Oligorotaxane Radicals Under Orders

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Supporting Information

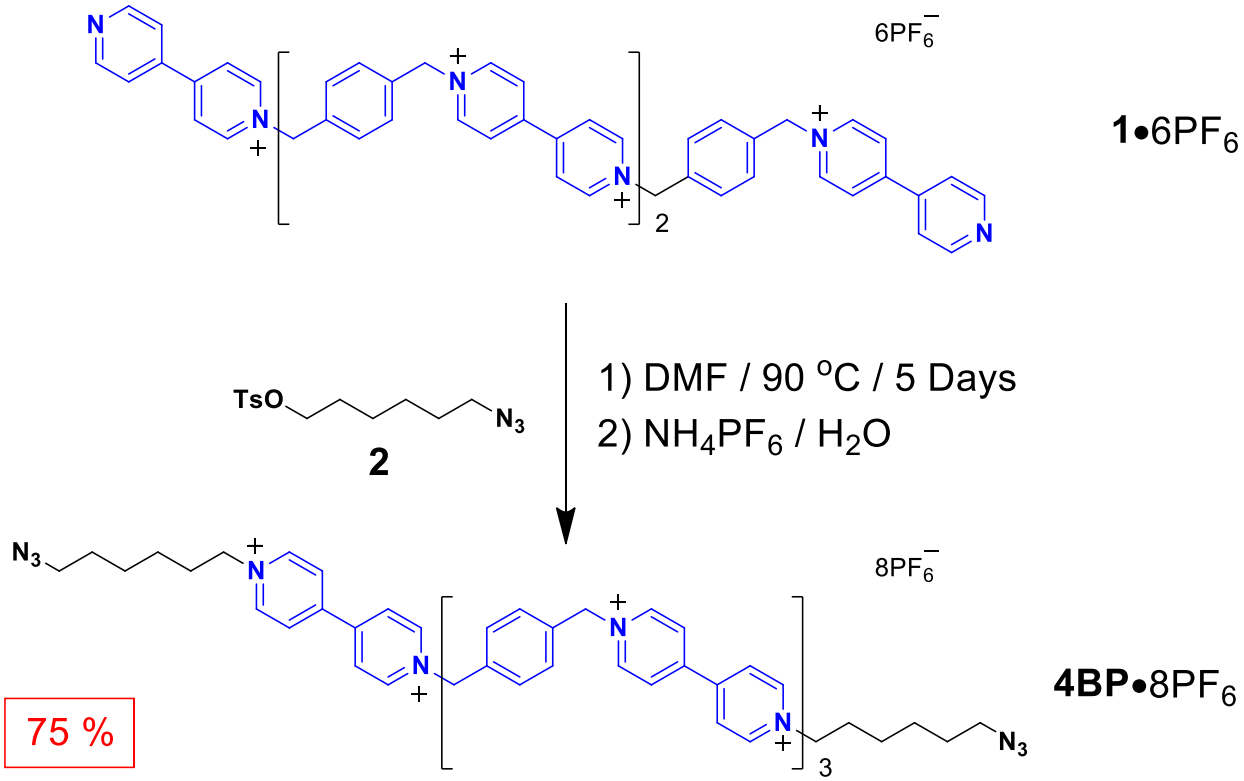
Table of Contents

1. Materials and General Methods

Chemicals were purchased as reagent grade and used without further purification. Commercial grades of anhydrous MeCN and *N*,*N*-dimethylformamide (DMF) were used as solvents in all reactions. Benzyl viologen **BnV**•$2PF_6$ and compounds **1**•$6PF_6$ and **3**•$8PF_6$ were prepared[1,2] according to literature procedures. Thin layer chromatography (TLC) was performed on silica gel 60F254 (E Merck). Column chromatography was carried out on silica gel 60F (Merck 9385, 0.040–0.063 mm). High performance liquid chromatography (HPLC) was performed on a preparative RP-HPLC instrument, using a C_{18} column (Agilent, 10μm packing, 30 mm × 250 mm). The eluents employed were MeCN and H_2O, both mixed with 0.1 % (v/v) trifluoroacetic acid (TFA). The detector was set to $\lambda = 254$ nm. HPLC Analyses were performed on an analytical RP-HPLC instrument, using a C_{18} column. For UV/Vis/Near Infrared (NIR) studies, all sample preparations were completed in an Argon-filled atmosphere. Samples were loaded into quartz 1 cm tubes and sealed with a clear ridged UV doming epoxy (IllumaBond 60-7160RCL) and used immediately after preparation. Nuclear magnetic resonance (NMR) spectra were recorded at 298 K on Bruker Avance 500 and 600 spectrometers, with working frequencies of 500 and 600 MHz for ^1H, and 125 and 150 MHz for ^{13}C nuclei, respectively. Chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents.[3] EPR Spectra were recorded using a Bruker Elexsys E580-X EPR spectrometer, equipped with a variable Q dielectric resonator (ER-4118X-MD5-W1). Samples were prepared by reduction with cobaltocene and the solution was loaded into quartz 1.4 mm tubes and sealed with a clear ridged UV doming epoxy (IllumaBond 60-7160RCL). Samples were used immediately after preparation. Solution CW-EPR spectra were collected with a 0.4 G modulation amplitude 5.12 ms time constant and 20.48 ms conversion time. High-resolution mass spectra were measured on an Agilent 6210 Time-of-Flight (TOF) LC-MS, using an ESI source, coupled with Agilent 1100 HPLC stack, using direct infusion (0.6 mL min^{-1}). Measurements at X-band (9.5 GHz) were performed with a Bruker Elexsys E580, equipped with a variable Q dielectric resonator (ER-4118X-MD5-W1). Cyclic voltammetry experiments were performed on a Princeton Applied Research 263 A Multipurpose instrument interfaced to a PC, using a glassy carbon working electrode (0.071 cm^2, Cypress system). The electrode surface was polished routinely with an alumina/water slurry on a felt surface immediately before use. The counter electrode was a Pt coil and the reference electrode was an AgCl coated Ag wire. The concentrations of the samples were 1 mM in 100 mM electrolyte solutions of tetrabutylammonium hexafluorophosphate ($TBAPF_6$) in MeCN.

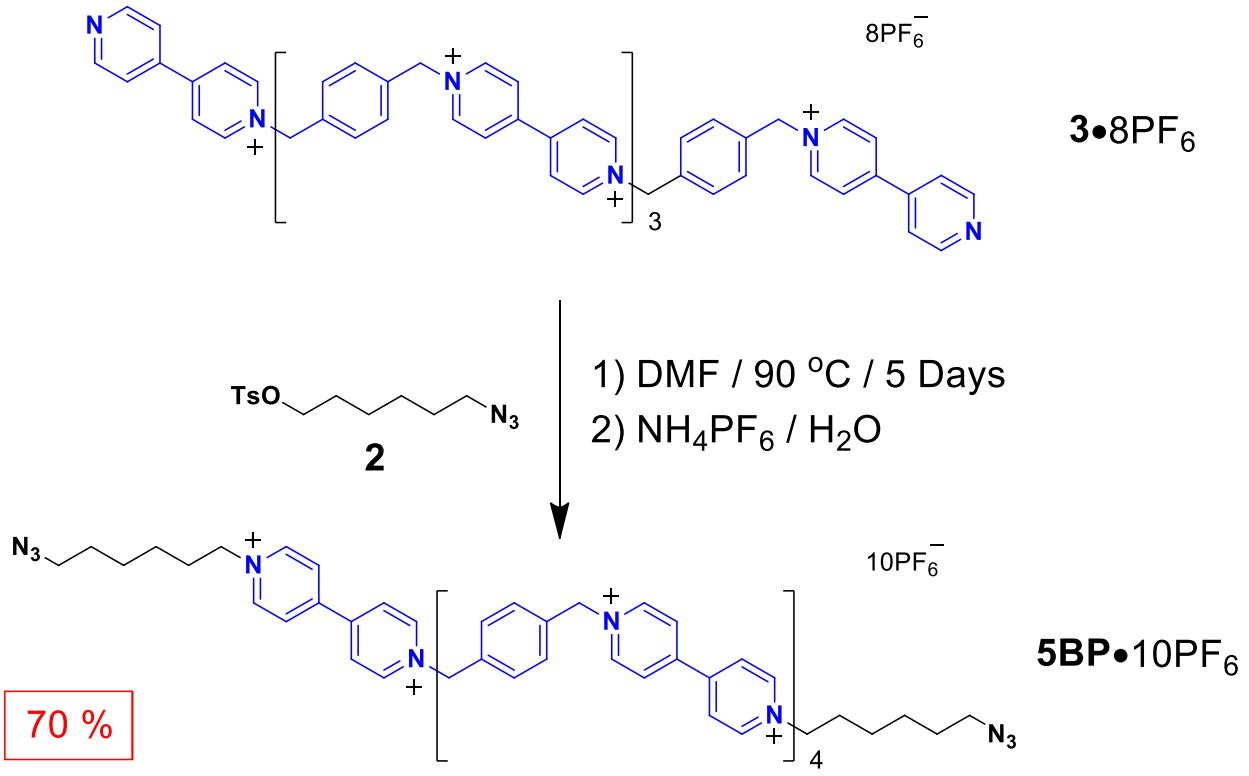
2. Synthetic Protocols

Scheme S1. One-Step Synthesis of 4BP•8PF$_6$ from 1•6PF$_6$



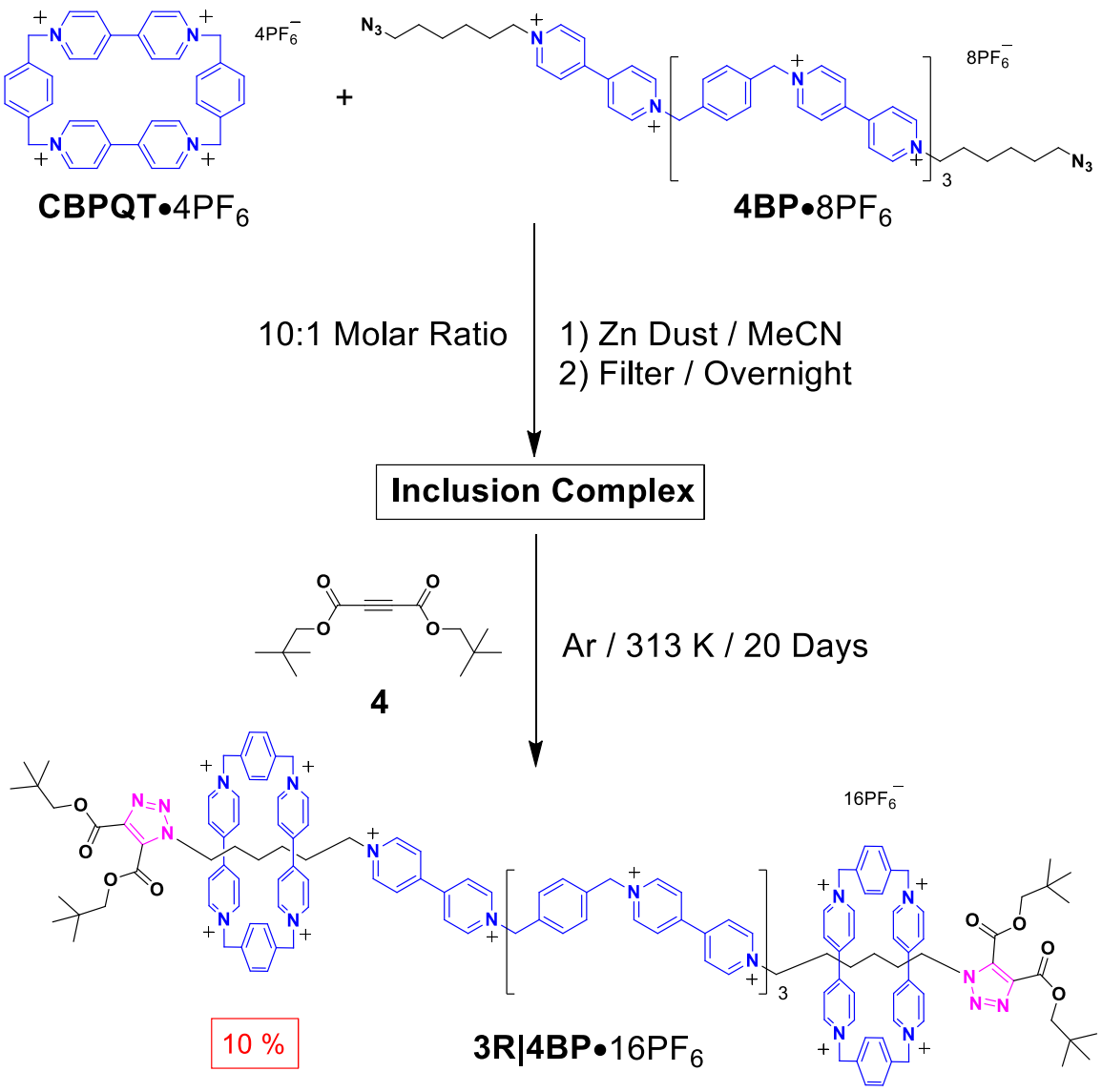
4BP•8PF$_6$: **1**•6PF$_6$ (90 mg, 0.05 mmol) and **2** (148 mg, 0.5 mmol) were dissolved in DMF (10 mL) at room temperature. The reaction mixture was heated to 90 °C for 5 days and cooled down to room temperature, then Me_2CO was added to the solution. The resulting precipitate was filtered off, washed with Me_2CO, re-dissolved in H_2O, and re-precipitated by adding an excess of NH_4PF_6. The solid was filtered off and washed with H_2O, MeOH and finally Et_2O to afford **4BP**•8PF$_6$ as a yellow solid (85 mg, 75 %). ^{1}H NMR (500 MHz, CD_3CN): δ = 8.98 (d, *J* = 6.9 Hz, 12H), 8.92 (d, *J* = 6.9 Hz, 4H), 8.42 (d, *J* = 5.1 Hz, 12H), 8.39 (d, *J* = 5.1 Hz, 4H), 7.62 (s, 12H), 5.87 (s, 12H), 4.64 (t, *J* = 7.6 Hz, 4H), 3.33 (t, *J* = 6.8 Hz, 4H), 2.05 (p, *J* = 7.4 Hz, 4H), 1.69 – 1.60 (m, 4H), 1.51 – 1.38 (m, 8H). ^{13}C NMR (126 MHz, CD_3CN): δ = 150.1, 145.3, 134.0, 130.0, 127.2, 127.2, 126.8, 63.5, 50.5, 30.4, 27.8, 25.3, 24.7. HRMS (ESI): *m/z* calcd for $C_{76}H_{80}F_{36}N_{14}P_6$ $[M - 2PF_6]^{2+}$ 1029.7279, found 1029.7287.

Scheme S2. One-Step Synthesis of 5BP•10PF$_6$ from 3•8PF$_6$



5BP•10PF$_6$: **3**•8PF$_6$ (70 mg, 0.03 mmol) and **2** (89 mg, 0.3 mmol) were dissolved in DMF (10 mL) at room temperature. The reaction mixture was heated to 90 °C for 5 days and cooled down to room temperature, then Me_2CO was added to the solution. The resulting precipitate was filtered off, washed with Me_2CO, re-dissolved in H_2O, and re-precipitated by adding an excess of NH_4PF_6. The solid was filtered off and washed with H_2O, MeOH and finally Et_2O to afford **5BP**•10PF$_6$ as a yellow solid (61 mg, 70 %). ^{1}H NMR (500 MHz, CD_3CN): δ = 8.98 (d, *J* = 6.9 Hz, 16H), 8.92 (d, *J* = 6.9 Hz, 4H), 8.42 (d, *J* = 5.1 Hz, 16H), 8.39 (d, *J* = 5.1 Hz, 4H), 7.62 (s, 12H), 7.61 (s, 4H), 5.87 (s, 16H), 4.64 (t, *J* = 7.6 Hz, 4H), 3.33 (t, *J* = 6.8 Hz, 4H), 2.05 (p, *J* = 7.4 Hz, 4H), 1. 69 – 1.60 (m, 4H), 1.51 – 1.38 (m, 8H). ^{13}C NMR (126 MHz, CD_3CN): δ = 150.1, 145.3, 134.0, 130.0, 127.2, 127.2, 126.9, 63.5, 50.5, 30.4, 27.8, 25.3, 24.7. HRMS (ESI): *m/z* calcd for $C_{94}H_{96}F_{48}N_{16}P_8$ $[M - 2PF_6]^{2+}$ 1304.7578, found 1304.7573.

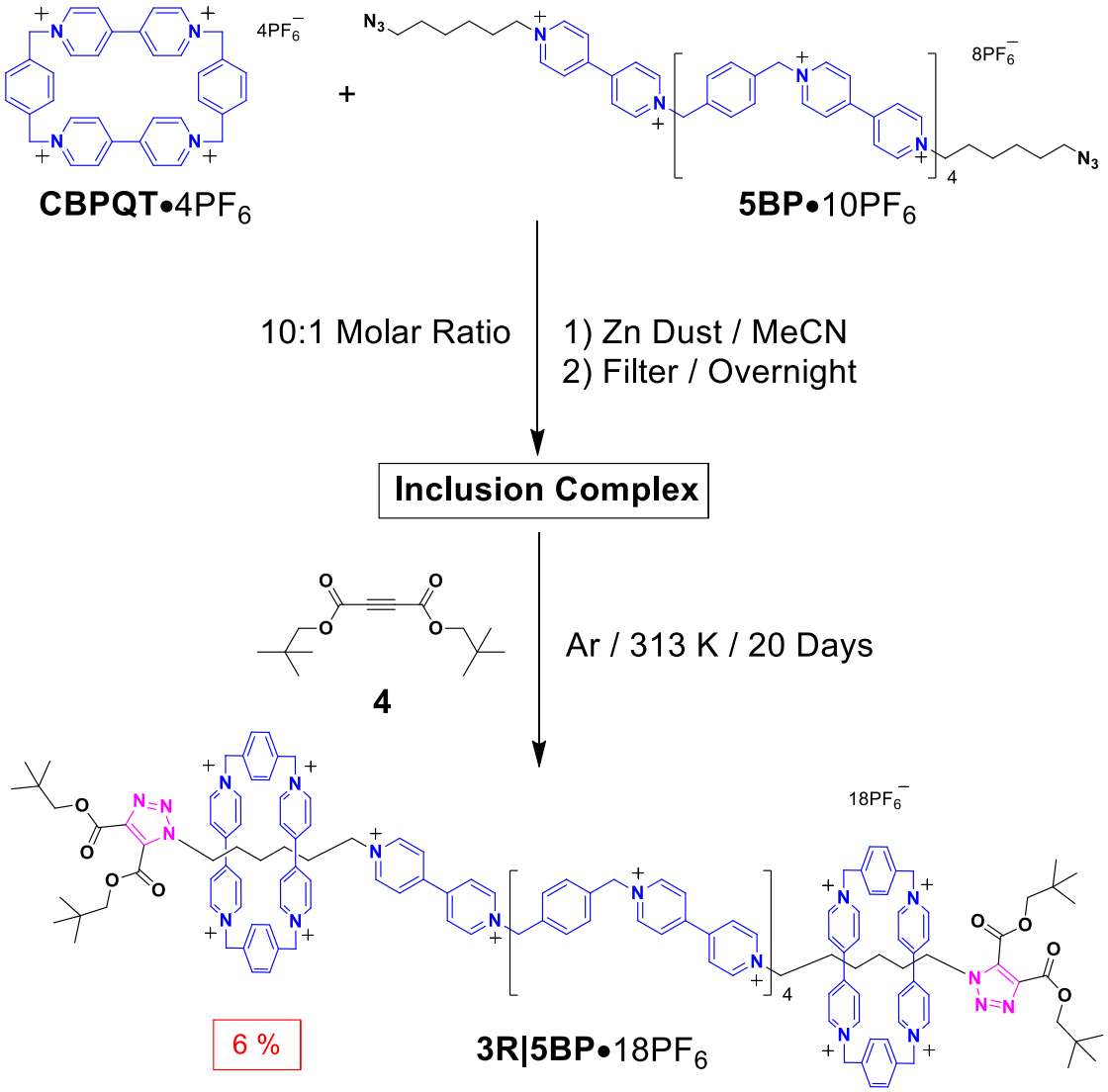
Scheme S3. Synthesis of 3R|4BP•16PF$_6$ Templated by Radical-Pairing Interactions



3R|4BP•16PF$_6$: **S3**•8PF$_6$ (46 mg, 0.02 mmol) and **CBPQT**•4PF$_6$ (220 mg, 0.2 mmol) were dissolved in degassed MeCN (20 mL) in an Ar-filled glove box. An excess of Zn dust was added to this solution. After stirring for 30 mins, the colorless solution turned dark purple and the solid was filtered off. The purple filtrate was stirred overnight before compound **4** (51 mg, 0.2 mmol) was added. The reaction mixture was then heated to 40 °C and stirred under an Ar atmosphere for 20 days, during which time the reaction was monitored by RP-HPLC. The solvent was evaporated off, and the residue was purified by prep-HPLC (H_2O–MeCN, 0.1% TFA, 0–75% MeCN in 35 min). The fraction was combined and the solvent was evaporated off, and the solid was re-dissolved in H_2O, and precipitated by addition of an excess of NH_4PF_6. The solid was filtered off

and washed with H_2O, MeOH and finally Et_2O to afford **3R|4BP•16PF$_6$** as a white solid (9 mg, 10 %). ^{1}H NMR (500 MHz, d_6-Me_2CO): δ = 9.57 (d, *J* = 7.2 Hz, 12H), 9.51 (d, *J* = 6.2 Hz, 8H), 9.48 (d, *J* = 6.2 Hz, 8H), 9.28 (d, *J* = 6.2 Hz, 4H), 8.90 (d, *J* = 6.4 Hz, 16H), 8.84 (d, *J* = 6.4 Hz, 4H), 8.82 – 8.78 (m, 12H), 7.90 – 7.80 (m, 12H), 7.77 (s, 16H), 6.36 – 5.99 (m, 28H), 4.78 (t, *J* = 8.4 Hz, 3H), 4.38 (s, 4H), 4.25 (s, 4H), 2.63 (t, *J* = 8.4 Hz, 4H), 1.60 (br, 4H), 1.14 (s, 18H), 1.12 (s, 18H), 0.09 (br, 4H), –0.58 (br, 4H), –1.46 (br, 4H). ^{13}C NMR (126 MHz, CD_3CN): δ = 158.6, 150.7, 148.5, 146.2, 146.1, 145.6, 145.4, 136.3, 135.0, 130.6, 130.5, 130.4, 127.7, 127.6, 127.5, 76.7, 75.1, 64.9, 64.2, 48.9, 31.4, 31.3, 28.5, 28.3, 28.2, 25.9, 25.8, 25.7, 25.4. HRMS (ESI): *m/z* calcd for $C_{176}H_{188}F_{78}N_{22}O_8P_{13}$ $[M - 3PF_6]^{3+}$ 1540.6775, found 1540.6770.

Scheme S4. Synthesis of 3R|5BP•18PF$_6$ Templated by Radical-Pairing Interactions



3R|5BP•18PF$_6$: **5BP**•10PF$_6$ (58 mg, 0.02 mmol) and **CBPQT**•4PF$_6$ (220 mg, 0.2 mmol) were dissolved in degassed MeCN (20 mL) in an Ar-filled glove box. An excess of Zn dust was added to this solution. After stirring for 30 mins, the colorless solution turned dark purple and the solid was filtered off. The purple filtrate was stirred overnight before compound **4** (51 mg, 0.2 mmol) was added. The reaction mixture was then heated to 40 °C and stirred under an Ar atmosphere for 20 days, during which time the reaction was monitored by RP-HPLC (H_2O–MeCN, 0.1% TFA, 0–75% MeCN in 35 min). The solvent was evaporated off, and the residue was purified by prep-HPLC. The fraction was combined and the solvent was evaporated off, and the solid was re-dissolved in H_2O, and precipitated by addition of an excess of NH_4PF_6. The solid was filtered off and washed with H_2O, MeOH and finally Et_2O to afford **3R|5BP**•18PF$_6$ as a yellow solid (6 mg, 6 %). ^{1}H NMR (500 MHz, *d*$_6$-Me_2CO): δ = 9.57 (d, *J* = 7.2 Hz, 12H), 9.51 (d, *J* = 6.2 Hz, 8H), 9.48 (d, *J* = 6.2 Hz, 8H), 9.28 (d, *J* = 6.2 Hz, 4H), 8.90 (d, *J* = 6.4 Hz, 16H), 8.84 (d, *J* = 6.4 Hz, 4H), 8.82 – 8.78 (m, 12H), 7.90 – 7.80 (m, 12H), 7.77 (s, 16H), 6.36 – 5.99 (m, 28H), 4.78 (t, *J* = 8.4 Hz, 3H), 4.38 (s, 4H), 4.25 (s, 4H), 2.63 (t, *J* = 8.4 Hz, 4H), 1.60 (br, 4H), 1.14 (s, 18H), 1.12 (s, 18H), 0.05 (br, 4H), –0.61 (br, 4H), –1.51 (br, 4H). ^{13}C NMR (126 MHz, CD_3CN): δ = 158.6, 150.7, 148.5, 146.2, 146.1, 145.6, 145.4, 136.3, 135.0, 130.6, 130.5, 130.4, 127.7, 127.6, 127.5, 76.7, 75.1, 64.9, 64.2, 48.9, 31.4, 31.3, 28.5, 28.3, 28.2, 25.9, 25.8, 25.7, 25.4. HRMS (ESI): *m/z* calcd for $C_{194}H_{204}F_{90}N_{24}O_8P_{15}$ $[M - 3PF_6]^{3+}$ 1724.7741, found 1724.7800.

3. ^{1}H NMR Spectroscopic Analysis of oligorotaxane 3R|4BP•16PF$_6$ and 3R|5BP•18PF$_6$.

Compound **3R|4BP**•16PF$_6$ has a simple ^{1}H NMR spectrum on account of its high symmetry and only four $BIPY^{2+}$ subunits. In its oxidized state, the positive-charged $CBPQT^{4+}$ rings are positioned

on the hexamethylene chains as a result of the Coulombic repulsions with the $BIPY^{2+}$ subunits of the thread, giving rise to the substantially lower resonating frequency (< 0 ppm) of protons on the hexamethylene chains. In addition, the methyl groups of the stopper separate into two set of peaks, as a result of heterotopic nature of the triazole rings.

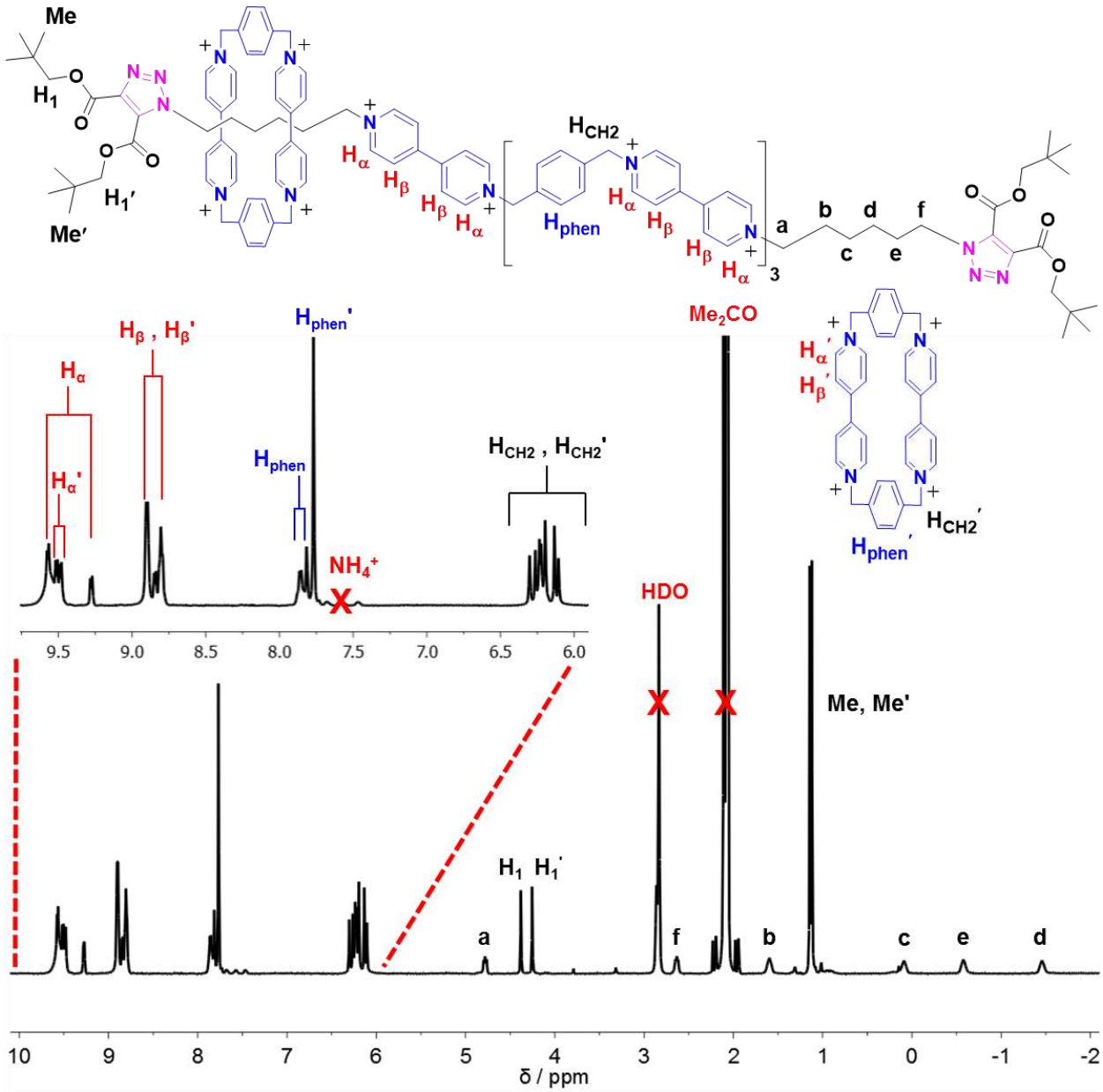


Figure S1. ^1H NMR spectrum (500 MHz, CD_3COCD_3, 298K) of oligorotaxane **3R|4BP**•16PF_6.

