | 2.966139 | -2.597964 | -0.842250 |
| 6 | 3.797332 | -1.517146 | -1.061730 |
| 6 | 3.496691 | -0.224017 | -0.528863 |
| 6 | 2.307810 | -0.160698 | 0.271680 |
| 6 | 1.035961 | -3.762284 | 0.113649 |
| 8 | 1.595411 | -4.853413 | 0.003961 |
| 7 | 4.240825 | 0.879763 | -0.716328 |
| 6 | 5.476067 | 0.677327 | -1.453589 |
| 7 | -0.306270 | -3.760383 | 0.492973 |
| 6 | -0.830824 | -5.085727 | 0.838632 |
| 6 | -1.238704 | -2.721051 | 0.265721 |
| 6 | -1.196748 | -1.926685 | -0.888141 |
| 6 | -2.127884 | -0.914049 | -1.072759 |
| 6 | -3.160100 | -0.719751 | -0.150571 |
| 6 | -3.238599 | -1.546145 | 0.968849 |
| 6 | -2.268211 | -2.512953 | 1.193929 |
| 6 | -4.214223 | 0.324385 | -0.355175 |
| 8 | -5.403815 | 0.071548 | -0.237736 |
| 7 | -3.778432 | 1.575995 | -0.742404 |
| 6 | -4.803236 | 2.553224 | -1.107740 |
| 6 | -2.497004 | 2.058362 | -0.362113 |
| 6 | -2.036446 | 1.862351 | 0.944279 |
| 6 | -0.762040 | 2.270944 | 1.302684 |
| 6 | 0.051325 | 2.904952 | 0.359854 |
| 6 | -0.426132 | 3.149367 | -0.930771 |
| 6 | -1.698212 | 2.730329 | -1.291637 |
| 6 | 1.454493 | 3.245905 | 0.674285 |
| 8 | 1.793518 | 3.007780 | 1.928940 |
| 6 | 3.186460 | 3.142423 | 2.252918 |
| 8 | 2.251354 | 3.671613 | -0.156692 |
| 3 | 3.638010 | 2.680421 | -1.036666 |
| 1 | 5.320572 | 0.315349 | -2.485001 |
| 1 | -2.303323 | -3.111307 | 2.098509 |
| 1 | -4.046326 | -1.405846 | 1.681100 |
| 1 | -0.422983 | -2.098278 | -1.628049 |
| 1 | -2.070374 | -0.287352 | -1.958316 |
| 1 | 0.615200 | -1.125740 | 1.115783 |
| 1 | 3.226044 | -3.566466 | -1.259875 |
| 1 | 4.689768 | -1.660428 | -1.660030 |
| 1 | 2.078857 | 0.779793 | 0.766830 |
| 1 | -0.393056 | 2.093697 | 2.306486 |
| 1 | 0.216718 | 3.643709 | -1.651300 |
| 1 | -2.062893 | 2.882426 | -2.302716 |
| 1 | -2.676550 | 1.370218 | 1.668945 |
| 1 | -4.336672 | 3.366508 | -1.663810 |
| 1 | -5.293320 | 2.959634 | -0.216707 |
| 1 | -5.552404 | 2.064798 | -1.729984 |
| 1 | -0.275815 | -5.504635 | 1.680210 |
| 1 | -0.724280 | -5.764820 | -0.011152 |
| 1 | -1.883295 | -4.999833 | 1.099619 |
| 1 | 6.022954 | 1.625318 | -1.521384 |
| 1 | 6.150686 | -0.047056 | -0.968251 |
| 1 | 3.256777 | 2.930392 | 3.316939 |
| 1 | 3.762201 | 2.413296 | 1.674404 |
| 1 | 3.526515 | 4.155769 | 2.035444 |