In the aromatic region of the spectrum, the signals for protons H_α and H_α' are well resolved. In particular, the resonances for H_α' on the $CBPQT^{4+}$ units appear as two set of peaks, presumably as a result of the free rotation of the $BIPY^{2+}$ units along the C–N bond being hindered by the hexamethylene chain. In contrast, the signals for protons H_β and H_β' on the dumbbell and the cyclophane $CBPQT^{4+}$, respectively, resonate at a similar frequencies, exhibiting overlapped peak signals. Protons on the hexamethylene chains were assigned unambiguously to resonances by identifying important through-bond couplings in the ^1H–^1H gCOSY (Figure S2) such as $H_a \leftrightarrow H_b$, $H_b \leftrightarrow H_c$, $H_c \leftrightarrow H_d$, $H_d \leftrightarrow H_e$ and $H_e \leftrightarrow H_f$.

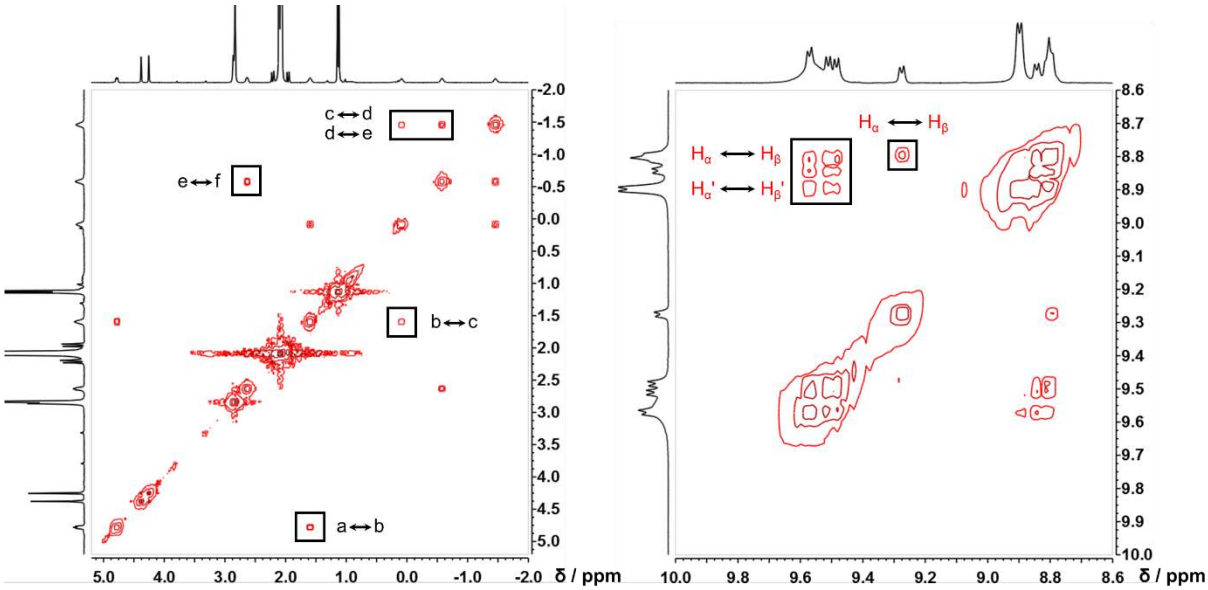


Figure S2. ^1H–^1H gCOSY spectrum (500 MHz, CD_3COCD_3, 298K) of oligorotaxane **3R|4BP•**$16PF_6$.

For compound **3R|5BP•**$18PF_6$, the ^1H NMR spectrum is more complicated because the dumbbell has one more $BIPY^{2+}$ subunit. Likewise, the protons of the hexamethylene chains can be assigned unambiguously to resonances by identifying important through-bond couplings in the ^1H–^1H gCOSY (Figure S4) including $H_a \leftrightarrow H_b$, $H_b \leftrightarrow H_c$, $H_c \leftrightarrow H_d$, $H_d \leftrightarrow H_e$ and $H_e \leftrightarrow H_f$.

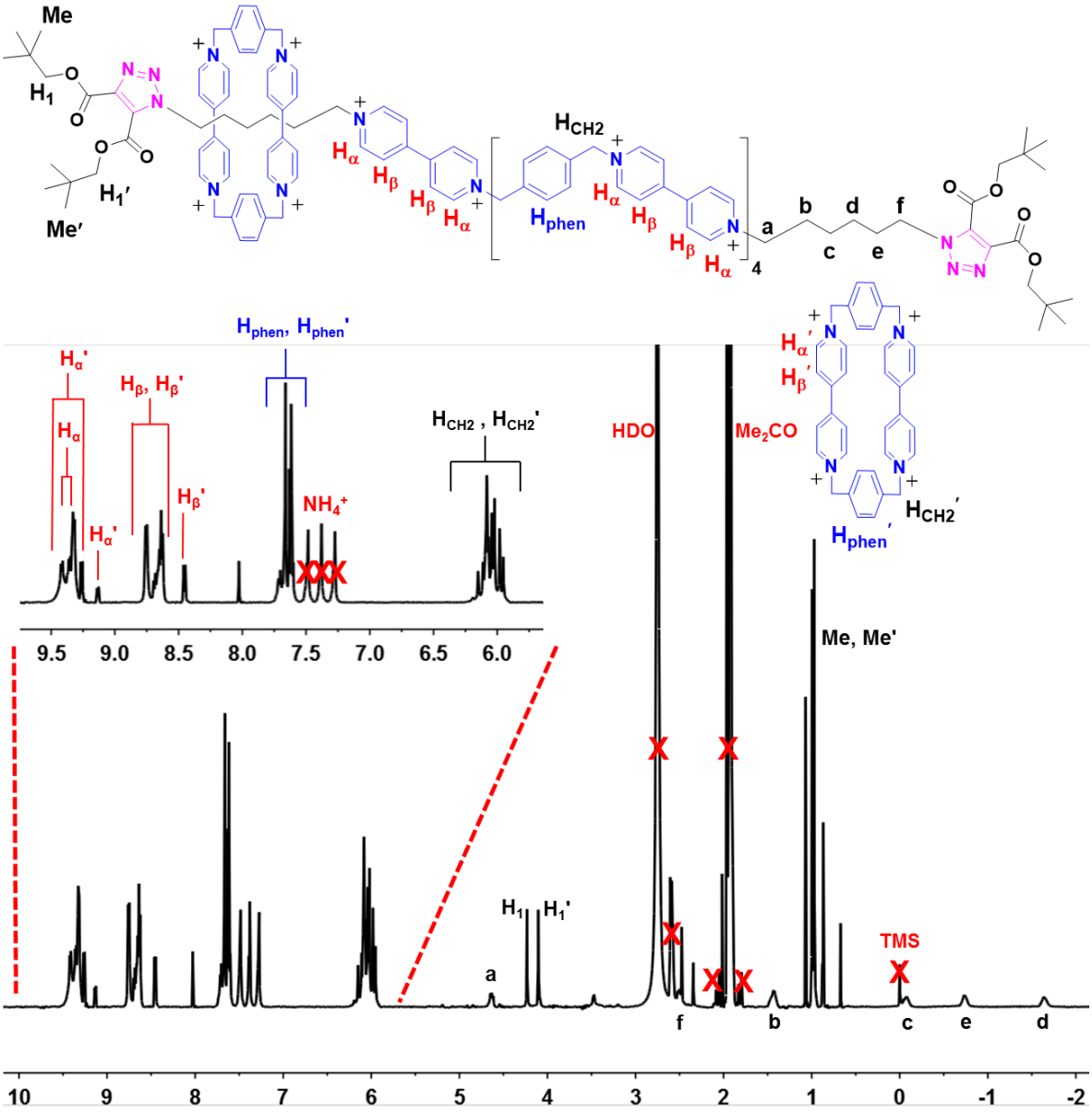


Figure S3. ^{1}H NMR spectrum (500 MHz, CD_3COCD_3, 298K) of oligorotaxane **3R**|**5BP**•18PF_6.

It is noteworthy that protons H_c, H_d and H_e of **3R**|**5BP**•18PF_6 resonate slightly upfield compared with those in **3R**|**4BP**•16PF_6, indicating that the **CBPQT**$^{4+}$ rings are pushed farther from the BIPY^{2+} subunits on the dumbbell, presumably on account of the higher Coulombic repulsions as one more BIPY^{2+} subunit is introduced into the rod portion of the dumbbell.

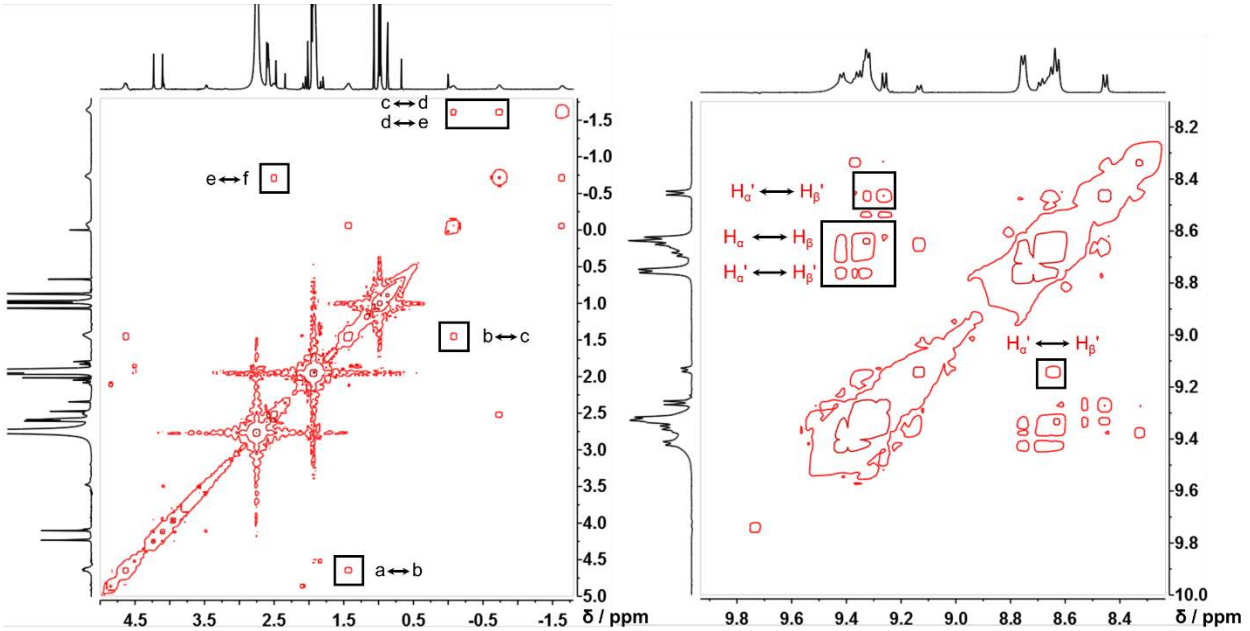


Figure S4. ^{1}H–^{1}H gCOSY spectrum (500 MHz, CD_3COCD_3, 298K) of oligorotaxane **3R**|**5BP**•$18PF_6$.

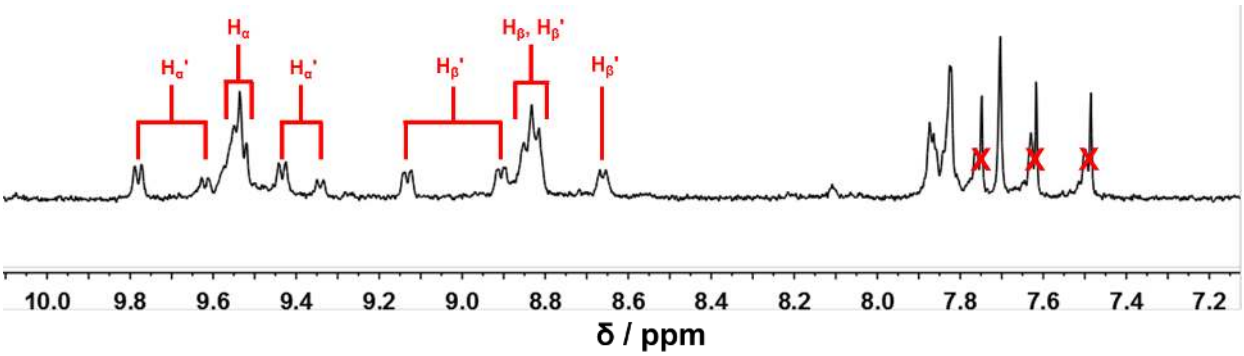


Figure S5. Partial ^{1}H NMR spectrum (400 MHz, CD_3COCD_3, 233K) of oligorotaxane **3R**|**5BP**•$18PF_6$.

The protons of the aromatic region can be assigned by recording (Figure S5) the ^{1}H NMR spectrum at 233 K. The integral value and the splitting pattern indicate that the α and β protons of the $BIPY^{2+}$ in the $CBPQT^{4+}$ rings separate into four sets of peaks, presumably as a result of the rotation of the $BIPY^{2+}$ units of the $CBPQT^{4+}$ rings around the hexamethylene chain is 'frozen' under lower temperatures. The crossed peaks correspond to proton resonances of NH_4^+ from NH_4PF_6.

4. HPLC and HRMS Characterizations of Oligorotaxanes 3R|4BP•16PF_6 and 3R|5BP•18PF_6

The HPLC traces and the HRMS spectra of **3R|4BP•**16PF_6 and **3R|5BP•**18PF_6 are shown in Figure S6 and Figure S7.

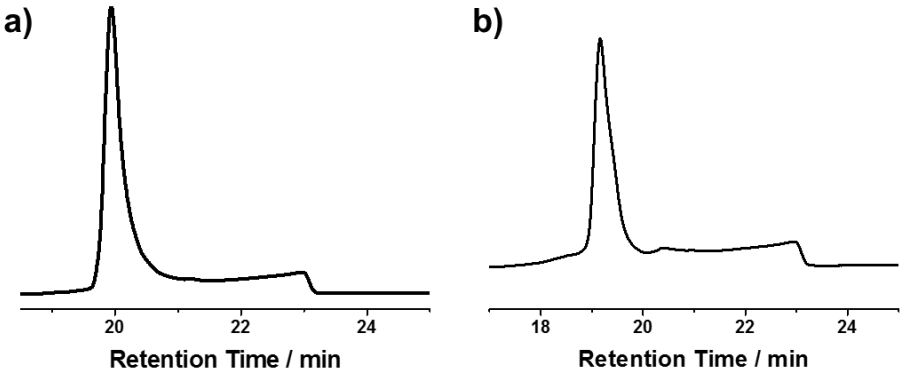


Figure S6. Analytical RP-HPLC chromatograms (H_2O–MeCN, 0.1% TFA, 0–100% MeCN in 60 min, λ = 254 nm) of a) **3R|4BP•**16PF_6 and b) **3R|5BP•**18PF_6. The higher charged oligorotaxane **3R|5BP•**18PF_6 has a shorter retention time on the column.

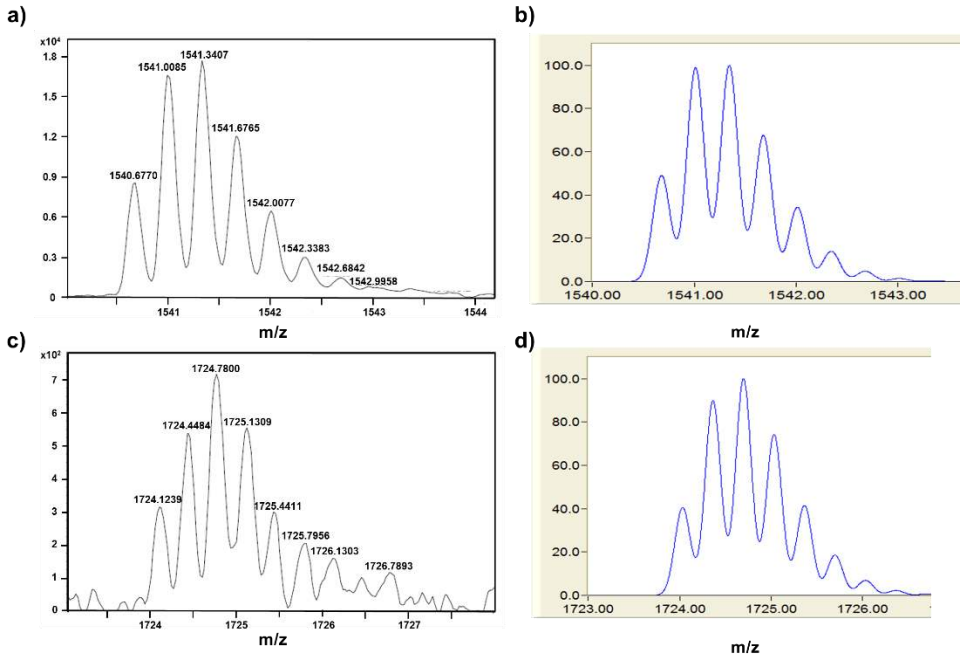


Figure S7. a–b) Experimental and simulated HRMS (ESI) spectra of **3R|4BP•**16PF_6. Calculated for $C_{176}H_{188}F_{78}N_{22}O_8P_{13}$: 1540.6775 $[M - 3PF_6]^{3+}$. c–d) Experimental and simulated HRMS (ESI) spectra of **3R|5BP•**18PF_6. Calculated for $C_{194}H_{204}F_{90}N_{24}O_8P_{15}$: 1724.7741 $[M - 3PF_6]^{3+}$.

5. Job plots of $4V^{4(\bullet+)}\subset 2CBPQT^{2(\bullet+)}$ and $5V^{5(\bullet+)}\subset 2CBPQT^{2(\bullet+)}$

In order to verify the binding stoichiometry between $CBPQT^{2(\bullet+)}$ and oligoviologen threads, we constructed a Job plot for $4V^{4(\bullet+)}$ and $CBPQT^{2(\bullet+)}$ (Figure S8), as well as $5V^{5(\bullet+)}$ and $CBPQT^{2(\bullet+)}$ (Figure S9) in MeCN.

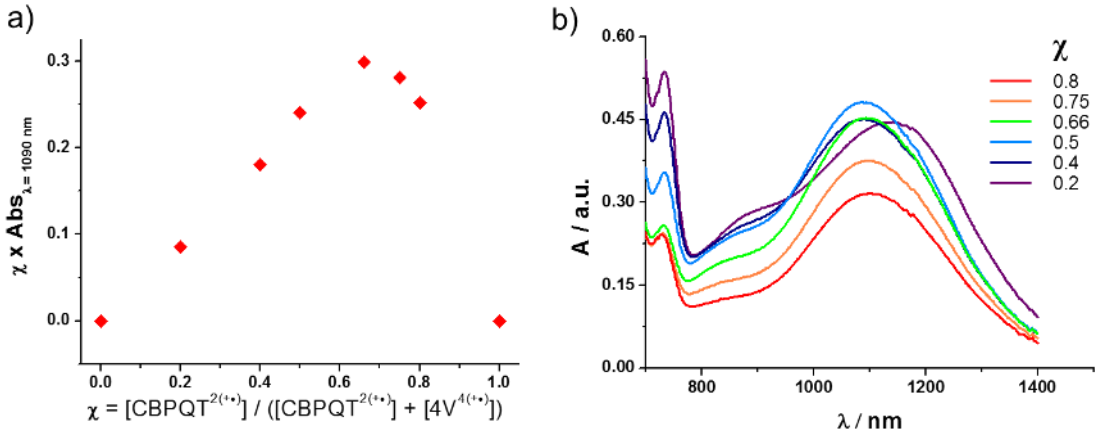


Figure S8. Determination of binding stoichiometry of $CBPQT^{2(\bullet+)}$ with respect to $4V^{4(\bullet+)}$ in MeCN using the method of continuous variation. (a) Job plot showing the intensity of the trisradical absorption band attributable to $4V^{4(\bullet+)}\subset 2CBPQT^{2(\bullet+)}$ host-guest complex against χ, which represents the $CBPQT^{2(\bullet+)}$:$4V^{4(\bullet+)}$ molar ratio. (b) Absorption spectroscopy data used in the Job plot. The spectra were recorded at 298 K with $[CBPQT^{2(\bullet+)}]+[4V^{4(\bullet+)}]$ = 50 μM.

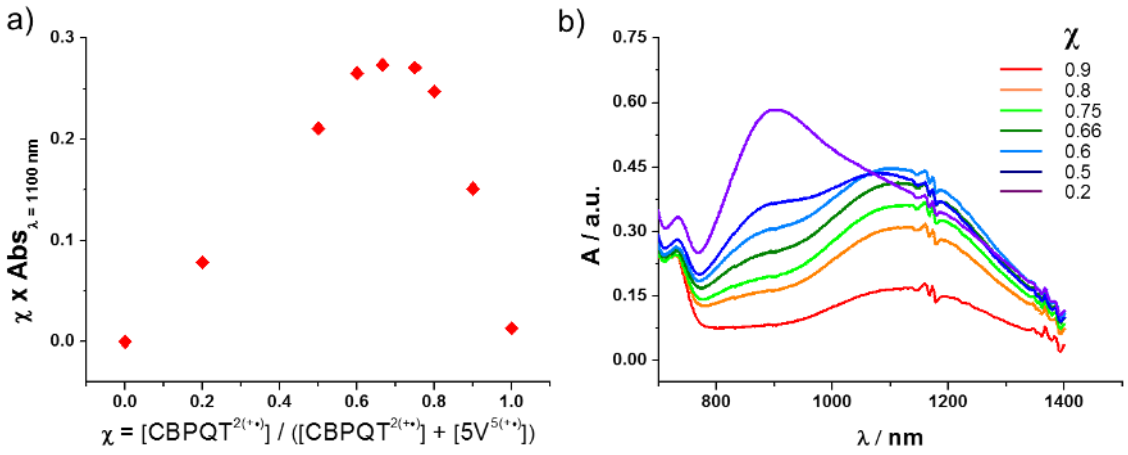


Figure S9. Determination of binding stoichiometry of $CBPQT^{2(\bullet+)}$ with respect to $5V^{5(\bullet+)}$ in MeCN using the method of continuous variation. (a) Job plot showing the intensity of the trisradical absorption band attributable to $5V^{5(\bullet+)}\subset 2CBPQT^{2(\bullet+)}$ host-guest complex against χ, which represents the $CBPQT^{2(\bullet+)}$:$5V^{5(\bullet+)}$ molar ratio. (b) Absorption spectroscopy data used in the Job plot. The spectra were recorded at 298 K with $[CBPQT^{2(\bullet+)}]+[5V^{5(\bullet+)}]$ = 50 μM.

The intensity of the trisradical complex absorption band at 1090 nm for $4V^{4(\bullet+)}$ and 1100 nm for $5V^{5(\bullet+)}$ was used for detecting the extent of binding as the molar ratio was varied. The Job plot is referenced to the concentration of $CBPQT^{2(\bullet+)}$. The maximum intensity of the trisradical complex band occurred at $\chi = 0.66$, where χ is the concentration of $CBPQT^{2(\bullet+)}$ divided by the sum of concentration of $CBPQT^{2(\bullet+)}$ and corresponding oligoviologen radical cationic species, indicating that both $4V^{4(\bullet+)}$ and $5V^{5(\bullet+)}$ bind two $CBPQT^{2(\bullet+)}$ units in solution.

6. UV/Vis/NIR Absorption Spectrophotometric Titration of $4V^{4(\bullet+)}$ and $5V^{5(\bullet+)}$ by $CBPQT^{2(\bullet+)}$

Figure S10 shows a spectrophotometric titration of $CBPQT^{2(\bullet+)}$ into a MeCN solution of $4V^{4(\bullet+)}$. This data was used to calculate a binding constant (K_a) of $3.3 \pm 0.8 \times 10^9$ M^{-2} based on the 1:2 binding model.

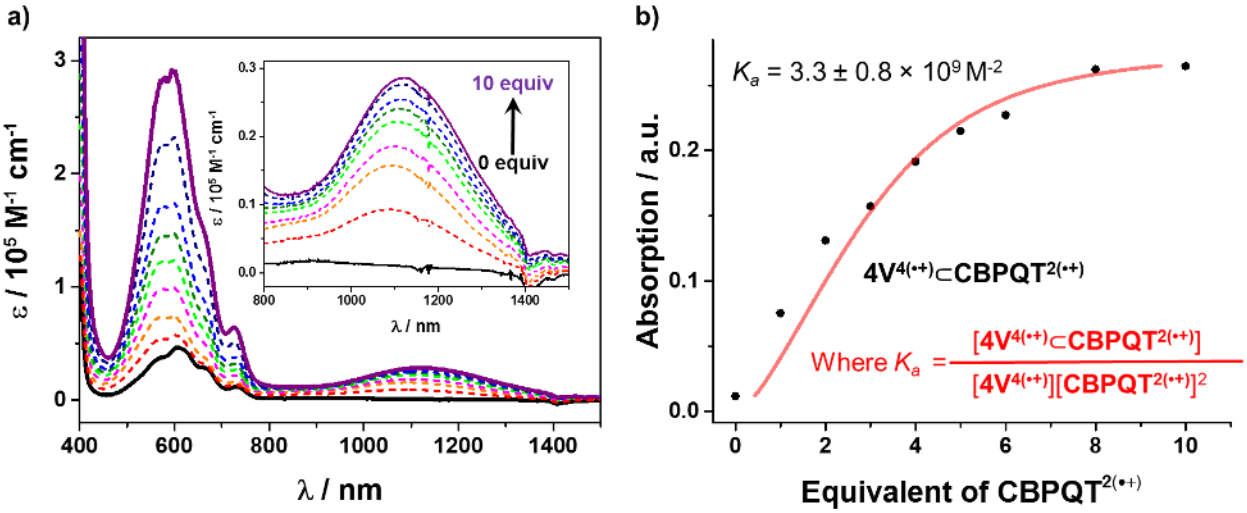


Figure S10. a) UV/Vis/NIR Absorption spectrophotometric titration experiment of $4V^{4(\bullet+)}$ by $CBPQT^{2(\bullet+)}$ at 298 K. Solvent: MeCN; black: $[4V^{4(\bullet+)}] = 10$ μM; purple: c ($CBPQT^{2(\bullet+)}$) / c ($4V^{4(\bullet+)}$) = 10. b) The simulated curve for the determination of the binding constant between $4V^{4(\bullet+)}$ and $CBPQT^{2(\bullet+)}$.