**3⁻d···Li⁺** transition state to macrocyclization (M06-2X/6-31G(d)/PCM geometry, Ultrafine integration grid)

$E_{Tot}$ = -1439.29184581 Hartree

| | | | |
|---|---|---|---|
| 6 | -0.440602 | -1.930204 | 0.867018 |
| 6 | -0.946638 | -2.872572 | -0.038525 |
| 6 | -0.059010 | -3.449149 | -0.952229 |
| 6 | 1.258269 | -3.023273 | -1.043486 |
| 6 | 1.746871 | -1.975380 | -0.221873 |
| 6 | 0.874059 | -1.516076 | 0.793861 |
| 6 | -2.372654 | -3.289776 | -0.074543 |
| 8 | -2.711610 | -4.435550 | -0.353229 |
| 7 | 2.993723 | -1.413441 | -0.362411 |
| 6 | 4.062458 | -2.332672 | -0.731553 |
| 7 | -3.334355 | -2.344301 | 0.244389 |
| 6 | -4.708459 | -2.835340 | 0.337777 |
| 6 | -3.121011 | -0.943151 | 0.131172 |
| 6 | -2.436052 | -0.411893 | -0.966953 |
| 6 | -2.136945 | 0.941586 | -1.014609 |
| 6 | -2.569334 | 1.795713 | 0.003066 |
| 6 | -3.333524 | 1.280746 | 1.050598 |
| 6 | -3.591188 | -0.082872 | 1.127758 |
| 6 | -2.302192 | 3.269670 | -0.036201 |
| 8 | -3.170623 | 4.079778 | 0.258936 |
| 7 | -1.061147 | 3.670989 | -0.477992 |
| 6 | -0.852220 | 5.110027 | -0.633096 |
| 6 | 0.105246 | 2.867213 | -0.286506 |
| 6 | 0.404577 | 2.343004 | 0.971569 |
| 6 | 1.536016 | 1.556467 | 1.149934 |
| 6 | 2.389748 | 1.277885 | 0.080188 |
| 6 | 2.123291 | 1.873915 | -1.154438 |
| 6 | 0.984755 | 2.649366 | -1.346279 |
| 6 | 3.635104 | 0.426755 | 0.247705 |
| 8 | 3.871092 | 0.228361 | 1.566752 |
| 6 | 4.984409 | -0.588277 | 1.894973 |
| 8 | 4.576321 | 0.541928 | -0.580622 |
| 3 | 3.763585 | -0.398971 | -2.018135 |
| 1 | 3.990547 | -2.738679 | -1.758941 |
| 1 | -4.129638 | -0.490541 | 1.978077 |
| 1 | -3.696214 | 1.952691 | 1.822237 |
| 1 | -2.106580 | -1.073686 | -1.761087 |
| 1 | -1.577139 | 1.340373 | -1.855035 |
| 1 | -1.082761 | -1.527449 | 1.645903 |
| 1 | -0.428879 | -4.224105 | -1.618410 |
| 1 | 1.909238 | -3.475600 | -1.785576 |
| 1 | 1.271815 | -0.838399 | 1.536239 |
| 1 | 1.766192 | 1.163047 | 2.133194 |
| 1 | 2.820111 | 1.764654 | -1.980083 |
| 1 | 0.771850 | 3.086592 | -2.317579 |
| 1 | -0.255319 | 2.551803 | 1.808666 |
| 1 | 0.022624 | 5.272152 | -1.263571 |
| 1 | -0.691616 | 5.592308 | 0.337621 |
| 1 | -1.732329 | 5.548416 | -1.102352 |
| 1 | -4.739967 | -3.713757 | 0.983085 |
| 1 | -5.088580 | -3.117503 | -0.649516 |
| 1 | -5.339172 | -2.050711 | 0.753993 |
| 1 | 5.021309 | -1.804292 | -0.659862 |
| 1 | 4.115292 | -3.203989 | -0.062551 |
| 1 | 5.222148 | -0.381224 | 2.938133 |
| 1 | 4.707690 | -1.640659 | 1.778967 |
| 1 | 5.839795 | -0.353658 | 1.258291 |