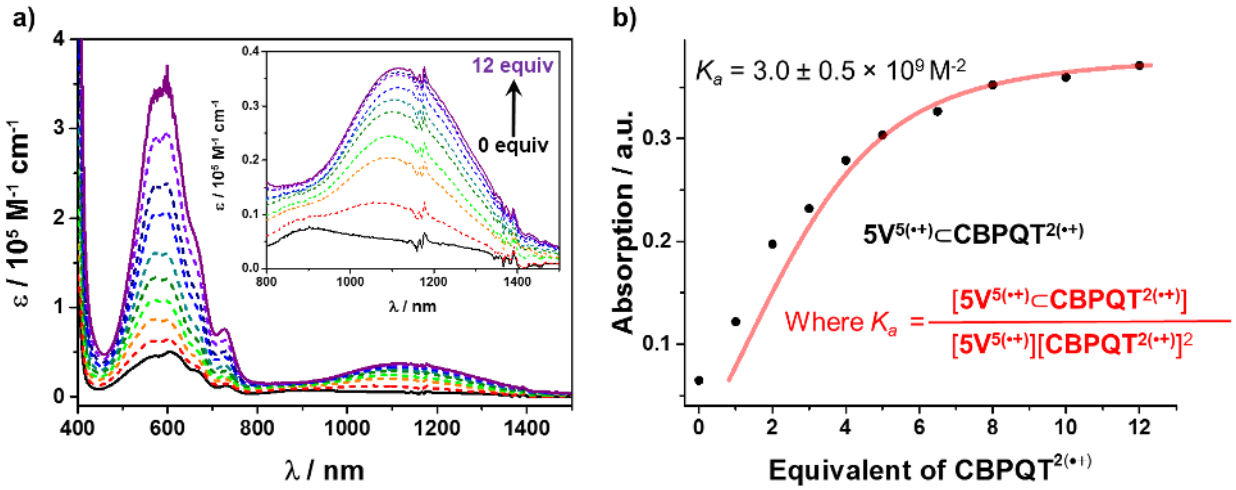


Figure S11. a) UV/Vis/NIR Absorption spectrophotometric titration experiment of $5V^{5(\bullet+)}$ by $CBPQT^{2(\bullet+)}$ 298 K. Solvent: MeCN; black: [$5V^{5(\bullet+)}$] = 10 μM; purple: c ($CBPQT^{2(\bullet+)}$) / c ($5V^{5(\bullet+)}$) = 12. b) The simulated curve for the determination of the binding constant between $5V^{5(\bullet+)}$ and $CBPQT^{2(\bullet+)}$.

Figure S11 shows a spectrophotometric titration of $CBPQT^{2(\bullet+)}$ into a MeCN solution of $5V^{5(\bullet+)}$. This data was used to calculate a binding constant (K_a) of 3.0 ± 0.5×10^9 M^{-2} based on the 1:2 binding model as well. It is noteworthy that this K_a value is comparable with that of $4V^{4(\bullet+)}$, indicating their similar abilities to bind $CBPQT^{2(\bullet+)}$ in MeCN. As $5V^{5(\bullet+)}$ is one viologen unit longer than $4V^{4(\bullet+)}$, the binding process is less entropically favored. Therefore, the binding enthalpy between $CBPQT^{2(\bullet+)}$ and $5V^{5(\bullet+)}$ is more negative to offset the additional entropy penalty. Moreover, this K_a value is also close to the square of the binding constant[4] between $CBPQT^{2(\bullet+)}$ and $MV^{\bullet+}$ (7.9 ± 5.5×10^4 M^{-1}), demonstrating that the strength of binding between viologen units and the $CBPQT^{2(\bullet+)}$ units is retained in the case of oligoviologens.

7. Variable-Temperature UV/Vis/NIR Spectroscopy of 3R|4BP•16PF$_6$

It is known[3] that the radical-pairing interactions become weaker at higher temperature in solution. The structural information for the oligorotaxanes under reducing conditions, therefore, can be obtained by monitoring the change of the UV/Vis/NIR absorption intensities at different temperatures. Based on this knowledge, we selected **3R|4BP•**16PF$_6$ as an example on which to perform a variable-temperature UV/Vis/NIR experiment.

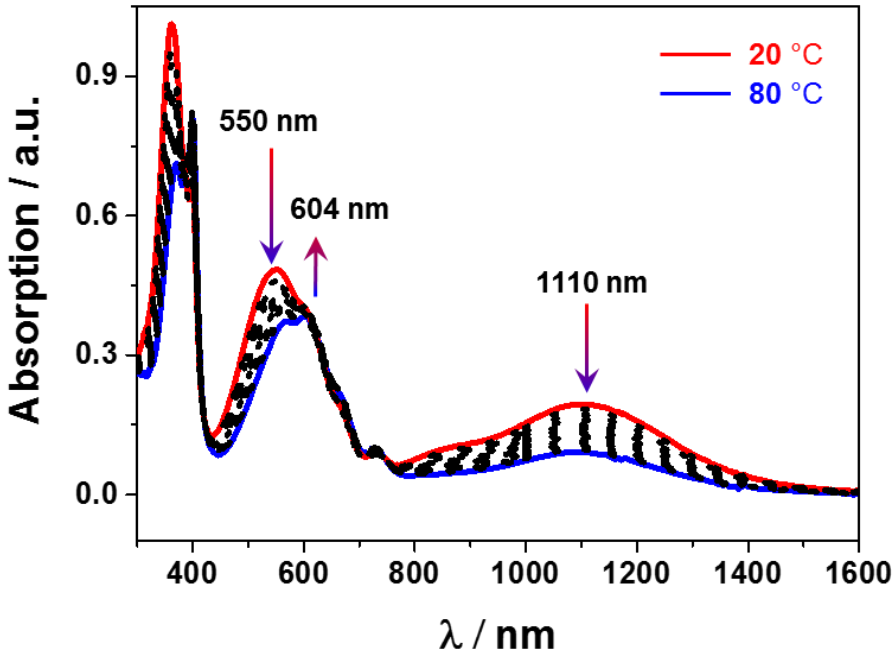


Figure S12. UV/Vis/NIR spectra of **3R|4BP•**16PF$_6$ recorded at different temperatures ranging from 20 °C to 80 °C in MeCN at a concentration of 100 μM. The arrows in the figure denote the changing trend of the absorption intensities.

The spectra (Figure S12) demonstrate that as the temperature of the solution increases, the absorption peaks centered at 550 and 1110 nm, which correspond to the formation of trisradical complex, decrease in their intensities. This observation suggest that the interactions between the CBPQT$^{2(\bullet+)}$ ring and the BIPY$^{\bullet+}$ units on the dumbbell are less favored at higher temperatures. As a result, the characteristic absorption band of unpaired BIPY$^{\bullet+}$ units, i.e., the one at 604 nm, becomes more dominant at higher temperatures.

8. Cyclic Voltammetry Titration of $4V^{4(\bullet+)}\subset 2CBPQT^{2(\bullet+)}$ and $5V^{5(\bullet+)}\subset 2CBPQT^{2(\bullet+)}$

In order to shed further light on the interacting mechanism between $4V^{4(\bullet+)}$ and $CBPQT^{2(\bullet+)}$, a CV titration experiment has been performed.

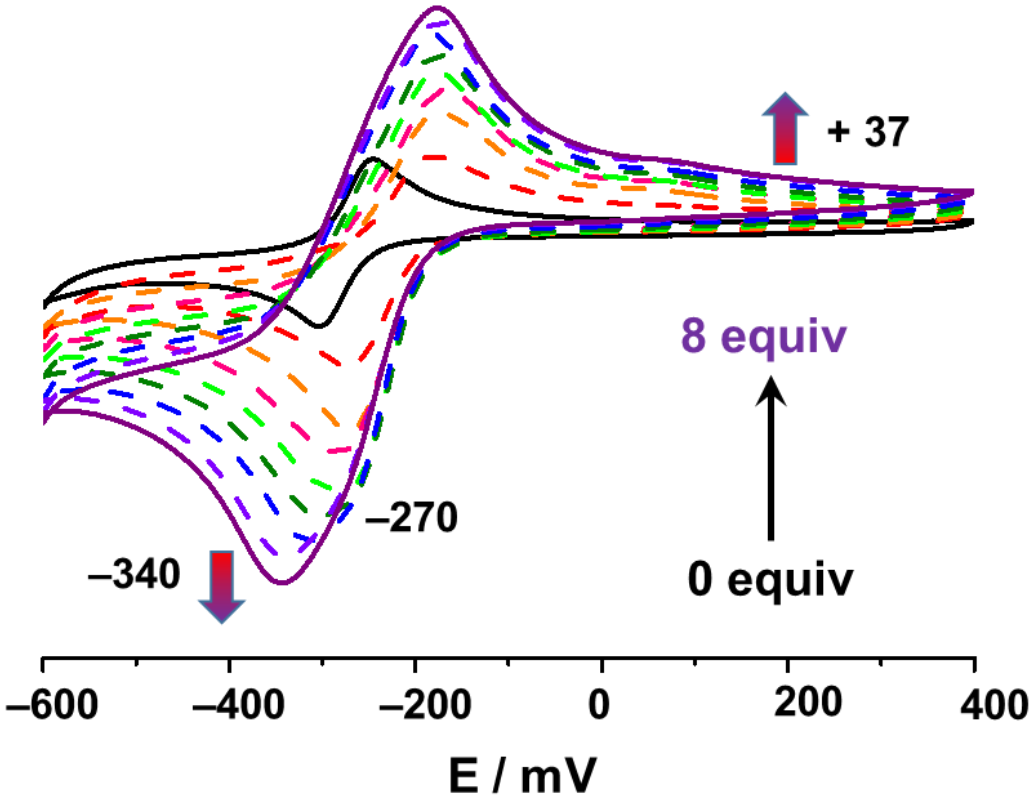


Figure S13. Cyclic voltammogram titration of $4V^{4(\bullet+)}\subset 2CBPQT^{2(\bullet+)}$. A glassy carbon working electrode, a platinum counter electrode, and a Ag/AgCl reference electrode were used in the characterization of 0.1 mM MeCN solutions of the $4V^{8+}$ at 298 K with 0.1 M $TBAPF_6$ serving as the electrolyte. A scan rate of 200 mV s^{-1} was used in all the analyses.

The result (Figure S13) shows that upon increasing the amount of $CBPQT^{4+}$ from 1 equiv to 10 equiv, a reduction peak at –340 mV gradually emerges. It shifts toward the reduction potential of free $CBPQT^{4+}$, indicating the saturation of binding between $4V^{4(\bullet+)}$ and $CBPQT^{2(\bullet+)}$ when an excess of $CBPQT^{4+}$ is added to the solution. In addition, as the equiv of $CBPQT^{4+}$ increases in the solution, a peak shoulder with a potential of +37 mV can be observed, which is shifted significantly in the positive direction, indicating the existence of the radical dimer—namely, $BIPY^{\bullet+}$ pimerization—a

structure generated from the one-electron oxidation of the trisradical complex between $4V^{4(\bullet+)}$ and $CBPQT^{2(\bullet+)}$.

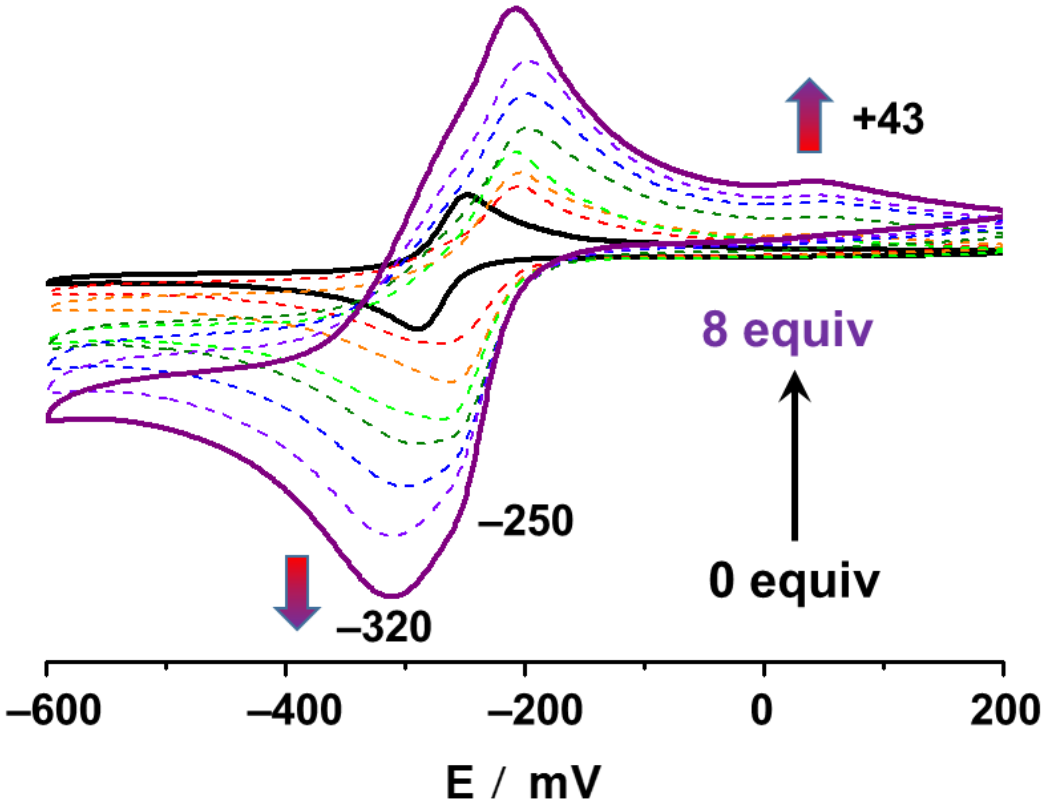


Figure S14. Cyclic voltammogram titration of $5V^{5(\bullet+)}\subset 2CBPQT^{2(\bullet+)}$. A glassy carbon working electrode, a platinum counter electrode, and a Ag/AgCl reference electrode were used in the characterization of 0.1 mM MeCN solutions of the $5V^{10+}$ at 298 K with 0.1 M $TBAPF_6$ serving as the electrolyte. A scan rate of 200 mV s^{-1} was used in all the analyses.

A CV titration experiment investigating (Figure S14) the binding between $5V^{5(\bullet+)}\subset 2CBPQT^{2(\bullet+)}$ has also been carried out. Similarly, the saturation of binding was also confirmed by the observation of the reduction peak at –320 mV. In addition, the formation of the $BIPY^{\bullet+}$ radical dimer can also be confirmed as a redox peak at +43 mV emerges upon oxidation. It is also noteworthy that this peak potential is shifted dramatically compared with that of the inclusion complex of $MV^{\bullet+}\subset CBPQT^{2(\bullet+)}$, presumably because the $BIPY^{\bullet+}$ dimers between $4V^{4(\bullet+)}$ and $5V^{5(\bullet+)}$ with $CBPQT^{2(\bullet+)}$ are more stable.

9. Differential Pulse Voltammetric Characterization of 3R|4BP•16PF$_6$

In order to gain a better understanding of the electron transfer processes during the formation of the radical states of these oligorotaxanes, as well as to find out how the mechanically interlocked structure affects the recognition between $BIPY^{\bullet+}$ radicals, we selected **3R|4BP•**16PF_6 as an example on which to perform a differential pulse voltammetry (DPV) experiment.

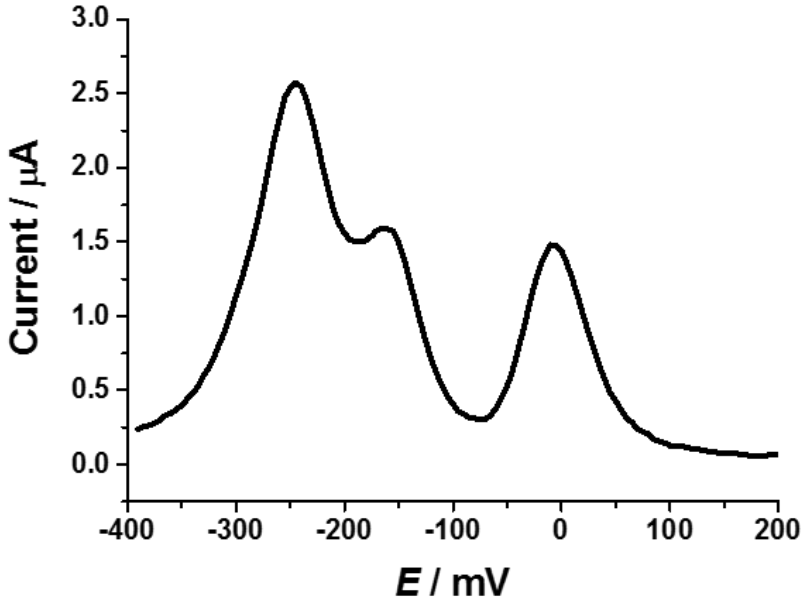


Figure S15. DPV Profile of **3R|4BP•**16PF_6. The ratio of the area under each peak (from right to left) is 1:1:2.

The DPV profile shows (Figure S15) three bands during the reduction process, an observation which agrees with the results from CV experiments where the reduction of **3R|4BP**$^{16+}$ to its radical state is complete after three steps. Comparison of the relative integrations associated with each band reveals a 1:1:2 ratio in relation to the numbers of electrons. Since a total number of eight electrons are involved during this reduction process, it can be concluded that the oligorotaxane **3R|4BP**$^{16+}$ receives two, followed by two, followed by four, electrons during the course of the three steps.

10. Redox Stimuli-Induced Contraction and Expansion of 3R|4BP•16PF$_6$

In order to gain an understanding of the changes in the lengths of the molecules during the redox-controlled switching processes of the oligorotaxanes, we selected **3R|4BP**•16PF$_6$ as an example and performed diffusion ordered spectroscopy (DOSY) on its oxidized state (Figure S16) and electron paramagnetic resonance (EPR) spectroscopy (Figure S17) on its reduced state.

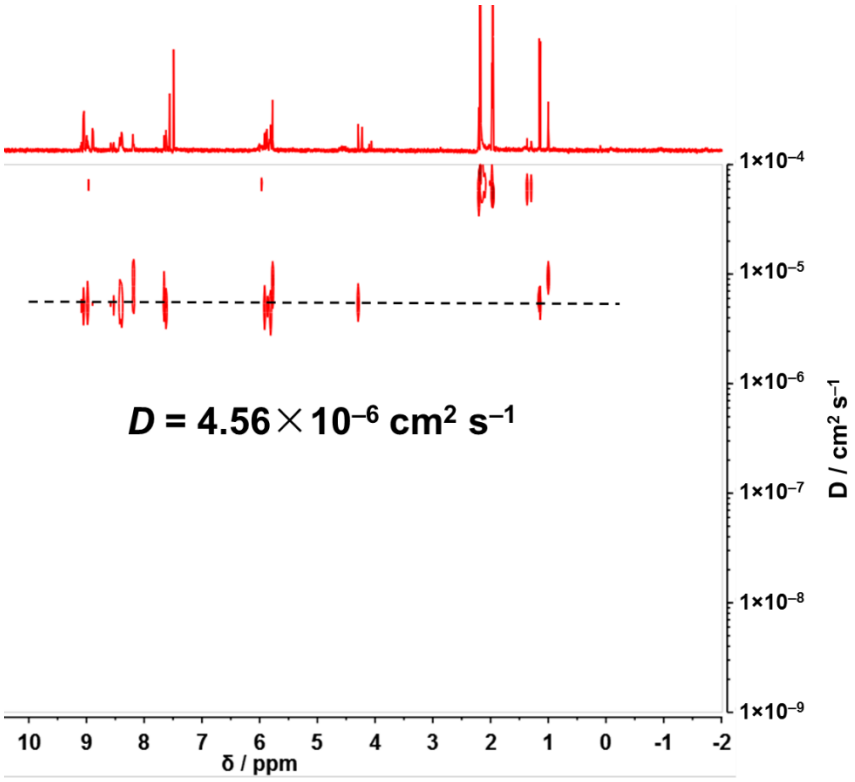


Figure S16. DOSY Spectrum (500 MHz, CD_3CN, 298 K) of **3R|4BP**•16PF$_6$.

The DOSY spectrum shows that the diffusion coefficient value (D) of **3R|4BP**•16PF$_6$ in CD_3CN is 4.6 × 10^{-6} cm^2 s^{-1}. Given the Einstein-Stokes equation $D = kT / 6\pi\eta r$, the radius (r) of **3R|4BP**•16PF$_6$ can be estimated as 1.4 nm. It should be noted, however, that this equation relates to spherical paritcles and so the DOSY can only give a rough estimation of molecular demensions.

On the other hand, the dimension of the reduced state of **3R|4BP**$^{16+}$, namely **3R|4BP**$^{8(\bullet+)}$, was investigated (Figure S17) by EPR spectroscopy. **3R|4BP**$^{8(\bullet+)}$ in MeCN (0.2 mM) can be generated by heterogeneous 8-electron reduction of **3R|4BP**$^{16+}$ using freshly activated Zn dust in a N_2-filled glovebox. The radical cation benzyl viologen (**BnV**$^{\bullet+}$) in MeCN (0.2 mM) was prepared in a similar fashion and used as a reference compound. A low sample concentration was employed in

order to avoid any intermolecular interactions, and the samples were subjected to EPR measurements immediately after their preparation. The **BnV**$^{\bullet+}$ solution at room temperature is blue-colored and shows (Figure S17a) the typical cw X-Band EPR spectrum of a viologen radical cation, for which the *g* factor is 2.0031. The hyperfine structure can be rationalized on the basis of the electron spin coupling to two equivalent N atoms and 12 H atoms, which can be divided further into two pairs of two methylene protons on the benzylic groups and two equivalent sets, each of four protons, on the bipyridinium core. In contrast, the EPR signal for the purple-colored **3R|4BP**$^{8(\bullet+)}$ under identical experimental conditions is four-fold weaker despite the fact that it contains eight viologen units per molecule. The weak intensity is indicative of a pronounced spin-pairing effect and is in line with the intramolecular diamagnetic π-dimerization. The detected weak EPR signal can be attributed to a small thermal population of paramagnetic co-conformations.

The cw-EPR spectrum of the octaradical **3R|4BP**$^{8(\bullet+)}$ even in frozen MeCN at 4.1 K shows (Figure S17b) only one unresolved resonance. No clear evidence for high multiplicity ($S > ½$) states can be observed, thus preventing the measurement of the zero-field splitting parameter *D* needed for estimation of the molecular diameter.

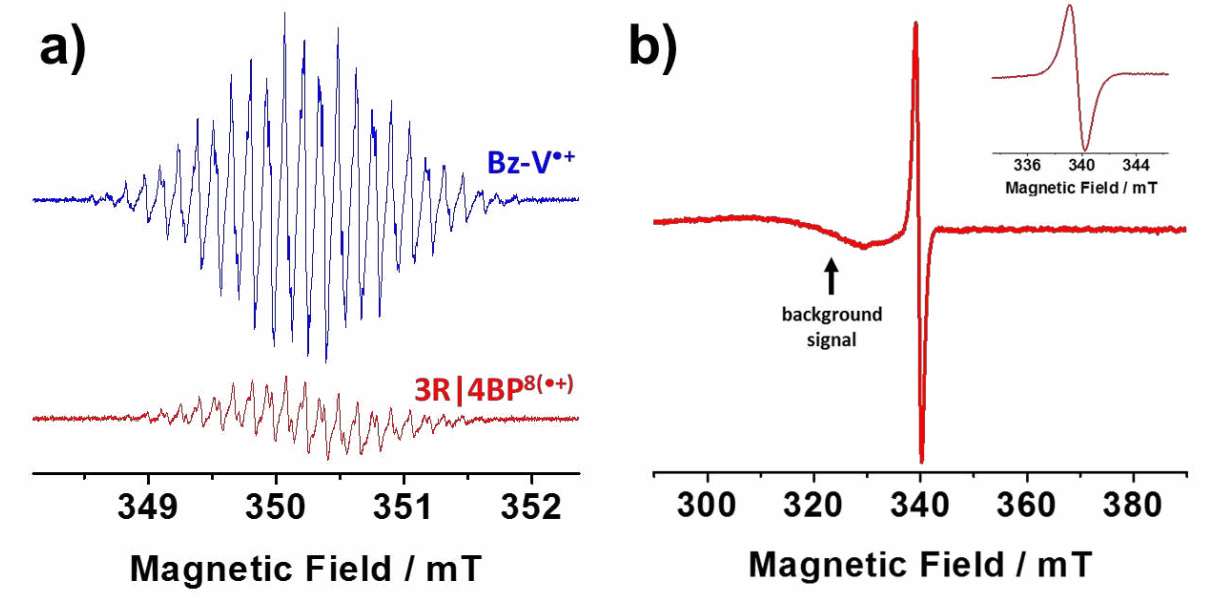


Figure S17. a) Cw-EPR spectra (X-Band) of the reference compound **BnV**$^{\bullet+}$ (blue line) and the oligorotaxane **3R|4BP**$^{8(\bullet+)}$ (red line) in MeCN at RT. b) Cw-EPR spectra (X-Band) of **3R|4BP**$^{8(\bullet+)}$ in frozen MeCN at 4.1 K. Concentration: 0.2 mM. Modulation Amplitude: 0.1 G. Microwave frequency: 9.8240. Power: 0.395 mW.

The change in the length of the oligorotaxane **3R|4BP**$^{16+}$ on reduction to **3R|4BP**$^{8(\bullet+)}$ is supported by computational analysis. Since **3R|4BP**$^{16+}$ is too large to be simulated by DFT calculations, we sought an approximation by comparing the "central regions" of **3R|4BP**$^{16+}$ and **3R|4BP**$^{8(\bullet+)}$. We measured the centroid-centroid distance between the two terminal BIPY^{2+} units in the simulated conformation (Figure S18a) of 4V^{8+} and the centroid-centroid distance between the two terminal BIPY$^{\bullet+}$ units — one on the 4V$^{4(\bullet+)}$ component and the other on the distant CBPQT$^{2(\bullet+)}$ ring — in the co-conformation (Figure S18b) of the oligopseudorotaxane 4V$^{4(\bullet+)}$⊂2CBPQT$^{2(\bullet+)}$. It turns out that, upon reduction, the molecular length contracts by 6 Å from 29.8 to 23.8 ÅThis result confirms our conclusion that the oligorotaxanes experience expansion–contraction movements during the redox-stimulated processes.

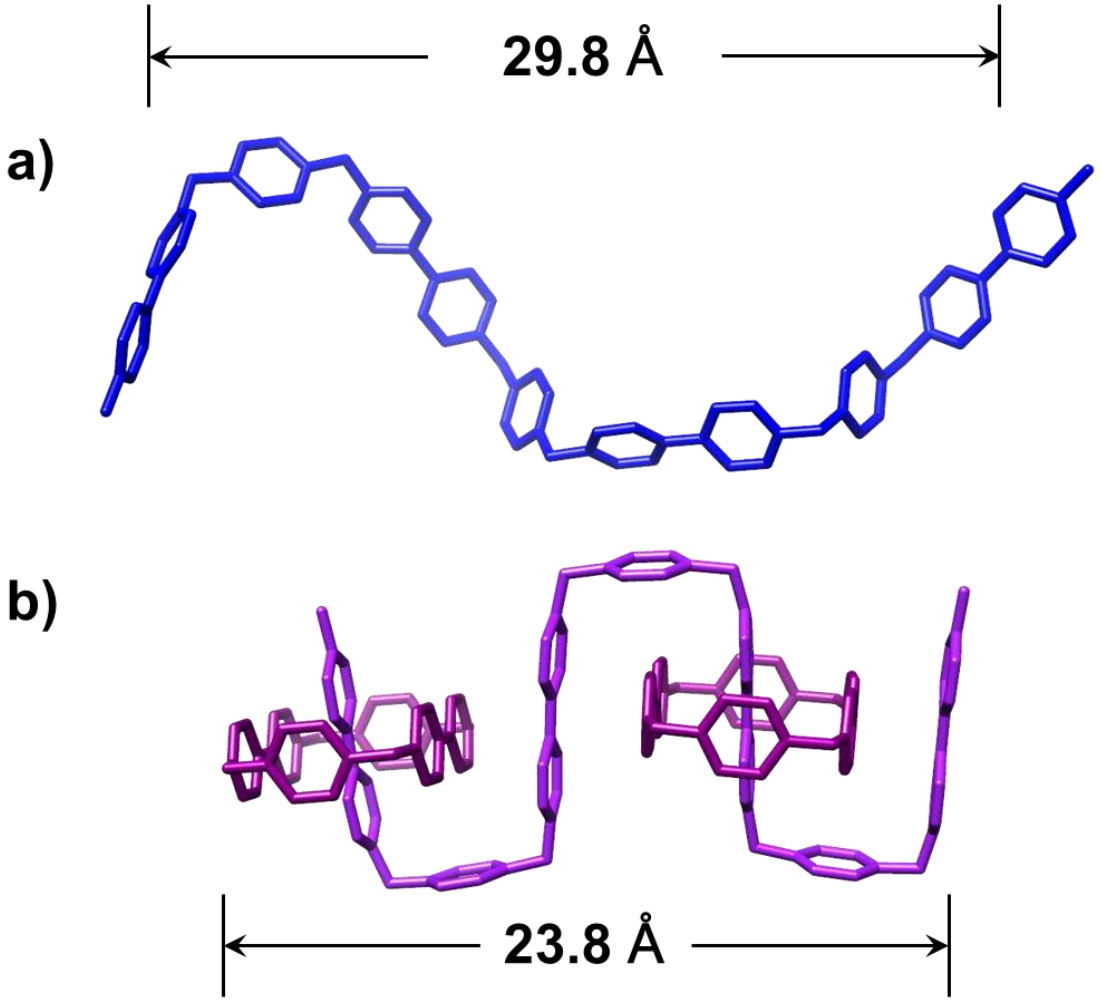


Figure S18. Comparison of the molecular lengths of a) 4V^{8+} and b) 4V$^{4(\bullet+)}$⊂2CBPQT$^{2(\bullet+)}$ measured on the simulated co-conformations.