**5a** reactant (M06-2X/6-31G(d)/PCM geometry, Ultrafine integration grid)

$E_{Tot}$ = -1670.28234120 Hartree

| | | | |
|---|---|---|---|
| 6 | 4.478117 | 0.279602 | -1.945681 |
| 6 | 4.032112 | 0.711122 | -0.692528 |
| 6 | 4.378676 | 1.991378 | -0.262405 |
| 6 | 5.159461 | 2.821879 | -1.066204 |
| 6 | 5.604197 | 2.381786 | -2.310433 |
| 6 | 5.259893 | 1.103486 | -2.749801 |
| 6 | 3.214827 | -0.241265 | 0.175237 |
| 7 | 2.626848 | 0.309101 | 1.372660 |
| 6 | 1.606692 | 1.174144 | 1.184535 |
| 6 | 1.015235 | 1.491913 | -0.077835 |
| 6 | -0.073165 | 2.338208 | -0.171046 |
| 6 | -0.608787 | 2.978393 | 0.953703 |
| 6 | 0.000476 | 2.738271 | 2.197136 |
| 6 | 1.050679 | 1.854595 | 2.314841 |
| 6 | -1.779073 | 3.874943 | 0.873716 |
| 8 | -1.898103 | 4.891623 | 1.550279 |
| 1 | 4.022101 | 2.333162 | 0.704610 |
| 7 | -2.758888 | 3.533318 | -0.058688 |
| 6 | -3.823277 | 4.511173 | -0.271223 |
| 6 | -3.070414 | 2.169660 | -0.313283 |
| 6 | -3.062870 | 1.237943 | 0.730892 |
| 6 | -3.328733 | -0.098091 | 0.478847 |
| 6 | -3.651325 | -0.521080 | -0.813455 |
| 6 | -3.721273 | 0.417441 | -1.844114 |
| 6 | -3.415474 | 1.751578 | -1.602050 |
| 6 | -4.047061 | -1.935633 | -1.089041 |
| 8 | -4.949507 | -2.206838 | -1.867863 |
| 7 | -3.411472 | -2.916263 | -0.350726 |
| 6 | -3.923166 | -4.279555 | -0.499499 |
| 6 | -2.025907 | -2.821391 | -0.009008 |
| 6 | -1.622986 | -3.034697 | 1.311057 |
| 6 | -0.271368 | -3.046433 | 1.629554 |
| 6 | 0.682935 | -2.882214 | 0.621738 |
| 6 | 0.281796 | -2.660205 | -0.697769 |
| 6 | -1.071635 | -2.612060 | -1.007674 |
| 6 | 2.115512 | -3.038191 | 0.979411 |
| 8 | 2.840534 | -3.540488 | -0.006022 |
| 6 | 4.214765 | -3.834116 | 0.287631 |
| 8 | 2.583708 | -2.782921 | 2.082071 |
| 3 | 2.605063 | -0.958203 | 2.859362 |
| 1 | -3.424477 | 2.472449 | -2.414133 |
| 1 | -4.002085 | 0.089159 | -2.839967 |
| 1 | -2.833031 | 1.567237 | 1.738654 |
| 1 | -3.322471 | -0.810284 | 1.297460 |
| 1 | -0.512744 | 2.526815 | -1.148012 |
| 1 | -0.386293 | 3.248765 | 3.075961 |
| 1 | 1.503453 | 1.675464 | 3.288406 |
| 1 | 1.418635 | 1.062118 | -0.987798 |
| 1 | 1.026451 | -2.541931 | -1.478007 |
| 1 | 0.053500 | -3.219938 | 2.650566 |
| 1 | -2.375382 | -3.194679 | 2.077570 |
| 1 | -1.396437 | -2.447751 | -2.030732 |
| 1 | -3.566377 | -4.880288 | 0.338219 |
| 1 | -3.583808 | -4.731106 | -1.438767 |
| 1 | -5.012063 | -4.249392 | -0.495218 |
| 1 | -3.381793 | 5.503992 | -0.352562 |
| 1 | -4.535561 | 4.512274 | 0.561958 |
| 1 | -4.352949 | 4.270928 | -1.193626 |
| 1 | 3.900998 | -1.042803 | 0.479843 |
| 1 | 2.469604 | -0.726130 | -0.486416 |
| 1 | 4.268399 | -4.576388 | 1.085483 |
| 1 | 4.628917 | -4.229617 | -0.636606 |
| 1 | 4.744167 | -2.929979 | 0.590859 |
| 1 | 5.417570 | 3.818473 | -0.719595 |
| 1 | 6.210569 | 3.029711 | -2.936095 |
| 1 | 5.597893 | 0.751442 | -3.720227 |
| 1 | 4.206394 | -0.716700 | -2.291850 |

**5b** reactant (M06-2X/6-31G(d)/PCM geometry, Ultrafine integration grid)

$E_{Tot}$ = -1784.76095849 Hartree

| | | | |
|---|---|---|---|
| 6 | 4.155523 | -0.684069 | -1.267272 |
| 6 | 3.708003 | -0.315269 | -0.000778 |
| 6 | 4.333689 | 0.765739 | 0.626941 |
| 6 | 5.374428 | 1.446290 | 0.010645 |
| 6 | 5.817583 | 1.058374 | -1.257765 |
| 6 | 5.202458 | -0.015789 | -1.903370 |
| 6 | 2.592842 | -1.106468 | 0.676358 |
| 7 | 2.003939 | -0.504070 | 1.849198 |
| 6 | 1.248390 | 0.593915 | 1.631376 |
| 6 | 0.902062 | 1.118483 | 0.346823 |
| 6 | 0.048763 | 2.197189 | 0.215648 |
| 6 | -0.467408 | 2.871229 | 1.330193 |
| 6 | -0.074632 | 2.426351 | 2.604229 |
| 6 | 0.735868 | 1.322443 | 2.752666 |
| 6 | -1.393028 | 4.014763 | 1.210910 |
| 8 | -1.378206 | 4.975627 | 1.974274 |
| 1 | 3.985145 | 1.075485 | 1.607738 |
| 7 | -2.288046 | 3.983658 | 0.141531 |
| 6 | -3.077777 | 5.192363 | -0.081521 |
| 6 | -2.844196 | 2.754975 | -0.307857 |
| 6 | -3.191590 | 1.758366 | 0.610848 |
| 6 | -3.700853 | 0.547247 | 0.170523 |
| 6 | -3.910409 | 0.323707 | -1.193116 |
| 6 | -3.621833 | 1.340312 | -2.105195 |
| 6 | -3.076904 | 2.542291 | -1.669997 |
| 6 | -4.557263 | -0.929200 | -1.689724 |
| 8 | -5.350274 | -0.910845 | -2.620307 |
| 7 | -4.292438 | -2.092679 | -0.992628 |
| 6 | -5.055851 | -3.277495 | -1.387594 |
| 6 | -3.003465 | -2.361862 | -0.432779 |
| 6 | -2.896570 | -2.735708 | 0.908430 |
| 6 | -1.659906 | -3.086450 | 1.433096 |
| 6 | -0.533249 | -3.105811 | 0.606173 |
| 6 | -0.637856 | -2.733739 | -0.736059 |
| 6 | -1.869442 | -2.343398 | -1.248083 |
| 6 | 0.743125 | -3.606362 | 1.176278 |
| 8 | 1.499821 | -4.225139 | 0.285676 |
| 6 | 2.698090 | -4.844123 | 0.777977 |
| 8 | 1.052932 | -3.511193 | 2.357559 |
| 3 | 1.451472 | -1.768734 | 3.230117 |
| 1 | -2.811062 | 3.315163 | -2.385001 |
| 1 | -3.815886 | 1.173652 | -3.160040 |
| 1 | -3.046657 | 1.936278 | 1.671227 |
| 1 | -3.973225 | -0.213611 | 0.894212 |
| 1 | -0.213713 | 2.542644 | -0.781727 |
| 1 | -0.436596 | 2.960940 | 3.479296 |
| 1 | 1.030922 | 0.996321 | 3.748374 |
| 1 | 1.307770 | 0.663753 | -0.549836 |
| 1 | 0.237696 | -2.761206 | -1.376290 |
| 1 | -1.564951 | -3.380499 | 2.473512 |
| 1 | -3.787400 | -2.748398 | 1.529244 |
| 1 | -1.965579 | -2.053514 | -2.290138 |
| 1 | -4.988673 | -4.017982 | -0.589330 |
| 1 | -4.666238 | -3.710035 | -2.316361 |
| 1 | -6.096006 | -2.992099 | -1.540554 |
| 1 | -2.427796 | 6.062197 | 0.008010 |
| 1 | -3.885578 | 5.282035 | 0.654131 |
| 1 | -3.508824 | 5.160184 | -1.082667 |
| 1 | 3.026192 | -2.069157 | 0.979984 |
| 1 | 1.843294 | -1.351600 | -0.101748 |
| 1 | 2.437372 | -5.630908 | 1.487606 |
| 1 | 3.188824 | -5.261024 | -0.098095 |
| 1 | 3.338421 | -4.107971 | 1.265446 |
| 1 | 5.859567 | 2.290161 | 0.491435 |
| 8 | 6.844213 | 1.786664 | -1.780646 |
| 1 | 5.519700 | -0.334099 | -2.889644 |
| 1 | 3.676981 | -1.517057 | -1.779933 |
| 6 | 7.304662 | 1.426342 | -3.067389 |
| 1 | 8.111989 | 2.118055 | -3.306604 |
| 1 | 7.688972 | 0.399686 | -3.079732 |
| 1 | 6.509336 | 1.521698 | -3.815721 |