11. Computational Details of Oligoviologens Folding with $CBPQT^{2(\bullet+)}$

The geometries were optimized at M06L/6-31G* level in the presence of the Poisson-Boltzmann solvation model for acetonitrile (ε=37.5 and R_0= 2.18 Å). Different C-C bond torsions are chosen as the initial structures to give different number of $BIPY^{2(\bullet+)}$ pairs. The single point energies were refined at M06/6-311++G** level. The optimized structures reported in the Figure 3 of the main text are provided below, with the calculated energies at each level. Units are in Hartree.

Co-conformation 3a

M06L/6-31G* in acetonitrile (A)	M06L/6-31G* in gas phase (B)	M06/6-311++G** in gas phase (C)	Total energy (C+A-B)
-6208.69096	-6206.86399	-6204.35455	-6206.18151

N1	-3.2675297147	3.8740747971	6.8603753271
N2	2.2135627877	3.3743762912	4.2234253702
C3	-2.0547628308	4.5059461563	6.8132339150
H4	-1.5057642291	4.5372576212	7.7512380461
C5	-1.5797925789	5.0660803791	5.6626678133
H6	-0.6161582503	5.5638063917	5.7180482225
C7	-2.3178954274	4.9975789455	4.4392407919
C8	-3.5938797947	4.3692106489	4.5482341791
H9	-4.2608354589	4.2897658993	3.6915296079
C10	-4.0261962255	3.8204045892	5.7215972830
H11	-4.9871573466	3.3201427869	5.8183947530
C12	-3.5922056964	2.9936817429	8.0052389467
H13	-3.1868945721	3.4665368832	8.9058236541
H14	-4.6823860915	2.9611297253	8.0998073623
C15	-3.0018656546	1.6275918956	7.7638114245
C16	-3.7479678636	0.6312338589	7.1276388779
H17	-4.8017683636	0.8040072662	6.9036368934
C18	6.4653861364	-7.6279387040	3.8326334890
H19	6.1986913244	-8.2815978518	4.6645925010
C20	7.1551973034	-8.1486386055	2.7316206807
C21	7.5283956601	-7.2818756502	1.7009495202
H22	8.0930433641	-7.6642194969	0.8497927854
C23	-1.6620812536	1.3720698790	8.0745747913
H24	-1.0745146494	2.1245070413	8.6021339232
C25	3.3453189530	4.1618491203	4.7618918720
H26	3.7125735114	3.6339614527	5.6476690721
H27	4.1410360486	4.1557268583	4.0098712408

C28	1.3440854809	2.7503461876	5.0768367950
H29	1.6769455181	2.6656608580	6.1088348727
C30	0.1459298391	2.2570423993	4.6462931898
H31	-0.4788251577	1.7641740806	5.3854813564
C32	-0.2674534932	2.3865043103	3.2848322357
C33	0.6808910595	3.0179535762	2.4248980793
H34	0.4883467724	3.1449431166	1.3629206082
C35	1.8664862514	3.4971884580	2.9039207732
H36	2.5985779304	3.9921536166	2.2704272167
N37	-4.0809533851	1.0623855617	1.9211565267
N38	-0.3704394011	9.2296247197	5.3930271146
N39	-0.7478133216	6.5263737445	0.7865395389
N40	-6.6294133274	6.9098761092	3.0366351586
C41	-3.1869426973	1.6327895738	1.0519008104
H42	-3.5239945102	1.7215251328	0.0224762287
C43	-1.9530709506	2.0494092295	1.4606183653
H44	-1.3020996199	2.4702674829	0.7013589632
C45	-1.5361145816	1.9213249998	2.8211811388
C46	-2.4861544183	1.2950118793	3.6839014997
H47	-2.2728860103	1.1136888025	4.7338853542
C48	-3.7140664420	0.9028489241	3.2280501476
H49	-4.4592898445	0.4409147262	3.8731829968
C50	-5.4969630249	0.9109198678	1.5129804855
H51	-5.5014135251	0.5980027123	0.4636050303
H52	-5.9282315947	0.1015280291	2.1113008021
C53	-6.2254509620	2.2139209443	1.7136320650
C54	-6.8114725943	2.5142024597	2.9470012167
H55	-6.8397221266	1.7576490523	3.7327471020
C56	-7.3647387930	3.7700482043	3.1796183936
H57	-7.8201054502	3.9890561824	4.1462832757
C58	-7.3413108674	4.7510802862	2.1832590753
C59	-6.7909694716	4.4378353866	0.9371369731
H60	-6.7930876751	5.1824428566	0.1400223667
C61	-6.2395197419	3.1809280328	0.7041558847
H62	-5.8166349618	2.9509321226	-0.2745743805
C63	-7.7848103556	6.1575371660	2.4929468363
C64	-0.2333307632	7.1467371707	-0.4307986259
C65	1.0397231541	9.3994259527	5.8098857161
H66	-8.5801348067	6.1877163916	3.2447576027
H67	0.8403649072	6.9576216935	-0.5120423355
H68	1.4656964877	10.2163948437	5.2189833757
H69	-8.1345022645	6.6911992821	1.6033823996
H70	-0.7402518720	6.7181222837	-1.2970905446
H71	1.0355290842	9.7061380539	6.8611897062

C72	-5.7537541607	7.5208279564	2.1879820567
C73	-2.0068503420	5.9877022952	0.8263478800
C74	-1.2681199734	8.6627696294	6.2560372323
H75	-6.0805586219	7.6156819197	1.1556773660
H76	-2.5441914876	5.9912771311	-0.1179122921
H77	-0.9527305472	8.6002066722	7.2940199352
C78	-4.5489468205	7.9977983434	2.6255766333
C79	-2.5361702595	5.4818708718	1.9800391061
C80	-2.4923584039	8.2289273219	5.8333042341
H81	-3.9281385090	8.5053424746	1.8950477768
H82	-3.5383144370	5.0630542026	1.9242513213
H83	-3.1575592487	7.8202120056	6.5870238380
C84	-4.1526311729	7.8671801457	3.9880475799
C85	-1.8049292916	5.5091224512	3.2083049136
C86	-2.8840708945	8.3402915051	4.4677227719
C87	-5.1066888549	7.2448467149	4.8414993855
C88	-0.5015453011	6.0815208659	3.1139735155
C89	-1.9349917192	8.9684369586	3.6121829843
H90	-4.9323794538	7.1311824045	5.9066797761
H91	0.1588485298	6.1403110594	3.9763686955
H92	-2.1481549353	9.1535637069	2.5636308671
C93	-6.2997142399	6.7843558377	4.3557072957
C94	-0.0134617882	6.5678003691	1.9360424058
C95	-0.7168528536	9.3775652102	4.0808315207
H96	-7.0465296190	6.3121964795	4.9884017116
H97	0.9777304348	7.0080612364	1.8491865557
H98	0.0277746624	9.8509795516	3.4457966661
N99	4.5897053383	-3.9274374509	2.3325407172
N100	-0.5785739727	-1.9220038419	5.2251479945
C101	3.5537666478	-4.2394875783	3.1745993748
H102	3.7989535361	-4.2694215805	4.2332389284
C103	2.2968378463	-4.4833837262	2.7049941050
H104	1.5309356037	-4.7005598048	3.4457422586
C105	1.9941169835	-4.4457767320	1.3078874992
C106	3.0887716770	-4.0642589615	0.4745804157
H107	2.9751197224	-3.9532976377	-0.6005433413
C108	4.3357917080	-3.8404687668	0.9910956369
H109	5.1878572064	-3.5727582369	0.3687351925
C110	5.9816894583	-3.9913668849	2.8366511495
H111	6.5947490978	-3.3476998467	2.1981896914
H112	5.9815192730	-3.5630420956	3.8449419584
C113	6.4673708314	-5.4186294830	2.8334408570
C114	6.1267508877	-6.2795635999	3.8838705924
H115	5.6011349064	-5.8906589090	4.7572255454

C116	-3.1579247509	-0.5815410985	6.7787611442
H117	-3.7554736223	-1.3494525688	6.2848461276
C118	-1.8080757256	-0.8215610620	7.0546568521
C119	-1.0711864992	0.1614761754	7.7238235925
H120	-0.0272512069	-0.0242324755	7.9806240343
C121	7.1872032474	-5.9311944718	1.7512196046
H122	7.4902088316	-5.2677101922	0.9397610149
C123	-1.1410916067	-2.0881371744	6.5850159059
H124	-1.8482613056	-2.9234747950	6.5416046232
H125	-0.3159448968	-2.3803966700	7.2428754533
C126	0.6832259767	-1.4203153119	5.0452397574
H127	1.2704925841	-1.2829067665	5.9496603204
C128	1.1745908738	-1.1339225204	3.8017725543
H129	2.1916106305	-0.7577480321	3.7537892458
C130	0.3915605080	-1.3339188851	2.6234456744
C131	-0.9206775695	-1.8386051600	2.8645505971
H132	-1.6124814157	-2.0272708498	2.0487017270
C133	-1.3713009263	-2.1082159589	4.1253573814
H134	-2.3680382243	-2.4965513879	4.3202120021
N135	-0.1877599317	-11.7760629198	-0.6085530940
N136	6.2162543702	-10.3104321444	2.0624989659
N137	1.9463267168	-0.6705559157	-1.2997627738
N138	0.6350492511	-8.5305940574	3.8351420499
N139	-1.8575877046	-5.4230960802	-0.2543360213
N140	3.9216534159	-6.7958630590	-2.2228733554
C141	0.8743746859	-11.5335629356	-1.4394370470
C142	5.1884368789	-10.6870280507	2.8846677730
C143	0.6735157350	-1.1450327655	-1.1258761479
H144	0.6448203142	-11.5083243303	-2.5017909652
H145	5.4081798538	-10.6764582383	3.9496441357
H146	0.1136714430	-1.3418395672	-2.0372423338
C147	2.1378771394	-11.3477569371	-0.9559562216
C148	3.9738168449	-11.0578528838	2.3872487640
C149	0.1411550155	-1.3430439756	0.1183121524
H150	2.9191222291	-11.1614754988	-1.6869901030
H151	3.2143918322	-11.3461776655	3.1092768741
H152	-0.8786051717	-1.7142459395	0.1591505522
C153	2.4136356955	-11.3634890754	0.4488161388
C154	3.7018074169	-11.0641708073	0.9833748601
C155	0.8945270854	-1.0832093799	1.3032595552
C156	1.2839217501	-11.6656224768	1.2731618195
C157	4.8161608576	-10.7011582516	0.1638788462
C158	2.2064992732	-0.5744304721	1.0695718059
H159	1.3706121778	-11.7449995276	2.3548130373

H160	4.7425876046	-10.6837324289	-0.9195004807
H161	2.8676707527	-0.3160553209	1.8907626323
C162	0.0388723029	-11.8498296705	0.7397162669
C163	6.0110248842	-10.3255610238	0.7082816282
C164	2.6954732734	-0.3894970198	-0.1922971027
H165	-0.8359682619	-12.0682826533	1.3496702317
H166	6.8585555665	-10.0157573095	0.1024436243
H167	3.6931544771	-0.0011786238	-0.3791163896
C168	2.5691502330	-0.6605293869	-2.6447161427
C169	7.4055390596	-9.6319696656	2.6256878376
C170	-1.5720271398	-11.6920373570	-1.1291171144
H171	1.7982392376	-0.3590770799	-3.3613115068
H172	7.6022467503	-10.0841426357	3.6037627026
H173	-1.5583759109	-12.0896567769	-2.1495402362
H174	3.3405169203	0.1167000104	-2.6338532354
H175	8.2548643692	-9.8589980175	1.9732833671
H176	-2.1942084985	-12.3552291816	-0.5190777064
C177	3.1387068963	-2.0182270430	-2.9738719041
C178	-2.0667902070	-10.2674932392	-1.0907084036
C179	4.3822495620	-2.4110883466	-2.4645749120
C180	-2.7679265798	-9.7801558730	0.0166475468
H181	4.9910398409	-1.6969833900	-1.9076684977
H182	-3.0412651505	-10.4593459413	0.8259060958
C183	4.8466404749	-3.7099444235	-2.6528137087
C184	-3.1355121967	-8.4375654152	0.0905123172
H185	5.8139498007	-4.0031961160	-2.2411399737
H186	-3.6894997649	-8.0741719119	0.9573887834
C187	4.0819616591	-4.6447957669	-3.3592771297
C188	-2.8102369603	-7.5548484388	-0.9432346799
C189	2.8701167848	-4.2340101829	-3.9212306632
C190	-2.1382054541	-8.0488564906	-2.0663334389
H191	2.2839690392	-4.9351239178	-4.5164544271
H192	-1.9085425445	-7.3805287966	-2.8974283031
C193	2.4025998939	-2.9352817321	-3.7294572226
C194	-1.7718986520	-9.3890195679	-2.1397099075
H195	1.4543256105	-2.6318324599	-4.1747779410
H196	-1.2592478217	-9.7583926167	-3.0287302817
C197	4.4899141296	-6.0959329739	-3.4013072019
C198	-3.0676213835	-6.0766965072	-0.8057740669
C199	0.0216580373	-9.0929203743	5.0614746922
H200	5.5767178679	-6.2243295790	-3.3658756238
H201	-3.8980067695	-5.8624570136	-0.1246303559
H202	4.1163053768	-6.6040254873	-4.2964566795
H203	-3.2850353627	-5.6000225758	-1.7673544871

H204	0.4280027336	-8.5342315803	5.9112864267
C205	2.6042227356	-7.1728233172	-2.2281393562
C206	-0.8432802550	-5.0406497099	-1.0883249693
C207	1.9465656022	-8.1328698648	3.8338944649
H208	2.1224390292	-7.1674747854	-3.2025679405
H209	-1.0931875876	-5.0046112631	-2.1457983005
H210	2.4249235130	-8.0941055305	4.8097569927
C211	1.9536674777	-7.5447017472	-1.0862314990
C212	0.3924060707	-4.7073552315	-0.6106863740
C213	2.5964950635	-7.7934756442	2.6810882719
H214	0.9180163959	-7.8562893298	-1.1855828421
H215	1.1322302668	-4.3886640258	-1.3396404235
H216	3.6325019885	-7.4804103483	2.7741578073
C217	2.6102561009	-7.5283331288	0.1841299987
C218	0.7011651497	-4.7627111871	0.7840261697
C219	1.9461547613	-7.8529328801	1.4083491100
C220	3.9904183741	-7.1706063918	0.1323645526
C221	-0.3936887890	-5.1526038549	1.6117127578
C222	0.5799994907	-8.2636919236	1.4617686254
H223	4.6116801535	-7.1752022087	1.0252668856
H224	-0.2936965282	-5.2093977859	2.6920175998
H225	-0.0276974412	-8.3380313088	0.5611231595
C226	4.5987637677	-6.8075217246	-1.0357919211
C227	-1.6138735943	-5.4777210246	1.0906028069
C228	-0.0263544102	-8.5957328632	2.6396005967
H229	5.6487857826	-6.5264332526	-1.0881378253
H230	-2.4537502589	-5.7835870430	1.7100206958
H231	-1.0629024076	-8.9244729983	2.6896291313
H232	-1.0533851931	-8.8898080663	5.0106477017
C233	2.8830460252	5.5595560994	5.0874503126
C234	2.1762748099	5.8043058095	6.2706539412
C235	1.6295608177	7.0576128163	6.5236813138
C236	1.7717359276	8.0987243052	5.5981222422
C237	2.5138734216	7.8668658490	4.4369335876
C238	3.0644427359	6.6100159345	4.1843536495
H239	2.0568611909	5.0084954647	7.0074246431
H240	1.0892820822	7.2283590363	7.4558699506
H241	2.6636412675	8.6749358821	3.7198865348
H242	3.6409478827	6.4458590931	3.2729381565
C243	0.9588603091	-13.3056908379	5.1830627079
C244	-0.2571900953	-12.8679863953	4.6498890575
C245	-0.5810425593	-11.5125246838	4.6472109564
C246	0.3047515075	-10.5682456308	5.1751196651
C247	1.4993642752	-11.0129099117	5.7508331571

C248	1.8235009067	-12.3660317749	5.7537708308
H249	-0.9571401810	-13.5918978475	4.2303326333
H250	-1.5367416648	-11.1889447787	4.2306912952
H251	2.1827291426	-10.2950426602	6.2062070610
H252	2.7599889657	-12.6945832735	6.2060242026
C253	1.4010080786	-14.7364782392	5.0164891012
H254	2.0628941800	-15.0674181501	5.8229604035
H255	0.5589237951	-15.4330815809	4.9535571452
C256	3.4685436269	-14.3821375719	1.2918180932
C257	2.1005397054	-14.7588500282	1.3671681887
C258	1.4815897583	-14.9611753242	2.5701299712
N259	2.1588266452	-14.8312064255	3.7465982382
C260	3.4825181475	-14.5012261793	3.7201115412
C261	4.1430812645	-14.2848277172	2.5416173607
H262	1.5036133219	-14.9172101297	0.4744353660
H263	0.4360034675	-15.2476359096	2.6504695668
H264	3.9751137121	-14.4372568901	4.6868240041
H265	5.2022509237	-14.0603683690	2.6059105172
N266	5.4621276673	-13.8339165340	-2.4264725787
C267	6.1495424352	-13.7307510616	-1.2532263796
C268	5.5234234837	-13.8785918774	-0.0477254349
C269	4.1316361934	-14.1547382026	0.0348715860
C270	3.4505543533	-14.2257974838	-1.2112070419
C271	4.1210907843	-14.0729666322	-2.3947503727
H272	7.2164308998	-13.5456562934	-1.3424331532
H273	6.1428672383	-13.7997576348	0.8403267920
H274	2.3876973310	-14.4337495822	-1.2720268442
H275	3.6281067881	-14.1443057535	-3.3600281761
C276	6.1849960322	-13.7248703878	-3.6921934618
H277	5.4740079521	-13.7893605514	-4.5174064795
H278	6.7107784712	-12.7661703146	-3.7368534243
H279	6.9111828861	-14.5398218107	-3.7731413085
H280	-0.4074388215	8.2290788127	-0.4113260450

Co-conformation 3b

M06L/6-31G* in acetonitrile (A)	M06L/6-31G* in gas phase (B)	M06/6-311++G** in gas phase (C)	Total energy (C+A-B)
-6208.69356	-6206.99997	-6204.48428	-6206.17787

N1	1.5187190500	8.1021492117	-9.7721571611
N2	-1.4311777248	3.3907927315	-8.3955650602
C3	0.2755105437	7.7072501418	-9.3556989500
H4	-0.5047406074	7.7302168358	-10.1140360782
C5	0.0399851746	7.3208085505	-8.0684239014

H6	-0.9792016471	7.0303930694	-7.8196943154
C7	1.0808903338	7.2917103944	-7.0903317016
C8	2.3567145577	7.7205826540	-7.5682295737
H9	3.2236207471	7.7557312680	-6.9108241295
C10	2.5469592867	8.0989353290	-8.8656413459
H11	3.5121098732	8.4246275238	-9.2472855337
C12	1.8029475119	8.2443674815	-11.2176795978
H13	0.9165578819	8.6881168683	-11.6817793084
H14	2.6290384153	8.9559401491	-11.3194882678
C15	2.1372162897	6.9008455392	-11.8131506848
C16	3.4517405555	6.4237900330	-11.7933576862
H17	4.2574021878	7.0704200327	-11.4419377587
C18	8.5168399009	-13.5294478901	3.4943876063
H19	8.3546845052	-14.1762872184	4.3577903240
C20	9.2690020399	-13.9928975500	2.4087297728
C21	9.5040569003	-13.1286252620	1.3361026909
H22	10.1152113021	-13.4628866515	0.4962355570
C23	1.1274525553	6.0711784097	-12.3107461497
H24	0.1017931639	6.4393662415	-12.3663285484
C25	-2.8969368497	3.4482842379	-8.5957074257
H26	-3.0910732398	3.2628488141	-9.6572656399
H27	-3.3344513762	2.6221637449	-8.0246738741
C28	-0.5742199960	3.8617083191	-9.3522358688
H29	-1.0237278936	4.0795104901	-10.3191602160
C30	0.7588983016	4.0366975069	-9.1042362064
H31	1.3665410850	4.4065680759	-9.9264897485
C32	1.3240921649	3.7589149273	-7.8207771187
C33	0.3908387281	3.2649301875	-6.8587310600
H34	0.7031680027	3.0071280535	-5.8507720682
C35	-0.9301599303	3.0994441823	-7.1534178897
H36	-1.6500919479	2.7255815202	-6.4300733846
N37	5.4014082320	4.5931542917	-6.8912657756
N38	-3.0988666913	9.3448451770	-6.3708314639
N39	0.4278028511	5.9734258073	-3.0933516050
N40	3.7124446984	10.5761132156	-4.8418842757
C41	4.5682613496	4.0525888565	-5.9483249585
H42	5.0104812322	3.8867076116	-4.9695939020
C43	3.2689276658	3.7445975854	-6.2309367091
H44	2.6808066430	3.3158853652	-5.4246152117
C45	2.7010886189	3.9867974709	-7.5183523024
C46	3.6208056701	4.5133436457	-8.4762649208
H47	3.3178109286	4.7145609405	-9.5000080820
C48	4.9125763276	4.8103650683	-8.1488805729
H49	5.6178260049	5.2285174104	-8.8642722304

C50	6.6794698821	5.2102984088	-6.4703360628
H51	7.1154960157	4.5657199610	-5.6998673234
H52	7.3477885803	5.2027403274	-7.3375953029
C53	6.4228033407	6.6061531979	-5.9627047480
C54	6.4247076265	7.6925877773	-6.8430639014
H55	6.7164041101	7.5467859663	-7.8840816855
C56	6.0655599750	8.9630591454	-6.4005014824
H57	6.0807097469	9.8013735436	-7.0984563494
C58	5.6936088824	9.1733099588	-5.0686405176
C59	5.7168254988	8.0920607753	-4.1823731035
H60	5.4546032917	8.2442799687	-3.1343458748
C61	6.0795580059	6.8225022950	-4.6243999063
H62	6.0998772189	5.9914447732	-3.9181408448
C63	5.1753837857	10.5171732925	-4.6247714674
C64	0.1874233150	5.5927066494	-1.7045273658
C65	-4.3989569580	8.7593038456	-6.7724942239
H66	5.6240268005	11.3402015960	-5.1910977861
H67	-0.6323207261	4.8722021538	-1.6616384905
H68	-5.0565118406	8.7917541282	-5.8977013444
H69	5.3541085751	10.6992222371	-3.5602924909
H70	1.0898544057	5.1361764412	-1.2914712383
H71	-4.8277129000	9.4057980923	-7.5453114693
C72	2.8544138885	10.1349359555	-3.8764276894
C73	1.6686671276	6.3881444701	-3.4943011621
C74	-2.2524035661	9.8386651466	-7.3243067721
H75	3.2906683679	9.9631015287	-2.8956788520
H76	2.4458084997	6.3472306630	-2.7352084707
H77	-2.6868527618	9.9907923084	-8.3090356205
C78	1.5256533511	9.9441867185	-4.1354082809
C79	1.9024049600	6.8136610532	-4.7699373543
C80	-0.9465716103	10.1330054899	-7.0440126773
H81	0.9063081669	9.6221394723	-3.3036812409
H82	2.9205052974	7.1106943353	-5.0118320847
H83	-0.3506771567	10.5471076680	-7.8513798223
C84	0.9773547651	10.1676547555	-5.4317938062
C85	0.8631838030	6.8597416705	-5.7482302915
C86	-0.4017136967	9.9194464936	-5.7445582482
C87	1.9033739761	10.6634744652	-6.3931712397
C88	-0.4112656348	6.4186812997	-5.2803144752
C89	-1.3321410859	9.4432886284	-4.7752863184
H90	1.5921918439	10.9270085861	-7.3992179313
H91	-1.2772708626	6.3939093915	-5.9372828252
H92	-1.0466084615	9.2973263919	-3.7379529553
C93	3.2233467084	10.8428625893	-6.0890403349

C94	-0.6003517265	6.0013525355	-3.9950118065
C95	-2.6277592726	9.1579873949	-5.1029132988
H96	3.9435692321	11.2171116892	-6.8117477065
H97	-1.5637018508	5.6635643372	-3.6213604159
H98	-3.3482716589	8.7868714785	-4.3785111980
N99	6.1051746484	-10.1539539626	1.9359126633
N100	2.9375354021	2.0513229467	-11.7359971144
C101	5.1393179612	-10.5035071696	2.8404338331
H102	5.4466884344	-10.4925243327	3.8832046072
C103	3.8710360463	-10.8256331917	2.4517953003
H104	3.1697779155	-11.0942571125	3.2364325199
C105	3.4860891697	-10.8310020922	1.0727572021
C106	4.5166785732	-10.4231913130	0.1698919308
H107	4.3350828885	-10.3622581709	-0.8998814541
C108	5.7742662164	-10.1172211706	0.6061148282
H109	6.5763375868	-9.8272412695	-0.0690712328
C110	7.5173122226	-10.0392751626	2.3645858833
H111	8.0174392784	-9.3571388039	1.6692295555
H112	7.5170990227	-9.5662054532	3.3529551403
C113	8.1855211987	-11.3911876252	2.3991152958
C114	7.9840756773	-12.2448616661	3.4901480782
H115	7.4155862164	-11.8982003949	4.3538278731
C116	3.7431574244	5.1313428640	-12.2214366547
H117	4.7748203003	4.7763933903	-12.1996451449
C118	2.7259710677	4.2863759728	-12.6786065092
C119	1.4179800009	4.7773180059	-12.7377909316
H120	0.6179245001	4.1408613517	-13.1186293735
C121	8.9687625715	-11.8403663256	1.3325416338
H122	9.1683855002	-11.1748298987	0.4912572353
C123	3.0182018381	2.8396327871	-12.9862162851
H124	4.0232744182	2.6985305956	-13.3973020841
H125	2.2977342536	2.4125168053	-13.6913828376
C126	1.7272958765	1.6060700236	-11.2856224302
H127	0.9100520813	1.6490153707	-12.0013880569
C128	1.5695391885	1.1223760562	-10.0166142493
H129	0.5798803373	0.7644349080	-9.7467126807
C130	2.6520688734	1.0892138069	-9.0916890034
C131	3.9029222000	1.5219341682	-9.6194569472
H132	4.8123953270	1.4874150488	-9.0273246381
C133	4.0147530527	1.9975177326	-10.8950708846
H134	4.9592641200	2.3381000838	-11.3113476292
N135	2.2179952143	-18.3047325142	-0.5345333720
N136	8.5635708335	-16.2514975980	1.8670852528
N137	2.1918536392	-0.2790796295	-5.0757394766