**5c** reactant (M06-2X/6-31G(d)/PCM geometry, Ultrafine integration grid)

$E_{Tot}$ = -1784.76783307 Hartree

| | | | |
|---|---|---|---|
| 6 | -1.931600 | -2.870009 | 1.403060 |
| 6 | -2.619770 | -2.828995 | 0.189210 |
| 6 | -1.925916 | -2.632661 | -1.006793 |
| 6 | -0.544857 | -2.491441 | -0.993511 |
| 6 | 0.139597 | -2.516428 | 0.223170 |
| 6 | -0.554956 | -2.690978 | 1.422608 |
| 7 | -4.033954 | -3.038745 | 0.163532 |
| 6 | -4.474212 | -4.431774 | 0.225857 |
| 6 | 1.619324 | -2.413815 | 0.270636 |
| 8 | 2.247837 | -1.986243 | 1.228730 |
| 6 | -4.873225 | -2.142494 | -0.468267 |
| 8 | -5.918407 | -2.499657 | -0.992159 |
| 6 | -4.476769 | -0.701745 | -0.402535 |
| 6 | -3.915549 | -0.158307 | 0.756213 |
| 6 | -3.622073 | 1.193913 | 0.825409 |
| 6 | -3.847727 | 2.022382 | -0.279737 |
| 6 | -4.423792 | 1.482112 | -1.434280 |
| 6 | -4.753128 | 0.132707 | -1.485838 |
| 7 | -3.547764 | 3.408944 | -0.213039 |
| 6 | -4.679831 | 4.327295 | -0.329320 |
| 6 | -2.462000 | 3.873008 | 0.533756 |
| 8 | -2.551676 | 4.934248 | 1.144589 |
| 6 | -1.215091 | 3.085392 | 0.493004 |
| 6 | -0.810010 | 2.339140 | -0.621535 |
| 6 | 0.423723 | 1.712826 | -0.669402 |
| 6 | 1.341297 | 1.778709 | 0.427399 |
| 6 | 0.872758 | 2.492854 | 1.579162 |
| 6 | -0.336598 | 3.146444 | 1.592369 |
| 7 | 2.582904 | 1.256983 | 0.454766 |
| 6 | 3.109523 | 0.784005 | -0.811762 |
| 8 | 2.194589 | -2.890990 | -0.822884 |
| 6 | 3.627928 | -2.959610 | -0.837063 |
| 3 | 2.930265 | -0.169154 | 1.724348 |
| 6 | 4.625166 | 0.839553 | -0.831347 |
| 1 | -4.601548 | 2.122108 | -2.293250 |
| 1 | -5.212599 | -0.287606 | -2.375143 |
| 1 | -3.210896 | 1.616930 | 1.735870 |
| 1 | -3.740590 | -0.789741 | 1.621138 |
| 1 | -1.470524 | 2.266507 | -1.482867 |
| 1 | -0.632021 | 3.730986 | 2.460066 |
| 1 | 1.545693 | 2.568315 | 2.430627 |
| 1 | 0.688853 | 1.154290 | -1.561005 |
| 1 | 0.002864 | -2.361719 | -1.920591 |
| 1 | -0.008128 | -2.705305 | 2.359763 |
| 1 | -2.485728 | -3.024135 | 2.324089 |
| 1 | -2.474118 | -2.606454 | -1.943816 |
| 1 | -3.912552 | -4.941864 | 1.009896 |
| 1 | -4.308482 | -4.944077 | -0.728852 |
| 1 | -5.538054 | -4.454690 | 0.459134 |
| 1 | -4.305330 | 5.324756 | -0.556377 |
| 1 | -5.253634 | 4.373159 | 0.603644 |
| 1 | -5.333544 | 3.991403 | -1.134491 |
| 1 | 2.776261 | -0.247313 | -1.055278 |
| 1 | 2.764320 | 1.401367 | -1.655014 |
| 1 | 3.978621 | -3.489646 | 0.050436 |
| 1 | 3.879736 | -3.511078 | -1.739972 |
| 1 | 4.056157 | -1.956692 | -0.865294 |
| 6 | 5.418172 | 0.156377 | 0.106794 |
| 6 | 6.808312 | 0.228854 | 0.073575 |
| 6 | 7.436075 | 0.993303 | -0.910179 |
| 6 | 6.677947 | 1.678691 | -1.849325 |
| 6 | 5.286455 | 1.596297 | -1.796375 |
| 8 | 4.751094 | -0.598297 | 1.048200 |
| 1 | 7.407773 | -0.298276 | 0.806465 |
| 1 | 8.519883 | 1.047085 | -0.929684 |
| 1 | 7.159281 | 2.276188 | -2.616457 |
| 1 | 4.688450 | 2.134826 | -2.526905 |
| 6 | 5.489780 | -1.591203 | 1.750028 |
| 1 | 4.750628 | -2.211956 | 2.257323 |
| 1 | 6.068507 | -2.202394 | 1.050111 |
| 1 | 6.160435 | -1.136667 | 2.484904 |