N138	0.5683956411	-8.8393761807	4.1431304027
N139	-0.3192813136	-12.2634379816	-0.2166093541
N140	3.2335307507	-7.0605967162	-2.1769804544
C141	3.2016472105	-17.9251718587	-1.4032387373
C142	7.5988789123	-16.6715948155	2.7391841172
C143	3.4131031374	0.1269441824	-5.5361396300
H144	2.9388381192	-17.9503551430	-2.4576693731
H145	7.8626832762	-16.6324563691	3.7929136252
H146	4.2332731915	0.0637659129	-4.8260352038
C147	4.4438672811	-17.5623737274	-0.9643816907
C148	6.3879347111	-17.1302550462	2.3012814415
C149	3.5819723910	0.5783589731	-6.8160474017
H150	5.1781500391	-17.3117296804	-1.7225038946
H151	5.6915388360	-17.4787627058	3.0563104809
H152	4.5858855179	0.8785675549	-7.1025551145
C153	4.7663075502	-17.5498127610	0.4260263024
C154	6.0603934318	-17.1596953373	0.9139887315
C155	2.4972292229	0.6348571059	-7.7375815231
C156	3.7148766630	-17.9623900764	1.2934373580
C157	7.1193046590	-16.7760076618	0.0442888182
C158	1.2482329453	0.1920911567	-7.2140150513
H159	3.8557292134	-18.0249321838	2.3684067540
H160	7.0144524146	-16.8313658805	-1.0352821805
H161	0.3499554228	0.1724561076	-7.8225250876
C162	2.4863763032	-18.3152592979	0.8050694052
C163	8.3166998617	-16.3252203224	0.5265383017
C164	1.1239364763	-0.2472732989	-5.9245831613
H165	1.6724243311	-18.6415932340	1.4475329394
H166	9.1328886525	-16.0178311460	-0.1224323753
H167	0.1772012821	-0.5865218425	-5.5127996536
C168	2.0615044110	-0.8515357207	-3.7163061822
C169	9.6998755077	-15.4375741296	2.3570107779
C170	0.8246229594	-18.4586682148	-1.0126401002
H171	2.6660264427	-0.2336214785	-3.0438376212
H172	9.9781761267	-15.8234460533	3.3431325469
H173	0.8723964915	-18.8679788072	-2.0270547510
H174	1.0123172860	-0.7328865538	-3.4256450151
H175	10.5421780973	-15.5978964611	1.6764156045
H176	0.3379606000	-19.2005803964	-0.3713103417
C177	2.4891958930	-2.2965270129	-3.6534869385
C178	0.1226345708	-17.1252638693	-0.9723049956
C179	1.6565540610	-3.3065354245	-4.1458664163
C180	-0.5773054135	-16.7206877100	0.1683863110
H181	0.6849534442	-3.0528677942	-4.5713861198

H182	-0.7073123267	-17.4174991967	0.9976128279
C183	2.0513409098	-4.6386639467	-4.0910722370
C184	-1.1201531337	-15.4396868671	0.2497160100
H185	1.3910368785	-5.4118031144	-4.4852705584
H186	-1.6705918017	-15.1422297242	1.1439809403
C187	3.2872124329	-4.9924620145	-3.5405896125
C188	-0.9776352979	-14.5382036270	-0.8088575640
C189	4.1214587570	-3.9831997803	-3.0530252392
C190	-0.3072645505	-14.9556736964	-1.9634943170
H191	5.0943795033	-4.2378604283	-2.6309969999
H192	-0.2160304766	-14.2773649778	-2.8127546015
C193	3.7262387745	-2.6481028637	-3.1097083535
C194	0.2373133890	-16.2335690841	-2.0441893014
H195	4.3859016853	-1.8729098785	-2.7183893306
H196	0.7493197909	-16.5442361138	-2.9558757998
C197	3.6951554753	-6.4412996757	-3.4442066948
C198	-1.4425805288	-13.1102148055	-0.6774397722
C199	0.0855182414	-9.4262771471	5.4136817044
H200	4.7844930338	-6.5528347621	-3.4748128707
H201	-2.2562001310	-13.0065568944	0.0480258545
H202	3.2725130180	-7.0345220948	-4.2616574020
H203	-1.7870190837	-12.6997858449	-1.6325966634
H204	0.5439417967	-8.8609907383	6.2315135871
C205	1.9899878269	-7.6196789679	-2.0876957728
C206	0.5893341509	-11.7839192210	-1.1242615065
C207	1.8571288412	-8.4002043443	4.0332473541
H208	1.4391131910	-7.6996825468	-3.0210567102
H209	0.2816353581	-11.8255401193	-2.1657553773
H210	2.4060300359	-8.3039865169	4.9665324919
C211	1.4741820893	-8.0421294498	-0.8913694251
C212	1.7986600480	-11.2866855452	-0.7342857815
C213	2.4066902721	-8.0832519690	2.8215346960
H214	0.4728886080	-8.4610023630	-0.9105971521
H215	2.4544736880	-10.9249780122	-1.5208648878
H216	3.4243215295	-7.7066147784	2.8262842604
C217	2.2055803602	-7.8894849135	0.3231283237
C218	2.1923730887	-11.2508035860	0.6400817708
C219	1.6600949180	-8.2178999306	1.6125904335
C220	3.5136669729	-7.3488944241	0.1711029112
C221	1.1888397697	-11.7083579252	1.5489004901
C222	0.3153928708	-8.6506855887	1.7803251739
H223	4.1717553862	-7.2043681746	1.0228671340
H224	1.3471997278	-11.6964816654	2.6253638875
H225	-0.3608467705	-8.7399031595	0.9353985496

C226	3.9858648058	-6.9415602317	-1.0460444521
C227	-0.0049110044	-12.2063880465	1.1119081292
C228	-0.1889985686	-8.9583845424	3.0123594952
H229	4.9699809850	-6.4965290675	-1.1717065528
H230	-0.7651840683	-12.5866551515	1.7918143084
H231	-1.2140762759	-9.2883484634	3.1587642822
H232	-0.9971218601	-9.2687739664	5.4560444142
C233	-3.4305163361	4.7858238973	-8.1506898244
C234	-3.5045839729	5.8528865135	-9.0506481905
C235	-3.8725178852	7.1231952573	-8.6150568973
C236	-4.1717661735	7.3542175220	-7.2688815331
C237	-4.1390357403	6.2782654013	-6.3757439373
C238	-3.7744996955	5.0071781918	-6.8126924050
H239	-3.2748196590	5.6892008480	-10.1044429147
H240	-3.9285007326	7.9448226604	-9.3302564359
H241	-4.4026561706	6.4343624786	-5.3281976967
H242	-3.7580414480	4.1784888357	-6.1031599904
C243	1.2680182206	-13.5773712291	5.2992485848
C244	0.0036287874	-13.1903653719	4.8456832146
C245	-0.4013998330	-11.8587762718	4.9257731283
C246	0.4520610495	-10.8877881262	5.4589778640
C247	1.7031575773	-11.2823369936	5.9446768825
C248	2.1045399802	-12.6118501884	5.8681342578
H249	-0.6768113465	-13.9368617754	4.4315776018
H250	-1.3928475199	-11.5724789261	4.5720662954
H251	2.3674531778	-10.5434837216	6.3947282747
H252	3.0798842477	-12.9026477599	6.2598656485
C253	1.7742166155	-14.9820158397	5.0917635833
H254	2.4197986850	-15.3121020992	5.9124770405
H255	0.9562000143	-15.7043788192	4.9981497743
C256	3.9792950266	-14.5718429290	1.4297861387
C257	2.6086998932	-14.9723462137	1.4626143889
C258	1.9503865632	-15.1788407304	2.6401924804
N259	2.5757015788	-15.0503553244	3.8487274585
C260	3.9056068647	-14.7156989637	3.8648207780
C261	4.6036587577	-14.4848861423	2.7145848066
H262	2.0325459544	-15.1078320428	0.5478627878
H263	0.8977754574	-15.4517813696	2.6800632429
H264	4.3603421989	-14.6575206819	4.8503567438
H265	5.6558978372	-14.2301080279	2.8155916331
N266	6.0074998341	-13.6462999209	-2.2024257957
C267	6.6361911010	-13.5096890491	-0.9953415301
C268	6.0048189198	-13.7947371973	0.1804834096
C269	4.6588410759	-14.2666788566	0.2131168971

C270	4.0403357147	-14.3829147286	-1.0721248031
C271	4.7126834285	-14.0858784481	-2.2217124074
H272	7.6633990251	-13.1553916882	-1.0361529853
H273	6.5755497484	-13.6385166817	1.0940364744
H274	3.0078476820	-14.7065611445	-1.1779500015
H275	4.2622365476	-14.1752145807	-3.2063617608
C276	6.7412913754	-13.4171742091	-3.4426885685
H277	6.0321143036	-13.2728271816	-4.2593740623
H278	7.3624007930	-12.5227005611	-3.3460167249
H279	7.3831350850	-14.2748764234	-3.6728920940
H280	-0.0764216294	6.4717043846	-1.1044182665

Co-conformation 3c

M06L/6-31G* in acetonitrile (A)	M06L/6-31G* in gas phase (B)	M06/6-311++G** in gas phase (C)	Total energy (C+A-B)
-6208.68304	-6206.95888	-6204.446	-6206.17016

N1	1.3528581733	8.1973332227	-9.9221225017
N2	0.4825039608	-2.5063650076	-10.6440125405
C3	0.1327071754	7.7048241142	-9.5489302919
H4	-0.6257479864	7.6812101354	-10.3280484996
C5	-0.1085282043	7.2833418506	-8.2722028722
H6	-1.1092861696	6.9170514890	-8.0555469923
C7	0.9062885350	7.3188862547	-7.2697039487
C8	2.1566317386	7.8487221620	-7.7036226665
H9	2.9991026736	7.9414913986	-7.0222697045
C10	2.3523793275	8.2580740624	-8.9896720042
H11	3.2996771805	8.6614160212	-9.3389228701
C12	1.6805279520	8.3754577882	-11.3523204737
H13	0.7822077665	8.7527650966	-11.8515318274
H14	2.4535056192	9.1482214696	-11.4167962224
C15	2.1308800784	7.0506452395	-11.9050855948
C16	3.4656119862	6.6544495482	-11.7791492449
H17	4.2026556252	7.3505129065	-11.3756468482
C18	8.6637272061	-13.6293227404	3.2452138524
H19	8.5592597342	-14.2215767120	4.1553078238
C20	9.3261250329	-14.1684466535	2.1362412758
C21	9.4910499338	-13.3730155745	0.9994667695
H22	10.0329697086	-13.7659896789	0.1377210952
C23	1.2091151145	6.1598580845	-12.4624397179
H24	0.1706755315	6.4669878300	-12.5951164356
C25	-0.9724078952	-2.4847903774	-10.9191601682
H26	-1.1054896137	-2.6673303973	-11.9904853258
H27	-1.4176275889	-3.3256199204	-10.3764007835

C28	1.3689823477	-2.0042592946	-11.5546202278
H29	0.9613567599	-1.7917180925	-12.5403380719
C30	2.6835742764	-1.7960530373	-11.2428596527
H31	3.3186870065	-1.4042968523	-12.0328366546
C32	3.1978675782	-2.0724451344	-9.9400383655
C33	2.2373227931	-2.6025190460	-9.0268289179
H34	2.5136025531	-2.8658380524	-8.0093429207
C35	0.9343231836	-2.7977733257	-9.3838714817
H36	0.1925226810	-3.2005635841	-8.6992223644
N37	7.2090325828	-1.1403807942	-8.8209687824
N38	-1.4323977935	3.4073610426	-8.6782046648
N39	0.2585882603	5.9671228492	-3.2832818954
N40	5.2663491867	4.7843322935	-6.8027444830
C41	6.3519708407	-1.7183941125	-7.9243277524
H42	6.7574149912	-1.8897213220	-6.9305393277
C43	5.0748344444	-2.0570654686	-8.2684830030
H44	4.4646866142	-2.5173676518	-7.4965241636
C45	4.5566527013	-1.8087402195	-9.5744190829
C46	5.5008720690	-1.2430464101	-10.4838620703
H47	5.2385839527	-1.0394553015	-11.5180227923
C48	6.7691169228	-0.9165411622	-10.0953055983
H49	7.4921428659	-0.4692595594	-10.7734290344
C50	8.4511830005	-0.4962344002	-8.3369893336
H51	8.8714153154	-1.1404128976	-7.5573267272
H52	9.1555444908	-0.4741074961	-9.1748117768
C53	8.1320108815	0.8856901490	-7.8260847162
C54	8.1412104372	1.9792537980	-8.6970941838
H55	8.4812499313	1.8505381864	-9.7255239501
C56	7.7277839687	3.2347314644	-8.2610902105
H57	7.7506281992	4.0790363181	-8.9514635165
C58	7.2926466934	3.4245218662	-6.9456715216
C59	7.3084911881	2.3373546133	-6.0662448583
H60	6.9976806078	2.4745213856	-5.0295064557
C61	7.7263151741	1.0816410405	-6.5015080332
H62	7.7428651049	0.2455424753	-5.8007998326
C63	6.7205307547	4.7530752876	-6.5211784687
C64	0.0137638133	5.5850344095	-1.8958233980
C65	-2.6884118226	2.7850147623	-9.1551996530
H66	7.1775320039	5.5843242273	-7.0685559705
H67	-0.7617629173	4.8166256944	-1.8626539934
H68	-3.3957860052	2.7953005157	-8.3197026549
H69	6.8498657343	4.9386299384	-5.4501506397
H70	0.9341891769	5.1884322368	-1.4610661360
H71	-3.0915548598	3.4214262456	-9.9499306056

C72	4.3685694958	4.3313410680	-5.8757422673
C73	1.4784651859	6.4525546548	-3.6619598336
C74	-0.5479782057	3.9298150279	-9.5796734238
H75	4.7616960977	4.1717904083	-4.8749496558
H76	2.2410347504	6.4667072925	-2.8878157699
H77	-0.9308511200	4.0736193671	-10.5873584407
C78	3.0564672930	4.1146194198	-6.1957133040
C79	1.7107031699	6.8858401112	-4.9362423247
C80	0.7303351256	4.2554570631	-9.2244931141
H81	2.4041750990	3.7817680596	-5.3934436618
H82	2.7117898392	7.2456095497	-5.1582118669
H83	1.3609866426	4.6898041720	-9.9956779179
C84	2.5650579479	4.3223472143	-7.5190677251
C85	0.6899105230	6.8618792075	-5.9312310261
C86	1.2111035962	4.0484236612	-7.8978535890
C87	3.5338670072	4.8206747995	-8.4418389351
C88	-0.5644660225	6.3511728932	-5.4873842367
C89	0.2395258202	3.5435760707	-6.9832057823
H90	3.2834049988	5.0489108994	-9.4759762346
H91	-1.4181969050	6.2856300604	-6.1560223865
H92	0.4723017049	3.3967761635	-5.9324460199
C93	4.8327409014	5.0284264884	-8.0751979413
C94	-0.7518355558	5.9290976632	-4.2017961191
C95	-1.0269146533	3.2268520159	-7.3841148359
H96	5.5818814878	5.4058988824	-8.7669546075
H97	-1.7013413115	5.5411069497	-3.8429862689
H98	-1.7763518127	2.8302201969	-6.7039725042
N99	6.1859730462	-10.3247970165	1.6590438091
N100	3.2292856373	2.2155996514	-11.7473509240
C101	5.2737644533	-10.6069414112	2.6400498835
H102	5.6414397522	-10.5268249577	3.6600074707
C103	3.9835857310	-10.9468463708	2.3472373868
H104	3.3274274780	-11.1578368705	3.1868100875
C105	3.5217727700	-11.0448783345	0.9953249396
C106	4.5002191716	-10.7061059203	0.0110940629
H107	4.2579327524	-10.7176341555	-1.0487762032
C108	5.7800441348	-10.3772675927	0.3520945321
H109	6.5429669943	-10.1383610468	-0.3848696265
C110	7.6236872029	-10.1974620078	1.9838678012
H111	8.0789684192	-9.5645189588	1.2150745001
H112	7.6937634760	-9.6652528589	2.9390549247
C113	8.2775135491	-11.5543740284	2.0521669728
C114	8.1474224967	-12.3389099200	3.2039215225
H115	7.6496097436	-11.9327309459	4.0850438993

C116	3.8598254210	5.3753498459	-12.1564767424
H117	4.9056251944	5.0817274440	-12.0513428352
C118	2.9305128064	4.4687307025	-12.6795124900
C119	1.6053158159	4.8815191513	-12.8468793982
H120	0.8744087457	4.1959369922	-13.2783567456
C121	8.9736922032	-12.0781416607	0.9591200559
H122	9.1177368787	-11.4677659751	0.0662485905
C123	3.3203136500	3.0417026629	-12.9721879638
H124	4.3492090912	2.9672586193	-13.3390822850
H125	2.6606396321	2.5929875930	-13.7221229471
C126	2.0236367050	1.6934899027	-11.3675093845
H127	1.2386418544	1.7196762934	-12.1201274152
C128	1.8341303533	1.1496891316	-10.1293025570
H129	0.8507855243	0.7341855741	-9.9191863838
C130	2.8782590936	1.1222724713	-9.1584204539
C131	4.1300210735	1.6358297537	-9.6137485138
H132	5.0153438548	1.6163522339	-8.9827201813
C133	4.2725733898	2.1727268990	-10.8606858234
H134	5.2194008118	2.5648589090	-11.2245122749
N135	2.0475611629	-18.6423817720	0.0455375100
N136	8.5538804100	-16.4495266990	1.7978085502
N137	2.3130365915	-0.4059421980	-5.2143311090
N138	0.7370084612	-8.8477978270	4.0852700130
N139	-0.3516479546	-12.5314692877	-0.0083258638
N140	3.2764236413	-7.2258304013	-2.3354188959
C141	2.9713270104	-18.3602069670	-0.9195375805
C142	7.6561687870	-16.7908687414	2.7707947811
C143	3.5389770806	0.0477066358	-5.6184088619
H144	2.6364832165	-18.4805296082	-1.9465836936
H145	7.9993684869	-16.6706539978	3.7950203425
H146	4.3344365679	-0.0183645368	-4.8801590791
C147	4.2422242971	-17.9751469304	-0.6016759002
C148	6.4137019817	-17.2720903200	2.4644832262
C149	3.7395834624	0.5487536912	-6.8743817910
H150	4.9245906037	-17.8060622874	-1.4281958005
H151	5.7757302561	-17.5520838994	3.2967571777
H152	4.7429664841	0.8900221610	-7.1159224336
C153	4.6596384692	-17.8368941167	0.7552552429
C154	5.9855512891	-17.4144995562	1.1117860031
C155	2.6877994153	0.6082150277	-7.8352313570
C156	3.6685361120	-18.1524887853	1.7276220822
C157	6.9751258144	-17.1078026273	0.1353577687
C158	1.4322066642	0.1157201843	-7.3698285720
H159	3.8834798374	-18.1160280251	2.7914591008

H160	6.7887289243	-17.2501230068	-0.9254405018
H161	0.5540320144	0.1047910304	-8.0084680023
C162	2.4063238373	-18.5315284872	1.3591694609
C163	8.2062363009	-16.6271786468	0.4893028869
C164	1.2742762183	-0.3691812720	-6.1009929007
H165	1.6357800973	-18.7845816142	2.0829818407
H166	8.9719385333	-16.3788280544	-0.2415202352
H167	0.3225924530	-0.7435863705	-5.7328595868
C168	2.1472877155	-1.0182760575	-3.8759394543
C169	9.7329160950	-15.6207978846	2.1427045676
C170	0.6255309063	-18.8136364974	-0.3281679204
H171	2.7157240167	-0.4079506444	-3.1660323169
H172	10.0820075608	-15.9488146500	3.1271890310
H173	0.6034789652	-19.3148177799	-1.3013480555
H174	1.0869883077	-0.9212320642	-3.6189778652
H175	10.5176580511	-15.8379634046	1.4108744027
H176	0.1701979583	-19.4835309282	0.4084411285
C177	2.5732237643	-2.4649974577	-3.8251016917
C178	-0.0460341337	-17.4649134157	-0.3699788106
C179	1.7411330147	-3.4651570985	-4.3396657752
C180	-0.6715873915	-16.9424896714	0.7655129622
H181	0.7756670537	-3.2008807261	-4.7727595614
H182	-0.7697707379	-17.5592426481	1.6600237942
C183	2.1222926505	-4.8017419370	-4.2897589142
C184	-1.1782119438	-15.6444292961	0.7604726836
H185	1.4607971030	-5.5656809729	-4.6995986317
H186	-1.6717526908	-15.2543479697	1.6523984606
C187	3.3461320828	-5.1719302067	-3.7235419004
C188	-1.0716128634	-14.8420829008	-0.3792549467
C189	4.1828842248	-4.1728232374	-3.2191945360
C190	-0.4741346888	-15.3767004197	-1.5255274814
H191	5.1471866981	-4.4391122566	-2.7847140859
H192	-0.4121232640	-14.7775601113	-2.4348278783
C193	3.8003148352	-2.8335790473	-3.2689762495
C194	0.0328800134	-16.6727580551	-1.5207844347
H195	4.4601961968	-2.0693163845	-2.8569039286
H196	0.4902233235	-17.0750245099	-2.4256934631
C197	3.7342361422	-6.6259370207	-3.6136735200
C198	-1.5040876025	-13.3980495834	-0.3466348968
C199	0.2936617451	-9.3740897835	5.3969084853
H200	4.8212983791	-6.7508344684	-3.6522779287
H201	-2.2792055721	-13.2267255238	0.4074562268
H202	3.2973243820	-7.2226135086	-4.4212101596
H203	-1.8917280318	-13.0602283554	-1.3135695498

H204	0.7805028754	-8.7726845294	6.1714235944
C205	2.0291474235	-7.7724268581	-2.2162225781
C206	0.5172438981	-12.1251570008	-0.9883230927
C207	2.0241304886	-8.4203989401	3.9237720911
H208	1.4611931008	-7.8629123060	-3.1383582410
H209	0.1614713077	-12.2368256715	-2.0091341914
H210	2.5984545922	-8.2910120995	4.8375294672
C211	1.5314718112	-8.1714468622	-1.0033599097
C212	1.7465711721	-11.6117973434	-0.6900517029
C213	2.5410220719	-8.1442770350	2.6890690890
H214	0.5264970587	-8.5829870600	-0.9972298872
H215	2.3664406183	-11.3113975358	-1.5296385590
H216	3.5606460313	-7.7744262976	2.6557392153
C217	2.2841705755	-8.0068699601	0.1970389810
C218	2.2063014544	-11.4855960039	0.6590652368
C219	1.7626755529	-8.3057752598	1.5042407634
C220	3.5947407674	-7.4822956569	0.0117819416
C221	1.2442023351	-11.8731648975	1.6417246919
C222	0.4223100068	-8.7330293365	1.7221165170
H223	4.2702745074	-7.3310285048	0.8482141821
H224	1.4448615951	-11.8009994316	2.7080022526
H225	-0.2778596381	-8.8443968543	0.8990334562
C226	4.0488275685	-7.0983287623	-1.2189363279
C227	0.0275986793	-12.3875629322	1.2959265744
C228	-0.0495770929	-9.0014959924	2.9777495621
H229	5.0350279795	-6.6659655328	-1.3675575400
H230	-0.7010847489	-12.7151445623	2.0351549998
H231	-1.0728122047	-9.3181488317	3.1620356668
H232	-0.7864014318	-9.2085509934	5.4666186903
C233	-1.5587219865	-1.1618393367	-10.4960098985
C234	-1.6126258955	-0.0925611023	-11.3953256656
C235	-2.0300145344	1.1677047906	-10.9745812008
C236	-2.3977106636	1.3879307785	-9.6434314873
C237	-2.3880905327	0.3077374293	-8.7547813271
C238	-1.9745668422	-0.9534523426	-9.1768295522
H239	-1.3269773028	-0.2470759783	-12.4367185947
H240	-2.0703298120	1.9901887953	-11.6901843901
H241	-2.7120303602	0.4517139363	-7.7227536174
H242	-1.9755866845	-1.7846486712	-8.4700793547
C243	1.4279019356	-13.5389840750	5.4720397689
C244	0.1530017686	-13.1605019881	5.0433771906
C245	-0.2339584885	-11.8214601070	5.0630841978
C246	0.6488360089	-10.8340466023	5.5091176531
C247	1.9124692348	-11.2178779160	5.9713265739

C248	2.2964051059	-12.5548763240	5.9546584937
H249	-0.5506389585	-13.9199031326	4.6968967590
H250	-1.2349155484	-11.5448619123	4.7290336268
H251	2.6007276815	-10.4643468076	6.3563470812
H252	3.2822237613	-12.8366398851	6.3263710718
C253	1.9079277043	-14.9594671724	5.3185359686
H254	2.5828565995	-15.2566031370	6.1281816146
H255	1.0783342448	-15.6742219056	5.2959433095
C256	3.9212150864	-14.7364914310	1.5345088497
C257	2.5553009713	-15.1332984568	1.6572954685
C258	1.9598063263	-15.2815990540	2.8763955106
N259	2.6466265876	-15.0970783517	4.0436009222
C260	3.9747356991	-14.7646708030	3.9749163976
C261	4.6102991821	-14.5899051342	2.7800027379
H262	1.9329152403	-15.3117004930	0.7810021780
H263	0.9110561212	-15.5507673425	2.9842613155
H264	4.4792668959	-14.6557922814	4.9314790696
H265	5.6661286301	-14.3318271866	2.8142935652
N266	5.7476288305	-13.9747466467	-2.2405280575
C267	6.4449364331	-13.7966429714	-1.0773920436
C268	5.8801078697	-14.0299291055	0.1429212259
C269	4.5356043024	-14.4904665677	0.2705987024
C270	3.8438346103	-14.6501117700	-0.9721419958
C271	4.4509829431	-14.4035073523	-2.1687289174
H272	7.4703191083	-13.4521075655	-1.1893333390
H273	6.5037078523	-13.8428978092	1.0152166398
H274	2.8038552774	-14.9653082194	-1.0061727304
H275	3.9444331016	-14.5270089435	-3.1218753672
C276	6.4111148446	-13.8018659960	-3.5281996717
H277	5.6576111612	-13.6812335882	-4.3085370547
H278	7.0451064374	-12.9113647869	-3.5019428324
H279	7.0303559745	-14.6757072368	-3.7608461035
H280	-0.3143029271	6.4539254635	-1.3133855357

Co-conformation 3d

M06L/6-31G* in acetonitrile (A)	M06L/6-31G* in gas phase (B)	M06/6-311++G** in gas phase (C)	Total energy (C+A-B)
-6208.68477	-6206.90408	-6204.38941	-6206.17010

N1	1.2298596002	8.3089628913	-9.8311233711
N2	-0.0368403632	-2.4514923036	-10.2047650148
C3	0.1210987648	7.8069125834	-9.2115277457
H4	-0.7832441434	7.7706940538	-9.8139283387
C5	0.1585061518	7.3906362665	-7.9086420209
H6	-0.7695184154	7.0191587279	-7.4837965747
C7	1.3632170905	7.4437067979	-7.1500560419
C8	2.4873576803	7.9841546138	-7.8347948618
H9	3.4514479752	8.0936262071	-7.3466959765
C10	2.4016051170	8.3876031448	-9.1338669246
H11	3.2483787046	8.8006330358	-9.6754401207
C12	1.2748444567	8.4657137991	-11.3014633736
H13	0.2945248382	8.8262458989	-11.6281407758
H14	2.0169941215	9.2367296933	-11.5299121956
C15	1.6236720097	7.1220015868	-11.8827299536
C16	2.9616960571	6.7196546922	-11.9393862364
H17	3.7523329600	7.4204461274	-11.6670741481
C18	6.0900101781	-7.3838374978	3.9997897483
H19	5.8292866739	-7.9312892661	4.9063841192
C20	6.9451222676	-7.9653485079	3.0573619410
C21	7.3027232537	-7.2243143296	1.9277421965
H22	7.9921899969	-7.6495433438	1.1971208243
C23	0.6284502555	6.2270141890	-12.2824564266
H24	-0.4161399510	6.5407979134	-12.2770369361
C25	-1.5172362297	-2.4229793495	-10.2181893511
H26	-1.8379190474	-2.6039229832	-11.2489308711
H27	-1.8655796574	-3.2587421959	-9.6019496950
C28	0.6680314636	-1.9445899146	-11.2578476307
H29	0.0904446342	-1.7273240290	-12.1525533390
C30	2.0159978592	-1.7316603533	-11.1846677331
H31	2.4976901773	-1.3400363388	-12.0751466859
C32	2.7559594867	-2.0118192997	-9.9987404115
C33	1.9797232506	-2.5544483108	-8.9337324280
H34	2.4364115808	-2.8254308161	-7.9863230436
C35	0.6330631595	-2.7497459310	-9.0502517848
H36	0.0256934300	-3.1560922256	-8.2452244907
N37	6.8989044255	-1.0562823984	-9.6076180495
N38	-1.4688677806	3.5222744478	-7.9960724913
N39	1.6163932950	6.1714945718	-3.0954476043
N40	5.4568173099	4.8943696668	-7.2551467517
C41	6.2211469473	-1.6529033407	-8.5803364289
H42	6.8015569698	-1.8381943421	-7.6799707125
C43	4.9037997325	-1.9960429997	-8.6934141170
H44	4.4455469791	-2.4762090053	-7.8335070102

C45	4.1582937397	-1.7327100500	-9.8790766481
C46	4.9170136742	-1.1449500053	-10.9347431085
H47	4.4729180069	-0.9350818793	-11.9036095715
C48	6.2349911094	-0.8160053817	-10.7766851305
H49	6.8207980630	-0.3546437361	-11.5677838067
C50	8.2131819711	-0.4243975715	-9.3473840790
H51	8.7630694504	-1.0836787416	-8.6682700219
H52	8.7531756247	-0.3955768445	-10.2993831731
C53	8.0180744752	0.9566487435	-8.7756637850
C54	7.9056371057	2.0616204830	-9.6253038173
H55	8.0637041403	1.9384153155	-10.6975187861
C56	7.6034360273	3.3202773083	-9.1130844476
H57	7.5308980379	4.1730437836	-9.7896432347
C58	7.4012312845	3.5019121572	-7.7412218809
C59	7.5408462971	2.4027935557	-6.8879452026
H60	7.4128808717	2.5317156393	-5.8121110874
C61	7.8482204465	1.1442818165	-7.3998264125
H62	7.9635681295	0.2989613553	-6.7197345671
C63	6.9360297143	4.8357832597	-7.2145431188
C64	1.6823957378	5.8375577891	-1.6743763024
C65	-2.7879343574	2.8961489368	-8.2375557732
H66	7.3138175449	5.6689296998	-7.8169089034
H67	0.9312375822	5.0784709316	-1.4453204611
H68	-3.3328079937	2.9104768811	-7.2880168264
H69	7.2431468611	4.9997035339	-6.1765789255
H70	2.6752502365	5.4479491973	-1.4391768691
H71	-3.3286180049	3.5285719368	-8.9496829520
C72	4.7156081911	4.4426264886	-6.1966422917
C73	2.7235053079	6.6285319065	-3.7479118993
C74	-0.7500018495	4.0470489973	-9.0342988163
H75	5.2668953433	4.2657934108	-5.2763753977
H76	3.6380614895	6.6605188187	-3.1620663512
H77	-1.2983212605	4.1887600088	-9.9633519249
C78	3.3692146462	4.2377249023	-6.2999493469
C79	2.6687500568	7.0289282455	-5.0545785810
C80	0.5686765425	4.3784153849	-8.8992124742
H81	2.8547852219	3.8983107396	-5.4059006015
H82	3.5967174514	7.3736544888	-5.4991457196
H83	1.0594566177	4.8116370040	-9.7677089861
C84	2.6657273686	4.4528364149	-7.5250139989
C85	1.4505786125	6.9934352430	-5.7911615108
C86	1.2725634991	4.1745738005	-7.6731889932
C87	3.4787482859	4.9460365079	-8.5939664142
C88	0.3224429056	6.5168108538	-5.0667968801

C89	0.4676032070	3.6626113907	-6.6102362825
H90	3.0786690482	5.1574547807	-9.5852057054
H91	-0.6641912064	6.4726035931	-5.5184502230
H92	0.8738134922	3.5088563921	-5.6153726474
C93	4.8204388453	5.1442915923	-8.4402780930
C94	0.4252819358	6.1280090319	-3.7596622783
C95	-0.8463073945	3.3431856822	-6.7897820101
H96	5.4516610442	5.5081802673	-9.2479812674
H97	-0.4252664760	5.7751306736	-3.1832272460
H98	-1.4681613565	2.9463536663	-5.9915032099
N99	3.9059421927	-4.2429104298	1.8212042623
N100	2.7169203732	2.2788429647	-11.7800518584
C101	2.8553467738	-4.5603058081	2.6396833936
H102	3.0417539343	-4.4645842142	3.7058219024
C103	1.6496883953	-4.9589049258	2.1401570469
H104	0.8689911387	-5.1826239700	2.8601282829
C105	1.4279962418	-5.0683297322	0.7340192499
C106	2.5329678037	-4.6815898806	-0.0803215603
H107	2.4704836845	-4.6942787836	-1.1656679588
C108	3.7282918323	-4.3080899024	0.4685054708
H109	4.5867557435	-4.0209234193	-0.1373238870
C110	5.2526074221	-4.0433541941	2.4010648456
H111	5.8205811840	-3.4106510409	1.7113035414
H112	5.1207992656	-3.4802962614	3.3314654022
C113	5.9050371330	-5.3786846958	2.6484020410
C114	5.5760808282	-6.1081786973	3.7974978385
H115	4.9252801068	-5.6670399799	4.5533744184
C116	3.2925611673	5.4271798546	-12.3300038778
H117	4.3415113846	5.1282104522	-12.3692188316
C118	2.2964691148	4.5179911777	-12.6998861039
C119	0.9629404649	4.9374749902	-12.6901269419
H120	0.1762688686	4.2477991348	-12.9990585107
C121	6.7893787257	-5.9431034491	1.7259740662
H122	7.0875460158	-5.3761784719	0.8425659916
C123	2.6445373415	3.0872479006	-13.0158273397
H124	3.6170587348	3.0072928916	-13.5118314141
H125	1.8959491952	2.6236906986	-13.6663510612
C126	1.5672877597	1.7666687973	-11.2423220101
H127	0.6917355704	1.7953338225	-11.8875892331
C128	1.5385777562	1.2258385579	-9.9915147311
H129	0.5857156205	0.8218643201	-9.6531867962
C130	2.7026456277	1.1822588279	-9.1653446962
C131	3.8858403611	1.6979589978	-9.7787761972
H132	4.8470719785	1.6711642409	-9.2674784207

C133	3.8664231474	2.2340046745	-11.0342948618
H134	4.7598389539	2.6196836526	-11.5214369751
N135	0.2406889769	-12.7101201587	-0.0569387027
N136	6.3023926147	-10.2996457569	2.7147445142
N137	2.6096257089	-0.4920842710	-5.2398337120
N138	0.2453071400	-8.8355804126	3.5699312599
N139	-2.1973823927	-6.6287388415	-0.8852919416
N140	3.5990513950	-7.3751215807	-2.5088937423
C141	1.3406422364	-12.4990259073	-0.8467909191
C142	5.2631278498	-10.6525064330	3.5368626344
C143	3.7817142301	-0.0086905807	-5.7594844297
H144	1.1997081507	-12.6778742929	-1.9096395793
H145	5.4247003498	-10.4775289870	4.5974762209
H146	4.6537113091	-0.0927643599	-5.1144360938
C147	2.5355649154	-12.1049334917	-0.3204394533
C148	4.1133480629	-11.2016421312	3.0463810615
C149	3.8368105742	0.5414679560	-7.0105953963
H150	3.3600243559	-11.9839720468	-1.0151085491
H151	3.3490039851	-11.4789464111	3.7677674000
H152	4.8042645525	0.9084001797	-7.3461208049
C153	2.7014489814	-11.8857523113	1.0841357012
C154	3.9259202156	-11.4139603587	1.6435522819
C155	2.6821501730	0.6292063234	-7.8483830601
C156	1.5351633906	-12.1351334059	1.8700896458
C157	5.0607239938	-11.0956613499	0.8368111113
C158	1.4898853932	0.1086286872	-7.2614880872
H159	1.5428569478	-12.0315937883	2.9537786636
H160	5.0635358316	-11.2791639296	-0.2341332664
H161	0.5431171567	0.1205160036	-7.7931252178
C162	0.3576939752	-12.5225028107	1.2926456911
C163	6.1888168113	-10.5436985492	1.3734537802
C164	1.4785421027	-0.4286852795	-6.0077062883
H165	-0.5409337725	-12.7102677257	1.8758161295
H166	7.0537142062	-10.2754574627	0.7712841382
H167	0.5749417695	-0.8253052605	-5.5505059699
C168	2.5613034206	-1.1621082415	-3.9229550739
C169	7.3720399927	-9.4030097194	3.2115346452
C170	-1.0894929131	-12.8933135916	-0.6808744647
H171	3.1865154355	-0.5788479687	-3.2382629106
H172	7.5517650113	-9.6695105881	4.2584843795
H173	-0.9368485700	-13.4528438731	-1.6094078372
H174	1.5265886058	-1.0806151787	-3.5733042130
H175	8.2777293620	-9.6288916152	2.6402000473
H176	-1.6861270956	-13.5185882081	-0.0079378238

C177	3.0123335541	-2.6043868357	-3.9386119458
C178	-1.7507819366	-11.5596341863	-0.9270834887
C179	2.2066671975	-3.6019256830	-4.4995057713
C180	-2.5930913047	-10.9941763871	0.0343525895
H181	1.2400038611	-3.3408831702	-4.9328451300
H182	-2.8605767522	-11.5666178542	0.9244287415
C183	2.5994666724	-4.9369232331	-4.4660973632
C184	-3.1097176801	-9.7123193468	-0.1396477802
H185	1.9595010525	-5.6968816274	-4.9161114768
H186	-3.7742007461	-9.2907947224	0.6161639387
C187	3.7953674703	-5.3170419028	-3.8451199262
C188	-2.7976534081	-8.9649616983	-1.2800250059
C189	4.5999255175	-4.3196961279	-3.2858530175
C190	-1.9802010249	-9.5426918564	-2.2579930087
H191	5.5329565804	-4.5814078415	-2.7844947234
H192	-1.7523573662	-8.9907449502	-3.1710515005
C193	4.2158423569	-2.9797808147	-3.3366625642
C194	-1.4632945140	-10.8243021858	-2.0828146531
H195	4.8375860036	-2.2243645774	-2.8543568098
H196	-0.8365666012	-11.2613924891	-2.8612734749
C197	4.1724838781	-6.7764540468	-3.7365926775
C198	-3.2576144671	-7.5319364692	-1.3898312756
C199	-0.4163872670	-9.2859908234	4.8176986743
H200	5.2580233952	-6.9129673129	-3.6854751976
H201	-4.1487133984	-7.3587160918	-0.7787338270
H202	3.8003266947	-7.3598946407	-4.5850102324
H203	-3.4816495017	-7.2352787475	-2.4196289197
H204	-0.0632245879	-8.6355672103	5.6247711875
C205	2.3359708573	-7.9059169324	-2.5198709016
C206	-1.1949345068	-6.1989128604	-1.7101474206
C207	1.5472477123	-8.4091512535	3.5810302770
H208	1.8704662838	-7.9910755019	-3.4990256729
H209	-1.3790958087	-6.3199541066	-2.7748787266
H210	1.9739522245	-8.2280041797	4.5646750843
C211	1.7035978498	-8.2850009817	-1.3695883443
C212	-0.0412016060	-5.6549543589	-1.2172429045
C213	2.2398922963	-8.1752124755	2.4256664216
H214	0.7028659039	-8.6972442731	-1.4700627365
H215	0.6957921737	-5.3263265110	-1.9432030675
H216	3.2604877600	-7.8121150653	2.5260161968
C217	2.3176530975	-8.1089620313	-0.0896510523
C218	0.1951633774	-5.5458176384	0.1878454065
C219	1.6378096676	-8.3709495993	1.1429005539
C220	3.6543088990	-7.6138950668	-0.1369376960

C221	-0.8963667328	-5.9639968736	1.0023374103
C222	0.2843555192	-8.8181925481	1.1812575568
H223	4.2360257330	-7.4673834298	0.7705762535
H224	-0.8582016775	-5.8751967913	2.0850939818
H225	-0.2920266550	-8.9658346069	0.2709232100
C226	4.2486851225	-7.2529570130	-1.3129666778
C227	-2.0351706868	-6.4925617776	0.4653340244
C228	-0.3622772655	-9.0454794605	2.3631318293
H229	5.2516829944	-6.8351831241	-1.3593424383
H230	-2.8628886378	-6.8398841033	1.0786229452
H231	-1.4048396112	-9.3532553854	2.4058324925
H232	-1.4908025251	-9.1148549368	4.6946755483
C233	-1.9932467124	-1.0873387501	-9.7062751315
C234	-2.1908964588	-0.0278099096	-10.5977400180
C235	-2.4990310907	1.2468944431	-10.1292714928
C236	-2.6069327770	1.4919138342	-8.7576042082
C237	-2.4555723990	0.4227465402	-7.8677388955
C238	-2.1540780655	-0.8537841941	-8.3367859591
H239	-2.1041317622	-0.2019480607	-11.6708652775
H240	-2.6543583868	2.0600066966	-10.8395909346
H241	-2.5874401206	0.5859464564	-6.7970184763
H242	-2.0408014693	-1.6761120284	-7.6283591456
C243	0.5933392226	-13.4309492393	5.4504996651
C244	-0.5619647972	-13.0875331663	4.7456435296
C245	-0.9151387435	-11.7499163328	4.5792336116
C246	-0.1151776994	-10.7317192516	5.1057754083
C247	1.0231047972	-11.0794718712	5.8412438537
C248	1.3713858574	-12.4146733467	6.0153848695
H249	-1.1960629316	-13.8729789630	4.3317909058
H250	-1.8244350226	-11.4969100535	4.0308985640
H251	1.6318546573	-10.2984591469	6.2982913930
H252	2.2561865895	-12.6693106220	6.5999505381
C253	1.0717120273	-14.8588676691	5.5033038002
H254	1.5543665168	-15.0995705784	6.4558950226
H255	0.2617623794	-15.5776307290	5.3425496712
C256	3.8574472490	-14.7076645174	2.2709567545
C257	2.5143912408	-15.1365487798	2.0840604119
C258	1.6579594026	-15.2668105774	3.1438784765
N259	2.0680323845	-15.0343181099	4.4253207359
C260	3.3648200916	-14.6682394258	4.6511583387
C261	4.2521385627	-14.5089294134	3.6265727982
H262	2.1191289523	-15.3550153119	1.0953872836
H263	0.6199943858	-15.5673141132	3.0251856294
H264	3.6376967474	-14.5107544224	5.6910314837

H265	5.2675380124	-14.2306322504	3.8909067951
N266	6.5510026129	-14.0913980305	-0.9646730445
C267	6.9451687342	-13.8629933765	0.3205093412
C268	6.0915374152	-14.0411292765	1.3738810286
C269	4.7589052592	-14.4953215698	1.1757687593
C270	4.3805872291	-14.6968194129	-0.1828908486
C271	5.2702661864	-14.5019748915	-1.2026801326
H272	7.9753062395	-13.5415971358	0.4499668771
H273	6.4832431456	-13.8240424698	2.3636057713
H274	3.3822812118	-15.0272626130	-0.4541422461
H275	5.0121424425	-14.6677366786	-2.2448974210
C276	7.5187900834	-13.9852638688	-2.0524252367
H277	6.9850832330	-13.8944045144	-3.0003054679
H278	8.1438632645	-13.1009043397	-1.9014989810
H279	8.1546970420	-14.8766893261	-2.0784311967
H280	1.4921089646	6.7303347114	-1.0677243088

Co-conformation 3e

M06L/6-31G* in acetonitrile (A)	M06L/6-31G* in gas phase (B)	M06/6-311++G** in gas phase (C)	Total energy (C+A-B)
-7013.50973	-7011.31315	-7008.47273	-7010.66930

N1	-3.5329575952	4.0164031520	6.0185144081
N2	1.7632271416	2.1450489191	4.5244339272
C3	-2.2443191260	4.4495311713	6.1715809588
H4	-1.8768165676	4.4764872193	7.1950070409
C5	-1.4838664952	4.8325925015	5.1054435715
H6	-0.4807026202	5.1893917666	5.3193596860
C7	-1.9876488753	4.7852214052	3.7680566521
C8	-3.3612843036	4.4064004183	3.6614555312
H9	-3.8703908332	4.3795836254	2.6979467282
C10	-4.0767600774	4.0134687916	4.7598485539
H11	-5.1095371660	3.6766149303	4.6971673975
C12	-4.1944522549	3.2932976839	7.1318035228
H13	-3.8964486850	3.7900231217	8.0615912831
H14	-5.2756753445	3.4186835849	7.0143141089
C15	-3.7876236290	1.8405583837	7.1088229109
C16	-4.5724843662	0.8912234315	6.4479937654
H17	-5.5465671562	1.1774422818	6.0479145185
C18	7.0298084453	-6.9878975919	3.0660032055
H19	7.0796075813	-7.6305307046	3.9456454478
C20	7.4529452460	-7.4751696061	1.8249350576
C21	7.4319985494	-6.6166049809	0.7215481590

H22	7.7927124357	-6.9703677467	-0.2453628852
C23	-2.5678862881	1.4350628512	7.6627648365
H24	-1.9619541243	2.1495851686	8.2217483801
C25	2.9461177278	2.6528399663	5.2572737968
H26	2.9496593348	2.1696529902	6.2399533752
H27	3.8364238440	2.3189373384	4.7152469362
C28	0.6158669012	1.8105110876	5.1893163578
H29	0.6977997273	1.7499773354	6.2726009136
C30	-0.5523512332	1.5620352886	4.5258165725
H31	-1.4128903003	1.2996418054	5.1350800028
C32	-0.6554706297	1.6759814961	3.1062831699
C33	0.5686321944	2.0149071517	2.4582689154
H34	0.6218856750	2.1073168542	1.3772941776
C35	1.7186833896	2.2425007006	3.1581386032
H36	2.6558410180	2.5112947002	2.6768411488
N37	-0.2113418181	11.9187692106	0.7827300080
N38	-5.1605769408	11.0278953279	5.7511802815
N39	-4.3789395407	1.2008641001	1.0719570482
N40	0.9498488467	8.6382363551	4.7966149750
N41	0.5462616038	5.5456481832	0.4199945209
N42	-5.4219294818	7.5898937402	1.8222772132
C43	-1.5247146671	11.7888766988	0.4366284343
C44	-3.8467427373	11.1293971227	6.1004014227
C45	-3.2497894789	1.5512768209	0.3813985968
H46	-1.7497095311	11.8766855760	-0.6226951903
H47	-3.6392774186	11.1331207323	7.1667261568
H48	-3.3828409265	1.7230983444	-0.6836831915
C49	-2.4932732045	11.5806909375	1.3784918647
C50	-2.8632725822	11.2425909666	5.1557000780
C51	-2.0379403790	1.6740924708	1.0004694414
H52	-3.5175403190	11.5184473031	1.0239728871
H53	-1.8447247030	11.3461652700	5.5155861479
H54	-1.1923827504	1.9415886431	0.3725545684
C55	-2.1706277008	11.4837863995	2.7605160081
C56	-3.1780150566	11.2702464354	3.7693307025
C57	-1.8872023168	1.4722438833	2.4049726076
C58	-0.7969500790	11.6535282782	3.0797630171
C59	-4.5530793241	11.1154603881	3.4484312750
C60	-3.0841070278	1.0710855998	3.0702642152
H61	-0.4409237591	11.6442868245	4.1060990812
H62	-4.9083074169	11.1097910363	2.4220120535
H63	-3.0884640078	0.8308829449	4.1292898949
C64	0.1386941762	11.8522657063	2.0986482399
C65	-5.5004432401	11.0116521689	4.4323151725

C66	-4.2747673607	0.9548105833	2.4107891006
H67	1.1959379574	11.9822594327	2.3152089983
H68	-6.5624970789	10.9352835604	4.2157200271
H69	-5.1945297467	0.6550568686	2.9088719819
C70	-5.7129901310	1.3993392764	0.4543281948
C71	-6.1920393039	11.0253028086	6.7885799042
C72	0.8302728395	11.8201297277	-0.2682705159
H73	-5.6441445910	1.0823209331	-0.5914030285
H74	-6.4066975946	12.0533161684	7.1008152285
H75	0.4468299831	12.3321299094	-1.1566217580
H76	-6.4116510825	0.7305502368	0.9675951258
H77	-7.1020823142	10.5700064351	6.3935033487
H78	1.7141841544	12.3597553130	0.0853636496
C79	-6.1043680640	2.8485686118	0.5831497193
C80	1.1013981481	10.3584102197	-0.5178843673
C81	-6.7157802201	3.3181441118	1.7502052924
C82	2.1229159583	9.6933764952	0.1657533509
H83	-7.0272266235	2.6113983225	2.5211843791
H84	2.8247322814	10.2635631043	0.7761917565
C85	-6.9383843934	4.6804097770	1.9341018307
C86	2.2514582936	8.3089985667	0.0696261386
H87	-7.4205237430	5.0307733432	2.8480248202
H88	3.0614650767	7.8049463777	0.6008382874
C89	-6.5552774427	5.6009114626	0.9532457129
C90	1.3562613437	7.5642852437	-0.7049932468
C91	-5.9820286879	5.1267524960	-0.2302433823
C92	0.3649712025	8.2365846989	-1.4259490331
H93	-5.7138379280	5.8282399441	-1.0208596116
H94	-0.3147615530	7.6740141976	-2.0666958645
C95	-5.7566233106	3.7652990989	-0.4130792444
C96	0.2407286288	9.6188836896	-1.3354282201
H97	-5.3100223181	3.4121909779	-1.3433702299
H98	-0.5379327384	10.1260853684	-1.9059607504
C99	-6.6680203136	7.0829235798	1.2006179257
C100	1.3880317700	6.0592076768	-0.6852571034
C101	2.2813169906	8.4318473897	5.4076916617
H102	-7.4928590074	7.3249230772	1.8783295735
H103	2.4026268079	5.6782862265	-0.5276142160
H104	3.0158783465	8.9868901344	4.8148042326
H105	-6.8197026423	7.6431760367	0.2720396589
H106	1.0051666460	5.6286105109	-1.6160723054
H107	2.2534868922	8.8753221268	6.4087411391
C108	-4.3380952966	7.8854340096	1.0413235177
C109	-0.8005632855	5.3459324867	0.2417568850

C110	-0.1773517597	8.5104414073	5.5672019450
H111	-4.5265609441	7.9229409819	-0.0284336732
H112	-1.1451865890	5.3843665702	-0.7885467580
H113	-0.0225111217	8.5607484048	6.6417965890
C114	-3.1076957447	8.1299123688	1.5820755673
C115	-1.6380764510	5.0950479657	1.2921132019
C116	-1.4119009360	8.3486369164	5.0105298783
H117	-2.3057407566	8.3764837706	0.8913592136
H118	-2.6867743751	4.9287368035	1.0608823278
H119	-2.2496147895	8.2683619662	5.6972723254
C120	-2.8832068329	8.0877132458	2.9932218921
C121	-1.1580900375	5.0602509404	2.6392870777
C122	-1.6006510355	8.3036275165	3.5911113192
C123	-4.0502703081	7.8051429857	3.7641917855
C124	0.2457068377	5.2833500400	2.7730234056
C125	-0.4064309778	8.4861053179	2.8320780465
H126	-4.0117499496	7.7549843995	4.8492902588
H127	0.7364018595	5.2480608483	3.7431172085
H128	-0.4176309568	8.4987041321	1.7416656983
C129	-5.2598246011	7.5551199846	3.1781694540
C130	1.0437941860	5.5199545612	1.6928561184
C131	0.8121694214	8.6215338318	3.4361565281
H132	-6.1498692308	7.3152771538	3.7548372771
H133	2.1156934109	5.6842720089	1.7863828750
H134	1.7345976189	8.7229431282	2.8677671560
H135	-5.8405483664	10.4512199014	7.6491830263
N136	4.3963464831	-3.5855700127	1.9273219146
N137	-1.6947086632	-2.1789076196	5.1297069939
C138	3.5364917413	-3.9543818206	2.9293505878
H139	3.9496927999	-3.9332791887	3.9347780926
C140	2.2419709267	-4.3102407360	2.6736199061
H141	1.6264001149	-4.5648865374	3.5305736489
C142	1.7229162237	-4.3422637987	1.3413116937
C143	2.6474667001	-3.9251219395	0.3364844060
H144	2.3599070788	-3.8737421794	-0.7126807104
C145	3.9337852273	-3.5793709655	0.6403969034
H146	4.6536362851	-3.2734431582	-0.1169171226
C147	5.8516841434	-3.4827364814	2.1941778560
H148	6.2667180805	-2.7687061312	1.4747506537
H149	5.9690314946	-3.0581374573	3.1968174127
C150	6.4949002965	-4.8401370479	2.0802008663
C151	6.5532099948	-5.6866433226	3.1921018364
H152	6.2308353673	-5.3221522635	4.1683725723
C153	-4.1211736711	-0.4172439701	6.2928314835

H154	-4.7491516961	-1.1425383952	5.7729362885
C155	-2.8713708273	-0.8051069611	6.7881749900
C156	-2.1132024024	0.1278416087	7.5027030758
H157	-1.1551007233	-0.1678781648	7.9325567433
C158	6.9594773092	-5.3119007126	0.8482283432
H159	6.9592304770	-4.6520800272	-0.0211433337
C160	-2.3213918995	-2.1742597517	6.4740978462
H161	-3.1096709971	-2.9347264722	6.4671285399
H162	-1.5573648318	-2.4837630446	7.1944584049
C163	-0.3820471925	-1.8202135269	4.9692439753
H164	0.2050441604	-1.7609984727	5.8828059943
C165	0.1513143990	-1.5682730896	3.7348910516
H166	1.2039763153	-1.3023211678	3.7011377384
C167	-0.6470549520	-1.6185417373	2.5513255728
C168	-1.9975668393	-2.0328395411	2.7647803174
H169	-2.6902879365	-2.1557904110	1.9361666510
C170	-2.4828220485	-2.2871677082	4.0151403546
H171	-3.5106968195	-2.5952104678	4.1899891093
N172	-0.0974859915	-11.9069513755	0.4823132030
N173	6.6009258320	-9.7350737147	1.4519097666
N174	0.8583420886	-0.6863258929	-1.3391753829
N175	1.0184366257	-8.2141248127	4.2374944163
N176	-2.2170631127	-5.6854701205	0.4058631625
N177	3.1294560109	-6.7160113704	-2.3747579764
C178	0.7399224924	-11.7118480969	-0.5869860149
C179	5.8291809084	-10.1004450886	2.5222872237
C180	-0.4503913233	-1.0411652726	-1.1623020276
H181	0.2973157524	-11.8683301729	-1.5670698085
H182	6.2972451304	-9.9876687959	3.4968723502
H183	-1.0600301916	-1.0697844969	-2.0616569396
C184	2.0457008491	-11.3571881876	-0.4201314850
C185	4.5623294787	-10.5839461649	2.3646369950
C186	-0.9547196049	-1.3296500722	0.0749424879
H187	2.6352960319	-11.2292890252	-1.3226767946
H188	4.0239858426	-10.8606187380	3.2678109785
H189	-2.0074752158	-1.5915608437	0.1206396778
C190	2.6195928442	-11.1670936393	0.8778699109
C191	3.9675848112	-10.7345998288	1.0714901060
C192	-0.1428042734	-1.2922960953	1.2496167883
C193	1.7209357499	-11.4226493191	1.9589050909
C194	4.8290215373	-10.3845160288	-0.0133389258
C195	1.2095439423	-0.8992927790	1.0144599079
H196	2.0406183171	-11.3394971001	2.9979657593
H197	4.5002437355	-10.4752489685	-1.0462446241

H198	1.9242804462	-0.8270388746	1.8306216800
C199	0.4137183834	-11.7582481071	1.7413541385
C200	6.0855407429	-9.8889683334	0.1934529885
C201	1.6739737672	-0.6288393901	-0.2417951407
H202	-0.2873936658	-11.9257803900	2.5565621272
H203	6.7372666897	-9.5868011416	-0.6227604880
H204	2.7060876773	-0.3485357125	-0.4382819873
C205	1.4446062087	-0.6280304858	-2.6987448000
C206	7.8238684678	-8.9283820899	1.6687618283
C207	-1.5588980946	-11.9897548681	0.2659947293
H208	0.6510349994	-0.2981972490	-3.3774363640
H209	8.3206424412	-9.3230715839	2.5617378836
H210	-1.7161033346	-12.5527387860	-0.6604205638
H211	2.2241377735	0.1408715475	-2.6917916456
H212	8.4855773356	-9.0954882907	0.8126685202
H213	-1.9857094856	-12.5752628362	1.0871969633
C214	1.9920544484	-1.9791958983	-3.0815730050
C215	-2.1583424883	-10.6078766220	0.1915549385
C216	3.3527758129	-2.2682169325	-2.9556661694
C217	-2.7578734820	-10.0192462511	1.3083809121
H218	4.0491998279	-1.4780162470	-2.6720328694
H219	-2.8811390975	-10.5990334023	2.2251050205
C220	3.8276928202	-3.5596202511	-3.1861958182
C221	-3.2142715967	-8.7025032961	1.2585373439
H222	4.8934139062	-3.7688363255	-3.0808302666
H223	-3.6911402027	-8.2617201263	2.1351039506
C224	2.9504939176	-4.5846970252	-3.5494310124
C225	-3.0761137681	-7.9459821823	0.0912542448
C226	1.5938958841	-4.2816994731	-3.7221874119
C227	-2.5056776049	-8.5458971370	-1.0370649752
H228	0.9020337985	-5.0588033368	-4.0494577032
H229	-2.4222251737	-7.9817125926	-1.9672655720
C230	1.1200808586	-2.9953541247	-3.4903403333
C231	-2.0564597916	-9.8615746083	-0.9885128993
H232	0.0602907418	-2.7790064104	-3.6330662380
H233	-1.6289858597	-10.3160074292	-1.8830288053
C234	3.4171908749	-6.0157240696	-3.6495364639
C235	-3.4245924917	-6.4798080776	0.0767438742
C236	0.6446950927	-8.7208571841	5.5790090263
H237	4.4944582483	-6.0872956722	-3.8317601281
H238	-4.1961445049	-6.2331384974	0.8139729233
H239	2.9016992586	-6.5632200774	-4.4457694316
H240	-3.7746670642	-6.1452759255	-0.9051521406
H241	1.1679239691	-8.1041561492	6.3170681494