**5a→6a** transition state (M06-2X/6-31G(d)/PCM geometry, Ultrafine integration grid)

$E_{Tot}$ = -1670.26557667 Hartree

| | | | |
|---|---|---|---|
| 6 | 4.099942 | 1.206357 | -2.141613 |
| 6 | 4.184653 | 0.256198 | -1.123299 |
| 6 | 5.321602 | 0.260443 | -0.307347 |
| 6 | 6.331404 | 1.200466 | -0.484622 |
| 6 | 6.224299 | 2.156349 | -1.495373 |
| 6 | 5.109288 | 2.151582 | -2.327680 |
| 6 | 3.096896 | -0.781468 | -0.897474 |
| 7 | 2.449443 | -0.665567 | 0.403126 |
| 6 | 1.533446 | 0.365104 | 0.535428 |
| 6 | 1.067012 | 1.170416 | -0.530304 |
| 6 | 0.145061 | 2.185995 | -0.324302 |
| 6 | -0.325496 | 2.490611 | 0.953115 |
| 6 | 0.122834 | 1.712962 | 2.024681 |
| 6 | 0.992764 | 0.656168 | 1.817274 |
| 6 | -1.277335 | 3.618606 | 1.173761 |
| 8 | -1.101144 | 4.483944 | 2.020459 |
| 1 | 5.426154 | -0.500320 | 0.463693 |
| 7 | -2.363052 | 3.650628 | 0.312429 |
| 6 | -3.276521 | 4.783579 | 0.426687 |
| 6 | -2.934026 | 2.400907 | -0.086303 |
| 6 | -3.238559 | 1.458794 | 0.897999 |
| 6 | -3.679090 | 0.196126 | 0.537918 |
| 6 | -3.854399 | -0.123625 | -0.809793 |
| 6 | -3.645260 | 0.850348 | -1.786629 |
| 6 | -3.172115 | 2.110079 | -1.428492 |
| 6 | -4.308313 | -1.494786 | -1.208964 |
| 8 | -5.190028 | -1.666844 | -2.039058 |
| 7 | -3.714846 | -2.541664 | -0.538239 |
| 6 | -4.198204 | -3.885016 | -0.850264 |
| 6 | -2.344450 | -2.459969 | -0.109531 |
| 6 | -2.014248 | -2.551501 | 1.239882 |
| 6 | -0.678194 | -2.498702 | 1.632907 |
| 6 | 0.330393 | -2.396529 | 0.678081 |
| 6 | -0.003043 | -2.320609 | -0.675634 |
| 6 | -1.334388 | -2.341297 | -1.067569 |
| 6 | 1.766133 | -2.444175 | 1.126878 |
| 8 | 2.457066 | -3.290621 | 0.305930 |
| 6 | 3.730409 | -3.708951 | 0.774859 |
| 8 | 2.079996 | -2.354858 | 2.343671 |
| 3 | 3.270017 | -0.888621 | 2.270856 |
| 1 | -2.947651 | 2.856618 | -2.184676 |
| 1 | -3.818371 | 0.602967 | -2.829404 |
| 1 | -3.092128 | 1.715266 | 1.943466 |
| 1 | -3.889899 | -0.545082 | 1.301141 |
| 1 | -0.203389 | 2.768584 | -1.173611 |
| 1 | -0.243717 | 1.923493 | 3.026267 |
| 1 | 1.251554 | 0.026314 | 2.664822 |
| 1 | 1.424161 | 1.003280 | -1.537532 |
| 1 | 0.784247 | -2.251575 | -1.419408 |
| 1 | -0.405384 | -2.555873 | 2.681635 |
| 1 | -2.805882 | -2.654002 | 1.976579 |
| 1 | -1.603658 | -2.276527 | -2.118461 |
| 1 | -3.891488 | -4.558646 | -0.048733 |
| 1 | -3.788729 | -4.246222 | -1.801189 |
| 1 | -5.285375 | -3.863657 | -0.920524 |
| 1 | -2.693897 | 5.699179 | 0.525513 |
| 1 | -3.929916 | 4.684521 | 1.301963 |
| 1 | -3.889850 | 4.832573 | -0.474622 |
| 1 | 3.551914 | -1.774444 | -0.947889 |
| 1 | 2.385005 | -0.739633 | -1.736250 |
| 1 | 3.647540 | -4.182573 | 1.754720 |
| 1 | 4.100236 | -4.420430 | 0.037002 |
| 1 | 4.428183 | -2.865712 | 0.837860 |
| 1 | 7.207534 | 1.182377 | 0.156943 |
| 1 | 7.009579 | 2.892492 | -1.636394 |
| 1 | 5.020848 | 2.884499 | -3.124002 |
| 1 | 3.239426 | 1.204874 | -2.806378 |

**5b→6b** transition state (M06-2X/6-31G(d)/PCM geometry, Ultrafine integration grid)

$E_{Tot}$ = -1784.74485302 Hartree

| | | | |
|---|---|---|---|
| 6 | 3.992615 | 0.184602 | -1.723899 |
| 6 | 3.772166 | -0.716735 | -0.687429 |
| 6 | 4.785029 | -0.860446 | 0.271089 |
| 6 | 5.954068 | -0.120799 | 0.205341 |
| 6 | 6.149330 | 0.792297 | -0.839221 |
| 6 | 5.164684 | 0.940375 | -1.814263 |
| 6 | 2.502680 | -1.548983 | -0.606989 |
| 7 | 1.766485 | -1.391852 | 0.641278 |
| 6 | 1.096375 | -0.188044 | 0.792848 |
| 6 | 0.951196 | 0.783647 | -0.225091 |
| 6 | 0.264940 | 1.969242 | -0.004167 |
| 6 | -0.265252 | 2.277562 | 1.248502 |
| 6 | -0.133114 | 1.334550 | 2.272369 |
| 6 | 0.490764 | 0.120916 | 2.040099 |
| 6 | -0.952831 | 3.580317 | 1.490099 |
| 8 | -0.665389 | 4.325373 | 2.416831 |
| 1 | 4.665031 | -1.579553 | 1.078688 |
| 7 | -1.915360 | 3.921478 | 0.552647 |
| 6 | -2.545178 | 5.231686 | 0.686601 |
| 6 | -2.720201 | 2.871857 | 0.008704 |
| 6 | -3.309018 | 1.955575 | 0.882706 |
| 6 | -3.998774 | 0.863803 | 0.383213 |
| 6 | -4.140170 | 0.699233 | -0.996014 |
| 6 | -3.638030 | 1.667996 | -1.865266 |
| 6 | -2.914472 | 2.748184 | -1.366155 |
| 6 | -4.863173 | -0.493085 | -1.544370 |
| 8 | -5.692843 | -0.392217 | -2.437489 |
| 7 | -4.578269 | -1.695977 | -0.937072 |
| 6 | -5.329176 | -2.863600 | -1.393122 |
| 6 | -3.267755 | -1.965219 | -0.411237 |
| 6 | -3.092834 | -2.267156 | 0.936761 |
| 6 | -1.819760 | -2.556043 | 1.424182 |
| 6 | -0.727170 | -2.580765 | 0.560377 |
| 6 | -0.908286 | -2.292051 | -0.793266 |
| 6 | -2.170413 | -1.974206 | -1.275690 |
| 6 | 0.612570 | -3.007704 | 1.097955 |
| 8 | 1.164547 | -3.913890 | 0.235236 |
| 6 | 2.256521 | -4.664607 | 0.744647 |
| 8 | 0.816909 | -3.116353 | 2.336593 |
| 3 | 2.325601 | -2.000639 | 2.515058 |
| 1 | -2.466653 | 3.475797 | -2.036644 |
| 1 | -3.783751 | 1.549476 | -2.934569 |
| 1 | -3.190898 | 2.090666 | 1.954081 |
| 1 | -4.431519 | 0.136684 | 1.061853 |
| 1 | 0.155616 | 2.681045 | -0.818847 |
| 1 | -0.555328 | 1.546890 | 3.251496 |
| 1 | 0.499129 | -0.618929 | 2.836461 |
| 1 | 1.377840 | 0.615567 | -1.204971 |
| 1 | -0.058827 | -2.325410 | -1.467732 |
| 1 | -1.664813 | -2.782381 | 2.473998 |
| 1 | -3.954026 | -2.265005 | 1.598986 |
| 1 | -2.319722 | -1.743144 | -2.327002 |
| 1 | -5.254037 | -3.643075 | -0.633390 |
| 1 | -4.934631 | -3.246143 | -2.341972 |
| 1 | -6.372451 | -2.582050 | -1.532961 |
| 1 | -1.775161 | 5.975456 | 0.890310 |
| 1 | -3.273677 | 5.243918 | 1.506208 |
| 1 | -3.053108 | 5.474329 | -0.248228 |
| 1 | 2.773737 | -2.604228 | -0.696254 |
| 1 | 1.886833 | -1.328733 | -1.493702 |
| 1 | 1.963267 | -5.222636 | 1.635851 |
| 1 | 2.548424 | -5.346376 | -0.053736 |
| 1 | 3.105410 | -4.015025 | 0.988216 |
| 1 | 6.739356 | -0.235679 | 0.945794 |
| 8 | 7.325214 | 1.475827 | -0.818145 |
| 1 | 5.289524 | 1.633311 | -2.637949 |
| 1 | 3.235623 | 0.306785 | -2.495742 |
| 6 | 7.551733 | 2.408341 | -1.857561 |
| 1 | 8.528519 | 2.849602 | -1.662033 |
| 1 | 7.562937 | 1.915920 | -2.836626 |
| 1 | 6.788666 | 3.194934 | -1.857445 |