C242	1.8770230638	-7.2179736800	-2.1396907454
C243	-1.3715735538	-5.2612447142	-0.5822908515
C244	2.2938065663	-7.7766485312	3.9932191437
H245	1.2424626531	-7.3211154614	-3.0165885493
H246	-1.7667031575	-5.3121965376	-1.5945458456
H247	2.9187587812	-7.6413134751	4.8725068332
C248	1.4669144987	-7.5757609520	-0.8867049224
C249	-0.1193926260	-4.7927159661	-0.3021127201
C250	2.7346882962	-7.5122496929	2.7276270958
H251	0.4671235796	-7.9895168816	-0.7926301211
H252	0.4809473088	-4.4482602158	-1.1401355212
H253	3.7564134967	-7.1576144785	2.6257879976
C254	2.3197602064	-7.4204829923	0.2502793335
C255	0.3893622720	-4.7548344128	1.0324155229
C256	1.8911138229	-7.6966546897	1.5868404770
C257	3.6344855462	-6.9562220099	-0.0533418547
C258	-0.5425457022	-5.1706632977	2.0287595868
C259	0.5766460484	-8.1607190740	1.8915354880
H260	4.3922966948	-6.8531760502	0.7218869378
H261	-0.2864129681	-5.1384696225	3.0856752820
H262	-0.1626240247	-8.3312427339	1.1106350508
C263	3.9965201483	-6.6043886595	-1.3233006329
C264	-1.7881798510	-5.6251769755	1.7041792150
C265	0.1817482832	-8.4113146786	3.1740836907
H266	4.9864896897	-6.2237364518	-1.5689373864
H267	-2.5061738115	-5.9558731675	2.4506131230
H268	-0.8164770012	-8.7700439229	3.4171584147
H269	-0.4307271226	-8.5560193794	5.7037761030
C270	2.8922786103	4.1549188978	5.3667805942
C271	2.1069937567	4.7585023755	6.3560634449
C272	1.9588162816	6.1402893465	6.3979051243
C273	2.5829823401	6.9553912375	5.4450519276
C274	3.3970198214	6.3561318199	4.4805716327
C275	3.5534967171	4.9699319168	4.4439756721
H276	1.6122223574	4.1412558377	7.1079195817
H277	1.3517332113	6.5905879048	7.1843989475
H278	3.9216401218	6.9779429721	3.7527923811
H279	4.2001571889	4.5184100867	3.6899958718
C280	1.7827420095	-12.8811965461	5.6986845956
C281	0.4772843990	-12.5175941971	5.3570711829
C282	0.0923320116	-11.1777512882	5.3628037977
C283	1.0061408068	-10.1773070644	5.7066253316
C284	2.2989356069	-10.5466792294	6.0913071453
C285	2.6829596344	-11.8835994699	6.0876367185

H286	-0.2458321038	-13.2887251029	5.0878759137
H287	-0.9334845071	-10.9100781885	5.1020410023
H288	3.0115434150	-9.7822333385	6.4030891185
H289	3.6943097060	-12.1531804255	6.3938447710
C290	2.2597506334	-14.3015831474	5.5296521528
H291	3.0105889320	-14.5791984011	6.2762415762
H292	1.4417689083	-15.0268691467	5.5800752632
C293	3.9648842589	-14.1010814193	1.6058745783
C294	2.6240389975	-14.5122242471	1.8278398416
C295	2.1208020553	-14.6508372321	3.0942915664
N296	2.8935442939	-14.4303366173	4.1958250599
C297	4.1979593104	-14.0668599020	4.0279235592
C298	4.7412571088	-13.9090815612	2.7830043439
H299	1.9506525749	-14.7337796611	1.0042454865
H300	1.0966133437	-14.9602633555	3.2863836689
H301	4.7759092486	-13.9318104237	4.9382435336
H302	5.7940688856	-13.6506568928	2.7365904187
N303	5.6066455673	-13.6533232453	-2.3013309417
C304	6.3728000802	-13.4186478330	-1.1997862149
C305	5.8617529978	-13.5406840769	0.0639976789
C306	4.5132529961	-13.9256538292	0.2823207081
C307	3.7507019134	-14.1505915415	-0.8952441503
C308	4.3037620094	-14.0132807732	-2.1398470908
H309	7.4086609041	-13.1507022306	-1.3890277897
H310	6.5405891679	-13.3442202215	0.8885632296
H311	2.7119071875	-14.4605943200	-0.8544632751
H312	3.7417650653	-14.1945002804	-3.0517063047
C313	6.2068427174	-13.5922032448	-3.6337302787
H314	5.4163411580	-13.4850117549	-4.3788555174
H315	6.8802107549	-12.7331395612	-3.6904291728
H316	6.7712122467	-14.5102225961	-3.8286371335

Co-conformation 3f

M06L/6-31G* in acetonitrile (A)	M06L/6-31G* in gas phase (B)	M06/6-311++G** in gas phase (C)	Total energy (C+A-B)
-7013.48893	-7011.40759	-7008.57209	-7010.65344

N1	-4.2683422503	3.6929249574	9.2329465124
N2	-10.8993360973	2.4983260776	12.9028735267
C3	-5.6013657957	3.4065657212	9.1250059537
H4	-6.1377120924	3.9267709722	8.3360422553
C5	-6.2107301579	2.5106843517	9.9564144736
H6	-7.2704514640	2.3320116570	9.7953647286

C7	-5.4815771755	1.8035613719	10.9562539813
C8	-4.1170832714	2.1990268317	11.0909643208
H9	-3.4718102255	1.7750375304	11.8531935250
C10	-3.5492931685	3.0987080968	10.2330264789
H11	-2.5022751401	3.3841145012	10.2961502351
C12	-3.5685764136	4.3930171002	8.1285910808
H13	-4.2716751387	5.1225946938	7.7145651406
H14	-2.7214502830	4.9360888063	8.5601062260
C15	-3.1271059485	3.3838011279	7.0954811967
C16	-1.8442272570	2.8356896790	7.1336058157
H17	-1.1079196875	3.2227540360	7.8385993575
C18	6.1574297123	-4.8492762501	3.3317408872
H19	6.1621734514	-5.0656167511	4.4005149381
C20	6.5701370467	-5.8297321869	2.4220116543
C21	6.6100036654	-5.5122437955	1.0615574574
H22	6.9647719847	-6.2531023065	0.3432700013
C23	-4.0472624814	2.8837308681	6.1661272436
H24	-5.0479507194	3.3127672687	6.1062732620
C25	-12.3321300095	2.6380213090	12.5583323328
H26	-12.3812478268	3.0887748716	11.5622551537
H27	-12.7595089679	1.6317135101	12.4974989530
C28	-10.0006648460	3.4569845433	12.5170983987
H29	-10.3576804591	4.1668189635	11.7755885299
C30	-8.7360132401	3.5024103254	13.0312166823
H31	-8.0833230585	4.2894405379	12.6620205416
C32	-8.2852707119	2.5617877249	14.0062841770
C33	-9.2461214850	1.5645342963	14.3502815787
H34	-9.0072439568	0.7635307281	15.0457203397
C35	-10.5030713765	1.5616576344	13.8178181838
H36	-11.2498454353	0.8152107989	14.0816435315
N37	-9.7100229266	1.1611614600	18.3886264011
N38	-8.1380110081	7.2380978303	15.1157493738
N39	-4.3963336376	2.6978301964	15.7528899822
N40	-13.2484683675	6.2036382084	17.6773261378
N41	-7.0952898995	-1.5390216977	13.0507106903
N42	-6.7286753540	6.5118837139	20.4467035921
C43	-8.5104983614	1.7767986864	18.6329184753
C44	-9.3779553275	6.6699902635	14.9928822838
C45	-5.3063531451	1.7537075496	16.1434982279
H46	-7.8353358667	1.2392103673	19.2946880510
H47	-10.0745249202	7.1988556845	14.3465195544
H48	-4.9728531561	1.0727228246	16.9238432215
C49	-8.1960812317	2.9861779071	18.0773714794
C50	-9.7036380050	5.5177743475	15.6441866008

C51	-6.5480505097	1.6776572145	15.5814134552
H52	-7.2289526360	3.4150703424	18.3303983279
H53	-10.7118972507	5.1378260260	15.4984750868
H54	-7.2189541216	0.9144830172	15.9703494133
C55	-9.0997138048	3.6538705147	17.1939623364
C56	-8.7686568817	4.8532017325	16.4962289685
C57	-6.9754688330	2.5980670742	14.5773723432
C58	-10.3670796684	3.0146776645	17.0426399980
C59	-7.4826662762	5.4687318553	16.5781313489
C60	-5.9888183455	3.5566587499	14.1954670222
H61	-11.1568406858	3.4544617016	16.4393868511
H62	-6.6822759492	5.0396867933	17.1777375822
H63	-6.1802798490	4.2855398548	13.4131139048
C64	-10.6319910146	1.8030647935	17.6094256070
C65	-7.2013647398	6.6191411064	15.8988000849
C66	-4.7552115878	3.5903300547	14.7781475665
H67	-11.5773427104	1.2828853010	17.4708765051
H68	-6.2280658302	7.1024682672	15.9393602196
H69	-3.9959916369	4.3171589263	14.5012490874
C70	-3.1991589678	2.9589255587	16.5842612368
C71	-7.8167440060	8.4441502851	14.3596811643
C72	-9.8695790826	-0.2904261876	18.6382372200
H73	-2.8070661014	1.9911462705	16.9134902676
H74	-8.6527271767	9.1472418128	14.4132679305
H75	-9.3333824374	-0.5249867949	19.5632242626
H76	-2.4488694264	3.4252599186	15.9375278561
H77	-6.9287748844	8.9130126860	14.7881057250
H78	-10.9344283445	-0.4826006997	18.8035739626
C79	-3.5849122476	3.8510647778	17.7359651463
C80	-9.3284433800	-1.0500794398	17.4521552230
C81	-3.6029024331	5.2401824451	17.5715940245
C82	-10.1655399061	-1.4359389077	16.4023965551
H83	-3.2204940643	5.6824108136	16.6504287740
H84	-11.2431930823	-1.2906916404	16.4887954601
C85	-4.1065941620	6.0655081082	18.5729475253
C86	-9.6355105742	-2.0004630033	15.2418847921
H87	-4.1103292282	7.1469965395	18.4302713997
H88	-10.3019449416	-2.2899822785	14.4283591648
C89	-4.6037633094	5.5206061476	19.7608635400
C90	-8.2582019624	-2.1965116579	15.1122074796
C91	-4.5493443859	4.1350887112	19.9412439553
C92	-7.4263642328	-1.8545858439	16.1858885534
H93	-4.9017537926	3.6957978878	20.8753201174
H94	-6.3524848071	-2.0353766104	16.1194408572

C95	-4.0452573095	3.3090937218	18.9391584474
C96	-7.9528755790	-1.2813343285	17.3381746684
H97	-4.0099630127	2.2304649540	19.0963112248
H98	-7.2927844705	-1.0215143158	18.1675215149
C99	-5.2891795091	6.3973666223	20.7775126994
C100	-7.6479029650	-2.6756802596	13.8188083435
C101	-14.4441289990	5.9471226117	16.8421577014
H102	-4.8768737218	7.4113304044	20.7941514382
H103	-8.3808373454	-3.1805885599	13.1807451362
H104	-15.1940055924	5.4625828971	17.4758217956
H105	-5.2195058189	5.9867349857	21.7899710810
H106	-6.8222795969	-3.3738432051	13.9929196416
H107	-14.8375475634	6.9202576994	16.5317105940
C108	-7.5924796863	5.5190388615	20.8192796392
C109	-5.8041939788	-1.1388894269	13.2584955955
C110	-12.4265532362	7.2571840135	17.4007730645
H111	-7.2038920401	4.7944614823	21.5298293853
H112	-5.2182277431	-1.7554688678	13.9345121070
H113	-12.8244919938	8.0031564145	16.7180792839
C114	-8.8711675422	5.4665273582	20.3412268739
C115	-5.2842879899	-0.0449381257	12.6313468015
C116	-11.1862057089	7.3641645798	17.9659909673
H117	-9.5004078951	4.6602855699	20.7073816831
H118	-4.2402204015	0.1822551625	12.8280777943
H119	-10.6061637913	8.2467124392	17.7128011008
C120	-9.3621390670	6.4323639040	19.4157684928
C121	-6.0565294763	0.7324936058	11.7182132632
C122	-10.6862054305	6.3743160374	18.8604670161
C123	-8.4374695206	7.4629386150	19.0821115058
C124	-7.4099739919	0.3052659033	11.5647386735
C125	-11.5940024549	5.3160347580	19.1475381940
H126	-8.7113643149	8.2790174075	18.4191889663
H127	-8.0995312316	0.8232722184	10.9049417556
H128	-11.3403621824	4.5226799537	19.8439691201
C129	-7.1654671014	7.4745225624	19.5840795903
C130	-7.8890086783	-0.7945142253	12.2198576555
C131	-12.8220466536	5.2455969143	18.5541354483
H132	-6.4476996779	8.2532555156	19.3394700373
H133	-8.9112034807	-1.1462088932	12.1047759029
H134	-13.5220805952	4.4380107083	18.7505517787
H135	-7.6232615761	8.1994944218	13.3087728116
N136	3.6920835937	-2.1216166025	0.9488128841
N137	-1.7591921682	0.0765863632	3.2516763048
C138	2.9082456586	-1.9580703808	2.0581546007

H139	3.3899275879	-1.4914875339	2.9135174203
C140	1.6016078205	-2.3492967590	2.0719448974
H141	1.0503222019	-2.1692441793	2.9885881751
C142	0.9764671487	-2.9558658790	0.9360512698
C143	1.8242428263	-3.0699843572	-0.2067578837
H144	1.4624374256	-3.4858251231	-1.1465717999
C145	3.1324729190	-2.6740133476	-0.1690504640
H146	3.8146359486	-2.7813291873	-1.0107333494
C147	5.1635200621	-1.9871897322	1.0485834293
H148	5.5382747886	-1.6918485410	0.0629767618
H149	5.3684763455	-1.1666300241	1.7441430543
C150	5.7513739343	-3.2910924995	1.5214670207
C151	5.7515352650	-3.5964701101	2.8872722379
H152	5.4387188583	-2.8431585928	3.6115358207
C153	-1.5069969814	1.7695209001	6.3023755806
H154	-0.5147189153	1.3227736222	6.3770707989
C155	-2.4468482471	1.2275744833	5.4229485416
C156	-3.7125118826	1.8172922511	5.3405572114
H157	-4.4564172787	1.4150955283	4.6515644000
C158	6.2065039513	-4.2535419330	0.6159111207
H159	6.2551349566	-4.0170781076	-0.4487456999
C160	-2.1455087860	-0.0437891079	4.6761699962
H161	-3.0172295890	-0.7067295398	4.6953147485
H162	-1.3254371865	-0.5781359483	5.1726441845
C163	-0.4904737211	0.4557876490	2.9039768415
H164	0.1483668365	0.7874667508	3.7184353684
C165	-0.0514700312	0.3859798805	1.6105026284
H166	0.9684991761	0.7035257417	1.4201912526
C167	-0.8886971443	-0.1204654721	0.5710954270
C168	-2.2196655728	-0.4324575205	0.9652521155
H169	-2.9598174580	-0.7834291349	0.2513826592
C170	-2.6185907196	-0.3271466323	2.2688212573
H171	-3.6200318735	-0.5978569386	2.5927101415
N172	-1.1896299610	-10.1232831286	3.3338816004
N173	5.5854680086	-7.9647564805	3.0846133540
N174	0.5765776390	-1.0020899106	-3.3332892738
N175	-0.0615398701	-5.3953242361	5.2550671297
N176	-3.0665764538	-4.3457586631	1.0390347064
N177	2.4768176239	-6.8107368676	-1.2279293079
C178	-0.4065036116	-10.3643651794	2.2359347123
C179	4.8543264368	-7.8076387808	4.2332456907
C180	-0.7141412860	-1.2918486996	-2.9946133273
H181	-0.8923723353	-10.8857361770	1.4148988793
H182	5.3760368075	-7.3317829040	5.0596201409

H183	-1.3106738493	-1.7702776909	-3.7672324965
C184	0.9041049043	-9.9887673433	2.1930495469
C185	3.5611919556	-8.2353138847	4.3276825108
C186	-1.2178108021	-0.9824496176	-1.7623078878
H187	1.4512846342	-10.2343946156	1.2875189938
H188	3.0602148644	-8.0831237754	5.2800816116
H189	-2.2610726110	-1.2253751774	-1.5842771202
C190	1.5328035160	-9.3081551778	3.2865117512
C191	2.8954102415	-8.8757321626	3.2354226136
C192	-0.4085561488	-0.3685070355	-0.7615392944
C193	0.6856501034	-9.1071708458	4.4166664312
C194	3.7119190811	-9.0524376151	2.0774067730
C195	0.9160993629	-0.0526645523	-1.1708711171
H196	1.0492278158	-8.6308813163	5.3262873501
H197	3.3301293228	-9.5473568326	1.1872100473
H198	1.6098364787	0.4576905948	-0.5077116697
C199	-0.6244744422	-9.4965273821	4.4095664495
C200	4.9977928230	-8.5925541090	2.0220729696
C201	1.3745909464	-0.3766805186	-2.4193809924
H202	-1.2827337119	-9.3321665167	5.2599571630
H203	5.6205375121	-8.6989096057	1.1364297246
H204	2.3817996766	-0.1393744237	-2.7521934828
C205	1.1651580613	-1.5899230037	-4.5596332180
C206	6.8570519068	-7.2268336062	2.9093400131
C207	-2.6601556102	-10.2601564177	3.2390117449
H208	0.3855158119	-1.5978110257	-5.3281637695
H209	7.3674595865	-7.2271401425	3.8785726033
H210	-2.8632741708	-11.1157129363	2.5875883321
H211	1.9634560183	-0.9188962144	-4.8932491929
H212	7.4751986787	-7.7903637996	2.2029952694
H213	-3.0384188090	-10.5036430323	4.2378512922
C214	1.6709809657	-2.9728586441	-4.2349280241
C215	-3.2525027402	-8.9828355002	2.7017454185
C216	2.9338099087	-3.1399076333	-3.6559815287
C217	-3.7312603221	-7.9924556782	3.5632991761
H218	3.6050811275	-2.2839482759	-3.5653578854
H219	-3.7976630909	-8.1932737193	4.6344405102
C220	3.3446068063	-4.3887821729	-3.1982891136
C221	-4.1344448058	-6.7535859165	3.0660782383
H222	4.3229464965	-4.4869075239	-2.7257428744
H223	-4.5124094853	-5.9924491725	3.7509784645
C224	2.5069606501	-5.5038376014	-3.3032706657
C225	-4.0653031644	-6.4804790152	1.6970469091
C226	1.2642626876	-5.3457910808	-3.9247922224

C227	-3.6286290116	-7.4889655662	0.8297276357
H228	0.6079744342	-6.2077670162	-4.0499561474
H229	-3.6049390146	-7.3060679309	-0.2452251331
C230	0.8504315239	-4.0958760640	-4.3828314038
C231	-3.2282707616	-8.7251549571	1.3254954959
H232	-0.1275843654	-3.9944932995	-4.8548528964
H233	-2.8929892824	-9.4993904614	0.6339090589
C234	2.8870784324	-6.8093429760	-2.6522064108
C235	-4.3384079498	-5.0945883068	1.1717097757
C236	-0.5291452223	-5.2995535704	6.6568644511
H237	3.9696897080	-6.9745695194	-2.6808111905
H238	-4.9872845987	-4.5270914350	1.8466758654
H239	2.4023756287	-7.6655420628	-3.1333343262
H240	-4.8101697172	-5.1090002545	0.1837108941
H241	-0.0303358777	-4.4360011273	7.1092471889
C242	1.1848211857	-7.1245861851	-0.8948888749
C243	-2.3307355665	-4.4247285190	-0.1141167191
C244	1.2435292052	-5.1119424349	4.9383677030
H245	0.5956771456	-7.5793196555	-1.6873289034
H246	-2.8444264050	-4.8573604802	-0.9687447996
H247	1.8236213759	-4.6359913773	5.7250711981
C248	0.6891883447	-6.8982783836	0.3558994622
C249	-1.0444160598	-3.9709618135	-0.1799916705
C250	1.7600139091	-5.3893683055	3.7058956477
H251	-0.3379208648	-7.1981773722	0.5415741060
H252	-0.5398555313	-4.0593478416	-1.1379562061
H253	2.7955997050	-5.1115917204	3.5305991537
C254	1.4861336012	-6.2952341589	1.3809766822
C255	-0.3831841436	-3.4022411552	0.9547985822
C256	0.9716372808	-6.0039032030	2.6802258814
C257	2.8317887007	-6.0068676933	0.9971312822
C258	-1.1953123462	-3.3335768335	2.1247135826
C259	-0.3699376737	-6.3081755942	3.0642166281
H260	3.5479483323	-5.5785074001	1.6980640473
H261	-0.8109629079	-2.9116272303	3.0509125417
H262	-1.0736382387	-6.7760108493	2.3779371429
C263	3.2797586539	-6.2532575963	-0.2705773189
C264	-2.4786248698	-3.8011742554	2.1467965682
C265	-0.8395472511	-6.0089934950	4.3119366468
H266	4.3000335282	-6.0348339779	-0.5790486019
H267	-3.0998909136	-3.7667829808	3.0391126870
H268	-1.8597562603	-6.2331991197	4.6161853786
H269	-1.6043562556	-5.0902395384	6.6301949314
C270	-13.0203116103	3.4861856927	13.5957647991

C271	-12.9258948244	4.8807387597	13.5293842948
C272	-13.4327931499	5.6726851400	14.5535369744
C273	-14.0463717451	5.0893776891	15.6679642100
C274	-14.1742773457	3.6989547830	15.7171431176
C275	-13.6662454582	2.9049252441	14.6897251073
H276	-12.4533756054	5.3523288683	12.6663494144
H277	-13.3534881691	6.7586230194	14.4844941727
H278	-14.6705636096	3.2297551610	16.5674949391
H279	-13.7740396844	1.8207587348	14.7420374618
C280	0.4437281622	-9.0630499482	8.5293554417
C281	-0.8166508533	-8.8612148417	7.9604583168
C282	-1.1512032947	-7.6271788102	7.4055202889
C283	-0.2310184388	-6.5741784241	7.3984526641
C284	1.0100553490	-6.7621563602	8.0145333275
C285	1.3418387258	-7.9913767630	8.5747599031
H286	-1.5445020008	-9.6738398797	7.9547917034
H287	-2.1446712917	-7.4808470023	6.9763737409
H288	1.7236115413	-5.9390396706	8.0594054424
H289	2.3144931631	-8.1187121787	9.0508223060
C290	0.8965781876	-10.4386153439	8.9439861707
H291	1.6066969312	-10.4127413158	9.7764420913
H292	0.0649038739	-11.0946046213	9.2189604896
C293	2.7498285763	-11.6556307750	5.2882222743
C294	1.4123536921	-12.0119014871	5.6081520946
C295	0.8657332664	-11.6973701191	6.8233842032
N296	1.5871599010	-11.0495597649	7.7829001651
C297	2.8815741707	-10.7020747098	7.5198893415
C298	3.4692987223	-10.9867725706	6.3194583181
H299	0.7880559296	-12.5650746786	4.9130274038
H300	-0.1524027830	-11.9642657938	7.0950544242
H301	3.4096091665	-10.1969965333	8.3240816677
H302	4.5112402715	-10.7081204446	6.2045757034
N303	4.5888024153	-12.7774674929	1.6258181562
C304	5.3030901445	-12.1203179456	2.5839038178
C305	4.7247638874	-11.7133050535	3.7541226229
C306	3.3564110169	-11.9845618548	4.0276363973
C307	2.6378383596	-12.6285513632	2.9829357123
C308	3.2610676931	-13.0102064017	1.8271359769
H309	6.3559975672	-11.9652574972	2.3646338637
H310	5.3667918988	-11.2149595913	4.4743835686
H311	1.5848244629	-12.8706522696	3.0769591821
H312	2.7418330932	-13.5255614152	1.0242620324
C313	5.2660830074	-13.2532558940	0.4222786383
H314	4.5319027509	-13.7018936458	-0.2484314343

H315	5.7588567527	-12.4164349090	-0.0823145165
H316	6.0142616503	-14.0042881812	0.6935869166

Co-conformation 3g

M06L/6-31G* in acetonitrile (A)	M06L/6-31G* in gas phase (B)	M06/6-311++G** in gas phase (C)	Total energy (C+A-B)
-7013.48517	-7011.39524	-7008.55690	-7010.64683

N1	-4.6023258759	2.4931741159	10.1669481400
N2	-5.7505509684	-3.0938796109	11.0483284537
C3	-5.6818148371	1.6650815740	10.3244509439
H4	-6.2631873051	1.4749302771	9.4250561407
C5	-6.0079307766	1.1294099214	11.5373620313
H6	-6.8823128295	0.4860688082	11.5708179467
C7	-5.2380758689	1.3988990256	12.7099223137
C8	-4.1798468610	2.3371344602	12.5136359136
H9	-3.5577621219	2.6618480055	13.3449015869
C10	-3.8790411702	2.8370487116	11.2776395509
H11	-3.0619329655	3.5346675013	11.1107161280
C12	-4.2100793790	2.9652350424	8.8182804319
H13	-5.1368933600	3.1973794647	8.2822985008
H14	-3.6668036056	3.9051476100	8.9584512468
C15	-3.3778366663	1.9617087853	8.0528862254
C16	-1.9802993238	1.9966061643	8.1085676114
H17	-1.4806395089	2.7648991136	8.6987372324
C18	6.7570691559	-6.6668209664	2.6432118173
H19	6.7372669785	-7.1570328578	3.6172558624
C20	7.0376779202	-7.4143292474	1.4943588563
C21	7.1111830473	-6.7539614845	0.2643126801
H22	7.3662549381	-7.3157090754	-0.6355292756
C23	-3.9876870622	0.9759388891	7.2705963801
H24	-5.0748061051	0.9411551165	7.1905853021
C25	-7.0633770479	-3.5088064916	10.5051562346
H26	-7.0040673785	-3.4273843560	9.4145991278
H27	-7.2028699232	-4.5651755510	10.7583065308
C28	-5.0135536937	-2.1214081337	10.4314188111
H29	-5.3392824411	-1.8475669046	9.4300787213
C30	-3.9394552668	-1.5383441308	11.0413892346
H31	-3.4127058138	-0.7728433164	10.4772153478
C32	-3.5459865906	-1.8866934724	12.3680314491
C33	-4.3039983708	-2.9504217817	12.9432655182
H34	-4.0633392720	-3.3501297281	13.9235396931
C35	-5.3681940864	-3.5082177224	12.2960928246
H36	-5.9630216324	-4.3069612543	12.7310301868
N37	-10.4452211687	2.4945553837	19.3339765381

N38	-9.6353063230	7.4979467884	14.3910114305
N39	-0.6557525917	0.3498658834	14.5719381503
N40	-10.2581336828	1.0206669336	13.7421327785
N41	-5.7647277159	-0.8003758368	16.3275446523
N42	-5.1216272129	4.7451835073	16.8992832877
C43	-9.5953933633	3.5447793843	19.5329256818
C44	-10.5042237418	6.4658479744	14.1841836034
C45	-1.3070504163	-0.7065348865	15.1471967512
H46	-9.0865616442	3.5700987199	20.4924422945
H47	-11.0677702932	6.5011703063	13.2560951970
H48	-1.0701539976	-0.8940669090	16.1912068647
C49	-9.4176939520	4.5097484307	18.5832618702
C50	-10.6597164305	5.4675458701	15.1057091842
C51	-2.1939316979	-1.4717905935	14.4451450992
H52	-8.7464858622	5.3263394930	18.8319076553
H53	-11.3907994919	4.6975218321	14.8786531688
H54	-2.6595331815	-2.2960234835	14.9774204242
C55	-10.1073113735	4.4596791886	17.3376155183
C56	-9.9198533260	5.4603819790	16.3210179025
C57	-2.5167841589	-1.1901387009	13.0837783159
C58	-11.0168082405	3.3770111658	17.1941560471
C59	-9.0033195317	6.5369424158	16.4763646502
C60	-1.7641302261	-0.1216401896	12.5122764180
H61	-11.6319922770	3.2647846599	16.3060980802
H62	-8.3780612109	6.6337037814	17.3593399487
H63	-1.8721258518	0.1469509802	11.4654862909
C64	-11.1508959517	2.4250371436	18.1665098188
C65	-8.8855607612	7.5164912067	15.5273872780
C66	-0.8800634922	0.6133202179	13.2490602307
H67	-11.8253735437	1.5783756592	18.0676461388
H68	-8.2078771330	8.3585424267	15.6368613663
H69	-0.3019144871	1.4311073872	12.8270668168
C70	0.0874107775	1.3175947012	15.4088523770
C71	-9.5031574515	8.5483317033	13.3820763138
C72	-10.3386725248	1.3010688859	20.2038710947
H73	0.5782952711	0.7533776561	16.2083695592
H74	-10.4973087990	8.8654423764	13.0567451633
H75	-10.1462732430	1.6545660529	21.2220776288
H76	0.8675835880	1.7538378353	14.7770802370
H77	-8.9760972544	9.3998981859	13.8156173452
H78	-11.3069224178	0.7911857150	20.1928204661
C79	-0.8452200908	2.3706451367	15.9548459752
C80	-9.2240344066	0.4355734194	19.6720452883
C81	-1.2581924452	3.4361601343	15.1461076650

C82	-9.4921383931	-0.6249264229	18.8029916486
H83	-0.8382683762	3.5527314713	14.1458792447
H84	-10.5244239159	-0.9222693113	18.6146089918
C85	-2.1830708786	4.3654764210	15.6122173597
C86	-8.4508951309	-1.2994864267	18.1679925374
H87	-2.4820469835	5.1959455263	14.9709456397
H88	-8.6790045292	-2.1289963355	17.4970633203
C89	-2.7163934880	4.2549494296	16.9016234014
C90	-7.1221607573	-0.9184921776	18.3786602965
C91	-2.2827076507	3.2079306204	17.7186180364
C92	-6.8537752110	0.1072900396	19.2907291620
H93	-2.6619419657	3.1244810501	18.7379992152
H94	-5.8206186458	0.3874457104	19.5032478073
C95	-1.3579645330	2.2748807939	17.2500948494
C96	-7.8914308422	0.7751696576	19.9323874058
H97	-1.0238070643	1.4695272976	17.9050600771
H98	-7.6609955485	1.5742300021	20.6380834366
C99	-3.7940263334	5.2036735088	17.3656318415
C100	-6.0039216478	-1.5416020111	17.5866753266
C101	-11.0064042314	0.0302073103	12.9370429795
H102	-3.6440967093	6.2148905872	16.9731019396
H103	-6.2285665376	-2.5782787578	17.3132085549
H104	-11.6934281232	-0.4900738159	13.6114098460
H105	-3.8334660363	5.2693191865	18.4581675695
H106	-5.0631838071	-1.5440124543	18.1469408473
H107	-11.6070229816	0.5913200612	12.2132601189
C108	-5.7680431455	3.7412038845	17.5673244852
C109	-4.8779876831	0.2440284594	16.2710669823
C110	-9.7685176349	2.1575379786	13.1511964352
H111	-5.3715208912	3.5001140488	18.5512595141
H112	-4.2997490921	0.4188403932	17.1759237861
H113	-10.1556647782	2.3777675366	12.1599260270
C114	-6.8422663908	3.0947917397	17.0277539293
C115	-4.7103427896	0.9909831207	15.1395722702
C116	-8.8618252002	2.9598718787	13.7811665982
H117	-7.3056029446	2.3194390237	17.6338049211
H118	-3.9639095379	1.7835245406	15.1774846149
H119	-8.5287109329	3.8401264861	13.2395903088
C120	-7.3388793347	3.4160290069	15.7268309024
C121	-5.4706439813	0.7331078245	13.9553655581
C122	-8.3625668034	2.6542849816	15.0852479842
C123	-6.6740614330	4.5129732836	15.0968239541
C124	-6.4296789708	-0.3181560902	14.0863745434
C125	-8.9362825573	1.4865079655	15.6748278870

H126	-6.9877697138	4.8783503402	14.1218090971
H127	-7.0732420862	-0.6033637937	13.2563576115
H128	-8.6563837953	1.1581065453	16.6733102948
C129	-5.5983201918	5.1272690110	15.6724418457
C130	-6.5527635646	-1.0437773402	15.2336601490
C131	-9.8342589725	0.7060897590	15.0022669871
H132	-5.0656350614	5.9453026982	15.1943150439
H133	-7.2549914194	-1.8686870463	15.3319291189
H134	-10.2601769240	-0.1991928627	15.4305627470
H135	-8.9420005227	8.1730275082	12.5198609193
N136	4.6714085227	-3.0876068268	1.1397110341
N137	-0.5468499674	-0.7062568265	4.5859580363
C138	3.9088763978	-3.1707131409	2.2754562793
H139	4.4470968783	-3.0639139450	3.2135386757
C140	2.5592988597	-3.3640636186	2.2202500031
H141	2.0348709306	-3.4046001290	3.1696837291
C142	1.8621561786	-3.4994476071	0.9779362311
C143	2.6933814500	-3.3641812498	-0.1741532731
H144	2.2844546129	-3.4135335740	-1.1823786797
C145	4.0447465645	-3.1859562074	-0.0694641927
H146	4.6895560203	-3.1065923453	-0.9423214295
C147	6.1457885951	-3.1948581100	1.2301148710
H148	6.5681939556	-2.7040486553	0.3470506527
H149	6.4593396155	-2.6253469528	2.1115217507
C150	6.5484447762	-4.6446015831	1.3223326914
C151	6.5156197379	-5.2997241935	2.5584450267
H152	6.3092154495	-4.7327721274	3.4669278801
C153	-1.2149107334	1.0664458761	7.4094945651
H154	-0.1275464309	1.1069375092	7.4768715820
C155	-1.8255558379	0.0697344067	6.6419698210
C156	-3.2224728238	0.0361049095	6.5831195362
H157	-3.7258681191	-0.7403289759	6.0061717261
C158	6.8691842051	-5.3830037991	0.1794198486
H159	6.9400870902	-4.8808605585	-0.7877517599
C160	-0.9959640784	-0.9981491869	5.9716107480
H161	-1.5613433848	-1.9372726127	5.9234920700
H162	-0.0866317324	-1.1953481437	6.5471791989
C163	0.7809182861	-0.5566570136	4.2925025458
H164	1.4556366110	-0.5453678934	5.1441719882
C165	1.2279870414	-0.4377247605	3.0030211745
H166	2.2962081455	-0.3063853884	2.8657992337
C167	0.3280232410	-0.4702713714	1.8978474726
C168	-1.0447253506	-0.6120581924	2.2521302654
H169	-1.8265373065	-0.6270388591	1.4973314265

C170	-1.4448358227	-0.7219410511	3.5549865245
H171	-2.4908912153	-0.8233295885	3.8333327743
N172	-1.1570327824	-10.8470911911	1.2651182028
N173	5.8273661187	-9.5431169544	1.5553187374
N174	1.6348541929	-0.1971504213	-2.1559426421
N175	0.7961629373	-7.0128621503	4.4156004700
N176	-2.3133463234	-4.3783229068	0.7358926484
N177	2.8063195289	-6.5924274575	-2.3928279105
C178	-0.3902775880	-10.8661767083	0.1282960862
C179	5.0976077849	-9.6695341427	2.7073051603
C180	0.3120836154	-0.3800400358	-1.8625156905
H181	-0.9283791667	-11.0373239870	-0.8004496576
H182	5.6485680002	-9.5081969419	3.6303639396
H183	-0.3588349531	-0.4371405964	-2.7155655205
C184	0.9616781999	-10.6932509905	0.1722831586
C185	3.7702339172	-9.9903774350	2.6877545216
C186	-0.1336990233	-0.4612828305	-0.5722816854
H187	1.4882205768	-10.7326527039	-0.7763848142
H188	3.2709465383	-10.0810325479	3.6496218423
H189	-1.2024171669	-0.5833345596	-0.4302400051
C190	1.6587011478	-10.4690923457	1.4027412580
C191	3.0624179724	-10.2036578961	1.4618395683
C192	0.7656540850	-0.3675734040	0.5310667193
C193	0.8233998206	-10.5020927348	2.5606127552
C194	3.8777400634	-10.0993343960	0.2932543285
C195	2.1268212079	-0.1449795047	0.1784326379
H196	1.2319129235	-10.3801952739	3.5628938470
H197	3.4620958555	-10.2623173032	-0.6979429974
H198	2.8956059846	-0.0108491505	0.9351007260
C199	-0.5295996224	-10.6694144065	2.4663566180
C200	5.2002463539	-9.7656322801	0.3599308156
C201	2.5263802561	-0.0804294529	-1.1281421329
H202	-1.1773484870	-10.6737769369	3.3407814150
H203	5.8237883000	-9.6571259450	-0.5241792599
H204	3.5617701496	0.0856371965	-1.4152601554
C205	2.1241784035	-0.3972227698	-3.5401700239
C206	7.1674895330	-8.9141128883	1.5838376551
C207	-2.6276634538	-10.7196071070	1.1623105921
H208	1.3425573217	-0.0364167905	-4.2166629237
H209	7.6530129138	-9.2276734162	2.5140833301
H210	-2.9437846252	-11.3110524416	0.2964735162
H211	3.0082708520	0.2342068223	-3.6747311457
H212	7.7437378458	-9.3265022791	0.7489511243
H213	-3.0652499879	-11.1774486034	2.0559841081

C214	2.4287838357	-1.8590838431	-3.7519864687
C215	-3.0168136277	-9.2691661502	1.0251710432
C216	3.7245794826	-2.3572460559	-3.5934935225
C217	-3.3554121696	-8.5048037061	2.1454552362
H218	4.5527721251	-1.6662372326	-3.4302730039
H219	-3.4389396513	-8.9840451019	3.1228984944
C220	3.9677059439	-3.7300358327	-3.6440638963
C221	-3.6043674592	-7.1381356651	2.0243625620
H222	4.9870561886	-4.1019000613	-3.5233510803
H223	-3.8798518448	-6.5586956891	2.9070305886
C224	2.9203282528	-4.6314524297	-3.8521205672
C225	-3.5183657619	-6.5062258606	0.7802648839
C226	1.6309120717	-4.1276284901	-4.0589768374
C227	-3.2124147028	-7.2781621943	-0.3461739474
H228	0.8084832925	-4.8126862551	-4.2687222214
H229	-3.1766360841	-6.8099864277	-1.3307166473
C230	1.3881554256	-2.7591940956	-4.0101200144
C231	-2.9667358770	-8.6422424639	-0.2253716604
H232	0.3776130232	-2.3858768088	-4.1811941185
H233	-2.7420635741	-9.2286527703	-1.1172068727
C234	3.1395347581	-6.1199124879	-3.7561565434
C235	-3.6519132893	-5.0092666485	0.6637381545
C236	0.4207050595	-7.3026291693	5.8179331639
H237	4.1798955007	-6.3948751183	-3.9562507747
H238	-4.2609288636	-4.5891021566	1.4714061617
H239	2.5044867078	-6.6744017122	-4.4553239249
H240	-4.1015282081	-4.7073566233	-0.2878290341
H241	1.0545395106	-6.6799063185	6.4583369610
C242	1.5061603489	-6.8775869414	-2.0644801339
C243	-1.5728043747	-4.1880696938	-0.3989368730
C244	2.1046362722	-6.7711939260	4.0823193583
H245	0.8265763240	-6.9955937464	-2.9046537110
H246	-2.1156891746	-4.2918661966	-1.3351312103
H247	2.7790418374	-6.6139246897	4.9204838515
C248	1.1069782290	-7.0206151199	-0.7677826408
C249	-0.2440081969	-3.8756374044	-0.3473195469
C250	2.5184163432	-6.7106811398	2.7828259071
H251	0.0608851874	-7.2678941203	-0.5990232460
H252	0.2646979441	-3.7241929873	-1.2956650195
H253	3.5691044949	-6.4949974393	2.6101743039
C254	2.0157293698	-6.8511664949	0.3252638025
C255	0.4555880627	-3.7523085183	0.8951312080
C256	1.6103980832	-6.9139773832	1.6936773355
C257	3.3669282651	-6.6060364351	-0.0684812846

C258	-0.3689432687	-3.9237292052	2.0465083533
C259	0.2612476630	-7.1643437579	2.0909917427
H260	4.1642843423	-6.5093413793	0.6674742192
H261	0.0397341937	-3.8208938376	3.0486246631
H262	-0.5279650929	-7.3198040155	1.3554119315
C263	3.7183767872	-6.4675723831	-1.3808153111
C264	-1.6944319714	-4.2369958207	1.9478960579
C265	-0.1035478388	-7.2202221606	3.4049563007
H266	4.7399566756	-6.2582927541	-1.6917777370
H267	-2.3281772139	-4.3902520204	2.8183548203
H268	-1.1269148571	-7.4197081403	3.7164462012
H269	-0.6166955429	-6.9783791088	5.9546851288
C270	-8.1609289312	-2.6454636586	11.0765700458
C271	-8.4592674462	-1.4051926445	10.5006043882
C272	-9.3974646755	-0.5580892247	11.0830589086
C273	-10.0608222507	-0.9300203334	12.2584163193
C274	-9.7838977317	-2.1803320693	12.8178555184
C275	-8.8453229974	-3.0297980371	12.2331606891
H276	-7.9600776195	-1.1014608260	9.5784430125
H277	-9.6225126396	0.3995476496	10.6109475419
H278	-10.3147503854	-2.5017167757	13.7148825624
H279	-8.6494058644	-4.0052358997	12.6797109742
C280	0.9977768893	-11.5334534949	6.4475251496
C281	-0.2684355269	-11.0354967912	6.1283943923
C282	-0.4702938233	-9.6651313136	5.9699614018
C283	0.5909655922	-8.7681003552	6.1218082680
C284	1.8473963520	-9.2647526555	6.4846542384
C285	2.0488558045	-10.6313352742	6.6457092076
H286	-1.1048940408	-11.7251750841	6.0060620433
H287	-1.4678637602	-9.2910998535	5.7311214994
H288	2.6761201112	-8.5754097823	6.6498424004
H289	3.0345288737	-11.0001767038	6.9318718376
C290	1.2695543069	-13.0163978869	6.4422648306
H291	2.0372203209	-13.3022248729	7.1686188417
H292	0.3709399456	-13.6083019995	6.6419684285
C293	2.6401276660	-13.4853273166	2.4147956717
C294	1.2828890595	-13.6915579644	2.7823416274
C295	0.8795064907	-13.6282446620	4.0887131494
N296	1.7666829961	-13.3928081476	5.0981474709
C297	3.0868704249	-13.2213709443	4.7926185762
C298	3.5344630638	-13.2704127205	3.5021757324
H299	0.5193223489	-13.9118636450	2.0411086921
H300	-0.1537811219	-13.7789637303	4.3905449501
H301	3.7532877855	-13.0649280557	5.6365483006

H302	4.6029404616	-13.1576803912	3.3489996552
N303	3.9633301123	-13.6904007413	-1.6280648508
C304	4.8506377026	-13.4424111763	-0.6225511258
C305	4.4447791607	-13.3541806193	0.6797282173
C306	3.0811913554	-13.5241697987	1.0447152187
C307	2.1897890847	-13.7649286276	-0.0372587233
C308	2.6432990604	-13.8461938995	-1.3263125991
H309	5.8899594632	-13.3387800248	-0.9220209474
H310	5.2151784623	-13.1632296066	1.4216828976
H311	1.1273781330	-13.9171072947	0.1191332517
H312	1.9843783806	-14.0484016017	-2.1657246536
C313	4.4493518826	-13.8577995771	-2.9962200093
H314	3.6023053169	-13.8359860469	-3.6839763673
H315	5.1394278188	-13.0467259148	-3.2434332821
H316	4.9721797710	-14.8153444999	-3.0890023592

Co-conformation 3h

M06L/6-31G* in acetonitrile (A)	M06L/6-31G* in gas phase (B)	M06/6-311++G** in gas phase (C)	Total energy (C+A-B)
-7013.47898	-7011.56174	-7008.7199	-7010.63714

N1	-4.6165637901	2.5961304223	10.1002441283
N2	-5.7623661296	-3.1154509157	11.0553226496
C3	-5.7145654790	1.7966640034	10.2665714298
H4	-6.3165523296	1.6302042361	9.3759141283
C5	-6.0341701223	1.2617771584	11.4807161971
H6	-6.9255197118	0.6415945496	11.5245392851
C7	-5.2358703768	1.4926668863	12.6416163751
C8	-4.1605185235	2.4090709048	12.4383855473
H9	-3.5136376541	2.7061339693	13.2610954293
C10	-3.8683136418	2.9125482606	11.2013637705
H11	-3.0357361672	3.5886746856	11.0252144221
C12	-4.2137714589	3.0371054350	8.7447431238
H13	-5.1368518964	3.2735590939	8.2033173022
H14	-3.6550975788	3.9703979419	8.8676212498
C15	-3.3970813232	2.0023757696	8.0063937804
C16	-1.9985461156	2.0412055990	8.0357266288
H17	-1.4910049838	2.8300935871	8.5918617359
C18	0.0289151711	-8.4753095881	-9.9817616244
H19	0.2177306563	-9.0493388685	-10.8896652964
C20	-0.0476725930	-9.1313254335	-8.7482693086
C21	-0.3452408133	-8.3818608168	-7.6059009161
H22	-0.4462931275	-8.8828094849	-6.6417848692
C23	-4.0211889425	0.9875570459	7.2733718490

H24	-5.1103853672	0.9472938192	7.2164068444
C25	-7.0777306808	-3.5224286672	10.5156310694
H26	-7.0208969464	-3.4470287075	9.4239171238
H27	-7.2247290942	-4.5768182860	10.7721495693
C28	-5.0524199921	-2.1061981535	10.4651212385
H29	-5.3942093626	-1.8056767463	9.4766578565
C30	-3.9832899553	-1.5227698371	11.0811787785
H31	-3.4765198770	-0.7299682585	10.5362921231
C32	-3.5658172186	-1.9119211583	12.3892984570
C33	-4.2956458614	-3.0095847671	12.9367333125
H34	-4.0289286232	-3.4417815959	13.8962153853
C35	-5.3565252979	-3.5662312898	12.2832676793
H36	-5.9279046165	-4.3946485901	12.6939850848
N37	-10.4098070372	2.4682762109	19.3534275685
N38	-9.6512921869	7.4820901428	14.4110150474
N39	-0.6768756131	0.2992282559	14.6133005733
N40	-10.2454864974	1.0439644333	13.7451432487
N41	-5.7417650745	-0.7491592814	16.2365825269
N42	-5.1233745013	4.7337731037	16.9551482082
C43	-9.5626783561	3.5229263456	19.5476274662
C44	-10.5253432049	6.4526458678	14.2129895831
C45	-1.3100532488	-0.7775781302	15.1713312740
H46	-9.0422142300	3.5444889139	20.5012044112
H47	-11.0978087996	6.4895595728	13.2903994143
H48	-1.0584754931	-0.9866829831	16.2077225630
C49	-9.4023327051	4.4955086719	18.6021584620
C50	-10.6740615085	5.4549740231	15.1354198821
C51	-2.1968717219	-1.5365749405	14.4622141579
H52	-8.7346799121	5.3151852879	18.8486122331
H53	-11.4078283734	4.6852090312	14.9142837395
H54	-2.6468611119	-2.3800492160	14.9789731337
C55	-10.1018952122	4.4473415875	17.3620014992
C56	-9.9232485912	5.4460725481	16.3443681676
C57	-2.5378123404	-1.2238116988	13.1122855526
C58	-11.0128750596	3.3630672885	17.2253863817
C59	-9.0025556067	6.5197725055	16.4901257712
C60	-1.8011519938	-0.1361524631	12.5559249487
H61	-11.6392866996	3.2539364838	16.3436698890
H62	-8.3676415604	6.6124861642	17.3665218339
H63	-1.9178075726	0.1501873071	11.5150697152
C64	-11.1314640517	2.4047386602	18.1943480350
C65	-8.8900583504	7.4977613485	15.5401157001
C66	-0.9143158128	0.5884502670	13.2981970214
H67	-11.8056318345	1.5569291738	18.1005351673

H68	-8.2064900377	8.3358273413	15.6421306042
H69	-0.3445174798	1.4177880245	12.8873133689
C70	0.0623898620	1.2592206894	15.4617716801
C71	-9.5304194233	8.5350349069	13.4043849683
C72	-10.2805376404	1.2662067232	20.2088983395
H73	0.5446461619	0.6883042560	16.2615251582
H74	-10.5267398481	8.8855508545	13.1211159931
H75	-10.0717330552	1.6091860531	21.2275471216
H76	0.8498639874	1.6970873898	14.8400242748
H77	-8.9602077939	9.3659721888	13.8231251183
H78	-11.2459128027	0.7503297769	20.2107498465
C79	-0.8694193629	2.3134830047	16.0075794276
C80	-9.1703799167	0.4122454374	19.6491324978
C81	-1.2663149666	3.3896891266	15.2043949620
C82	-9.4457940420	-0.6280766093	18.7574472668
H83	-0.8366265242	3.5120141444	14.2087459758
H84	-10.4796798291	-0.9225079828	18.5724900646
C85	-2.1848140750	4.3246846966	15.6723126777
C86	-8.4104415995	-1.2855445476	18.0954899370
H87	-2.4715585023	5.1629252036	15.0355325678
H88	-8.6451475673	-2.0983328763	17.4063581951
C89	-2.7258200190	4.2108195791	16.9584437797
C90	-7.0798237098	-0.9079400802	18.3022226143
C91	-2.3101867703	3.1513250867	17.7687428565
C92	-6.8037014680	0.0937297531	19.2384105160
H93	-2.6969020687	3.0637910406	18.7850631708
H94	-5.7686608812	0.3686083250	19.4481888934
C95	-1.3935764061	2.2115801574	17.2978787075
C96	-7.8355708806	0.7449720280	19.9064801291
H97	-1.0730474217	1.3970615759	17.9482767797
H98	-7.5989275469	1.5262408077	20.6299284940
C99	-3.7913221724	5.1714440820	17.4260869910
C100	-5.9672992927	-1.5109513750	17.4863705055
C101	-10.9922182020	0.0586124242	12.9336465069
H102	-3.6269883233	6.1828040383	17.0394151136
H103	-6.1898688751	-2.5443172821	17.1987052524
H104	-11.6882865896	-0.4572640263	13.6020571208
H105	-3.8314043244	5.2314092013	18.5189136678
H106	-5.0212101430	-1.5194905124	18.0375797651
H107	-11.5834746489	0.6230599388	12.2046444470
C108	-5.7859572268	3.7361943659	17.6180303199
C109	-4.8598238654	0.2999001976	16.1884295140
C110	-9.7492304440	2.1817384992	13.1615340172
H111	-5.3988655551	3.4901831926	18.6045134139

H112	-4.2824901883	0.4709480779	17.0944062418
H113	-10.1248536800	2.4027612012	12.1658114990
C114	-6.8624537740	3.1017906126	17.0699656655
C115	-4.6990259234	1.0594090713	15.0644098539
C116	-8.8507857136	2.9836145479	13.8034036949
H117	-7.3379054951	2.3300793178	17.6703808511
H118	-3.9602054983	1.8585735294	15.1096500292
H119	-8.5117600469	3.8653367685	13.2676244193
C120	-7.3458306163	3.4295156670	15.7657281559
C121	-5.4605762853	0.8099518661	13.8794571116
C122	-8.3658565189	2.6748428997	15.1126512611
C123	-6.6679071212	4.5234983781	15.1446778917
C124	-6.4159557782	-0.2460865621	14.0018738939
C125	-8.9482954011	1.5076871852	15.6950171027
H126	-6.9725997257	4.8980109003	14.1712418039
H127	-7.0587757264	-0.5281546476	13.1692139499
H128	-8.6800632200	1.1825093774	16.6981895743
C129	-5.5891709646	5.1243782496	15.7273121473
C130	-6.5310482507	-0.9845863865	15.1419380747
C131	-9.8388927955	0.7290766068	15.0116397681
H132	-5.0471200776	5.9397283984	15.2549193614
H133	-7.2306039857	-1.8124103701	15.2347623309
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H141	3.6103938543	-4.0500820680	-10.9271704922
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C158	-0.5221851930	-7.0008330697	-7.6899992346
H159	-0.7642881100	-6.4312395235	-6.7901726000
C160	-1.0578543095	-0.9788219838	5.9055549348
H161	-1.6356960810	-1.9065447045	5.8116150008
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H164	1.3832458939	-0.4192222064	5.1124191932
C165	1.1533645023	-0.2212984828	2.9802490941
H166	2.2203222347	-0.0721146163	2.8498955673
C167	0.2598539638	-0.2477138982	1.8680864203
C168	-1.1171913990	-0.4065820379	2.2119862705
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C170	-1.5129151729	-0.5868800696	3.5072065082
H171	-2.5545243977	-0.7345847052	3.7807236748
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C180	0.2862452220	-0.2645665849	-1.8884830814
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H182	1.9441801084	-10.9840893303	-10.6333886639
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C185	3.8571456180	-10.8117011353	-9.6534175776
C186	-0.1732479959	-0.2412747410	-0.6036804264
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H188	4.3873343439	-10.8712354125	-10.6004111529
H189	-1.2493414295	-0.2861059990	-0.4682167321
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C191	4.5641935586	-10.6713715591	-8.4169290549
C192	0.7152773075	-0.1714648388	0.5103192776
C193	6.8207270494	-10.4305647437	-9.4886291888
C194	3.7224389171	-10.6610865622	-7.2628265894
C195	2.0954841864	-0.0605602657	0.1630812233
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H197	4.1400202221	-10.5821829933	-6.2624591613
H198	2.8656933652	0.0391550744	0.9224179919
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H204	3.5592211920	-0.0222434959	-1.4155038411
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C206	0.2660376321	-10.6036025178	-8.6569854174
C207	10.1488765092	-9.4833203669	-8.1041239404
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H210	10.5981273514	-9.8464038296	-7.1736012663
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H315	3.2377201914	-13.5739351067	-3.3944676385
H316	4.0935155168	-15.1394872754	-3.3490816592

References

(1) Sharrett, Z.; Gamsey, S.; Fat, J.; Cunningham-Bryant, D.; Wessling, R. A.; Singaram, B. The effect of boronic acid acidity on performance of viologen-based boronic acids in a two-component optical glucose-sensing system. *Tetrahedron Lett* **2007**, *48*, 5125–5129.

(2) Wang, Y.; Frasconi, M.; Liu, W.; Liu, Z.; Sarjeant, A. A.; Nassar, M. S.; Botros, Y. Y.; Goddard III, W. A.; Stoddart, J. F. Folding of oligoviologens induced by radical-radical interactions. *J. Am. Chem. Soc.* **2015**, *137*, 876–885.

(3) Fulmer, G. R.; Miller, A. J.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I. NMR chemical shifts of trace impurities: common laboratory solvents, organics, and gases in deuterated solvents relevant to the organometallic chemist. *Organometallics* **2010**, *29*, 2176–2179.

(4) Fahrenbach, A. C.; Barnes, J. C.; Lanfranchi, D. A.; Li, H.; Coskun, A.; Gassensmith, J. J.; Liu, Z.; Benitez, D.; Trabolsi, A.; Goddard III, W. A., Elhabiri, M.; Stoddart, J. F. Solution-phase mechanistic study and solid-state structure of a tris(bipyridinium radical cation) inclusion complex. *J. Am. Chem. Soc.* **2012**, *134*, 3061–3072.