**5c→6c** transition state (M06-2X/6-31G(d)/PCM geometry, Ultrafine integration grid)

$E_{Tot}$ = -1784.75464592 Hartree

| | | | |
|---|---|---|---|
| 6 | 2.196974 | -2.708070 | -1.260354 |
| 6 | 2.663148 | -2.502805 | 0.035626 |
| 6 | 1.760441 | -2.224034 | 1.065292 |
| 6 | 0.400843 | -2.159163 | 0.797317 |
| 6 | -0.069593 | -2.363086 | -0.501064 |
| 6 | 0.831855 | -2.623748 | -1.529765 |
| 7 | 4.063473 | -2.619357 | 0.332295 |
| 6 | 4.550812 | -3.974050 | 0.582423 |
| 6 | -1.545164 | -2.401532 | -0.794004 |
| 8 | -1.998074 | -2.348993 | -1.964969 |
| 6 | 4.754798 | -1.586429 | 0.924697 |
| 8 | 5.723690 | -1.779235 | 1.646655 |
| 6 | 4.290388 | -0.204201 | 0.580598 |
| 6 | 3.928418 | 0.118097 | -0.728991 |
| 6 | 3.484730 | 1.394406 | -1.030046 |
| 6 | 3.358466 | 2.350234 | -0.019094 |
| 6 | 3.778222 | 2.052498 | 1.276655 |
| 6 | 4.257951 | 0.778688 | 1.570126 |
| 7 | 2.790444 | 3.622173 | -0.338261 |
| 6 | 3.716548 | 4.738714 | -0.501728 |
| 6 | 1.623364 | 3.648111 | -1.085780 |
| 8 | 1.394808 | 4.543484 | -1.887888 |
| 6 | 0.661060 | 2.544388 | -0.799513 |
| 6 | 0.291462 | 2.233798 | 0.509921 |
| 6 | -0.634731 | 1.236425 | 0.779574 |
| 6 | -1.196028 | 0.453276 | -0.256625 |
| 6 | -0.770310 | 0.757554 | -1.576854 |
| 6 | 0.102498 | 1.797825 | -1.842470 |
| 7 | -2.107025 | -0.566045 | -0.071929 |
| 6 | -2.804259 | -0.602716 | 1.201036 |
| 8 | -2.156330 | -3.191474 | 0.139483 |
| 6 | -3.455762 | -3.663484 | -0.196192 |
| 3 | -3.233889 | -0.900524 | -1.671580 |
| 6 | -3.876937 | 0.465336 | 1.272421 |
| 1 | 3.692019 | 2.806877 | 2.053241 |
| 1 | 4.575212 | 0.527449 | 2.577552 |
| 1 | 3.200694 | 1.653114 | -2.045884 |
| 1 | 3.997694 | -0.631225 | -1.510257 |
| 1 | 0.725694 | 2.796247 | 1.333127 |
| 1 | 0.379889 | 2.025903 | -2.868758 |
| 1 | -1.152627 | 0.158801 | -2.400728 |
| 1 | -0.914791 | 1.058498 | 1.811222 |
| 1 | -0.306182 | -1.950873 | 1.594833 |
| 1 | 0.455028 | -2.775390 | -2.536152 |
| 1 | 2.907568 | -2.922632 | -2.053770 |
| 1 | 2.135209 | -2.064974 | 2.072786 |
| 1 | 4.153582 | -4.635264 | -0.189105 |
| 1 | 4.230716 | -4.336193 | 1.566550 |
| 1 | 5.639643 | -3.971997 | 0.544314 |
| 1 | 3.151226 | 5.670416 | -0.501378 |
| 1 | 4.272361 | 4.662922 | -1.443906 |
| 1 | 4.421424 | 4.736169 | 0.331255 |
| 1 | -3.275000 | -1.585349 | 1.295378 |
| 1 | -2.147633 | -0.503194 | 2.079086 |
| 1 | -3.436432 | -4.207129 | -1.142778 |
| 1 | -3.746406 | -4.327869 | 0.617397 |
| 1 | -4.174431 | -2.838746 | -0.261846 |
| 6 | -4.937133 | 0.470518 | 0.348577 |
| 6 | -5.929872 | 1.443713 | 0.394956 |
| 6 | -5.872066 | 2.440051 | 1.371954 |
| 6 | -4.833666 | 2.458933 | 2.292136 |
| 6 | -3.847736 | 1.472754 | 2.231584 |
| 8 | -4.944069 | -0.542346 | -0.596236 |
| 1 | -6.747219 | 1.439474 | -0.316582 |
| 1 | -6.648019 | 3.198230 | 1.401316 |
| 1 | -4.785907 | 3.231572 | 3.052323 |
| 1 | -3.036081 | 1.476008 | 2.954902 |
| 6 | -6.179399 | -0.810549 | -1.256514 |
| 1 | -6.037401 | -1.748543 | -1.794427 |
| 1 | -6.984401 | -0.921739 | -0.525092 |
| 1 | -6.428123 | -0.016572 | -1.966357 |

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