Supporting Information

Exploring the Conformational Space of Bridge-Substituted Dithienylcyclopentenes

Maic Fredersdorf[a,b,†], Robert Göstl[c,d,†], Andreas Kolmer[a], Volker Schmidts[a], Peter Monecke[b], Stefan Hecht[c,] and Christina M. Thiele[a,*]*

[†] contributed equally

[a] Technische Universität Darmstadt, Clemens-Schöpf-Institut für Organische Chemie und Biochemie, Alarich-Weiss-Straße 16, 64287 Darmstadt, Germany

[b] Sanofi-Aventis Deutschland GmbH, Department of Chemistry, Industriepark Hoechst, 65926 Frankfurt am Main, Germany

[c] Humboldt-Universität zu Berlin, Department of Chemistry, Brook-Taylor-Str. 2, 12489 Berlin, Germany

[d] current address: Technische Universiteit Eindhoven, Department of Chemical Engineering and Chemistry, Macromolecular and Organic Chemistry, 5600 MB Eindhoven, The Netherlands

Contents

Preparative Details

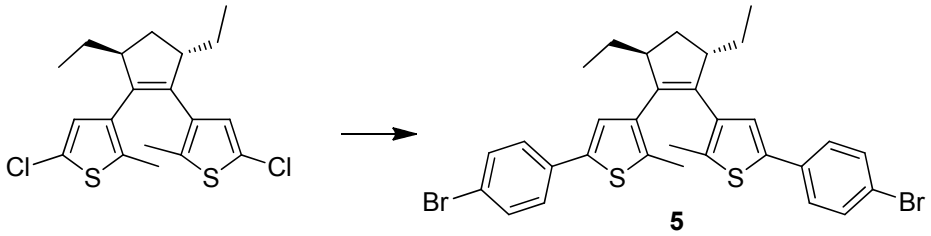
Ultrahigh-performance liquid chromatography / mass spectrometry (UPLC/MS) was performed on a Waters Acquity UPLC equipped with a Waters LCT Premier XE Mass detector for high-resolution MS (HR-MS, ESI^+-ionization) and with Waters Alliance systems (consisting of a Waters Separations Module 2695, a Waters Diode Array Detector 996 and a Waters Mass Detector ZQ 2000). TLC was performed on Merck Silica Gel 60 F254 TLC plates with a fluorescent indicator employing 254 nm UV-lamp for visualization.

Solvents and commercial starting materials were used as supplied. The solvents were dried before use, if necessary, employing an Innovative Technologies solvent purification system (multi-unit micro series). Silica gel for chromatography (0.035-0.070 mm, 60 Å) was used for column chromatography. The petroleum ether (PE) used had a boiling range of 40-60 °C.

All procedures linked to photochemistry were performed using spectrophotometric grade solvents. UV/vis-spectroscopy was performed on either a Varian Cary 50 or Varian Cary 60 UV/vis spectrophotometer equipped with a Peltier thermostated cell holder at 25 ± 0.05 °C. Analytical irradiation was performed on an Oriel 500 W mercury arc lamp model 68810 in an Oriel universal arc lamp housing model 66055 equipped with an Oriel 1/4 m grating monochromator model 77200, an Oriel timed shutter and water filter either at 313 nm or 280 nm for ring-closure or at 546 nm for ring-opening reactions.

Syntheses of DAEs **1**-**4** and of the precursors to **5** were carried out according to procedures already published.[1]

1,2-Bis(3-(5-*p*-bromophenyl-2-methylthienyl))-3,5-diethylcyclopent-1,2-ene 5



5

1,2-Bis(3-(5-chloro-2-methylthienyl))-3,5-diethylcyclopent-1,2-ene (0.46 g, 1.2 mmol) was dissolved in dry THF (5 mL) under Ar. To this solution was added dropwise *n*-BuLi (1.2 mL, 2.2 M) and the resulting brownish solution was stirred at rt for 30 min. Then, $B(OBu)_3$ (0.97 mL, 3.6 mmol) was added and the mixture was stirred for 1.5 h at rt. Meanwhile, 1-bromo-4-iodobenzene was dissolved in THF (5 mL) under Ar. To this solution was added $Pd(PPh_3)_4$ (0.14 g, 0.12 mmol) and the resulting mixture was stirred at rt for 5 min. Afterwards, aq. Na_2CO_3 sol. (10 mL, 2 M) and ethylene glycol (3 drops) were added. To this mixture, the solution containing the borate was added directly without any workup. The combined solutions were stirred at 40 °C for 16 h. Afterwards, the solution was diluted with 50 mL water, and extracted with CH_2Cl_2 (3 x 25 mL). The combined organic layers were dried over anhyd. $MgSO_4$ and the solvent was removed *in vacuo*.

The crude product was purified by column chromatography (silica, PE:CH_2Cl_2=10:1) and subsequent recrystallization from Hexane/CH_2Cl_2 to yield the target compound **5** as colorless needles (31%). **^{1}H-NMR (500 MHz, $CDCl_3$):** δ(ppm) = 7.44 (d, ^{3}J(H,H) = 8.6 Hz, 4H, CH_{ar}), 7.35 (d, ^{3}J(H,H) = 8.6 Hz, 4H, C*H*ar), 6.95 (s, 2 H, CH_{ar}), 3.11 (m, 2H, C*H*), 1.95 (t, ^{3}J(H,H) = 6.9 Hz, 2H, CH_2), 1.93 (s, 6 H, CH_3), 1.51 (m, 2H, CH_2), 1.19 (m, 2H, CH_2), 0.87 (t, ^{3}J(H,H) = 7.4 Hz, 6H, CH_3). **^{13}C-NMR (125 MHz, $CDCl_3$):** δ(ppm) = 139.1, 138.5, 136.3, 135.5, 133.7, 132.0, 126.9, 124.5, 120.7, 49.5, 34.0, 27.1, 14.4, 11.5. **HR-MS(ESI$^+$)**: *m/z* = 624.0213 (calcd. 624.0156 for $C_{31}H_{30}S_2Br_2^+$).

NOE Measurements

The NOE measurements were recorded at 300K without sample spinning on a Bruker AVANCE III 600 spectrometer equipped with a 5 mm triple-resonance broadband inverse probe with z-gradient and a proton resonance frequency of 600.4 MHz. For the quantitative determination of distances via the NOE, first T_1 relaxation time constants were measured using the inversion-recovery method, which is available as *t1ir* in the Bruker pulse sequence library. The relaxation delays in the 1D PFGSE NOE experiment with zero-quantum suppression (available in the Bruker pulse sequence library as *selnogpzs*) were set accordingly to 15 s (5 * T1 of the slowest relaxing group). For selective refocusing, a Gaussian pulse was chosen. The length of the Gaussian pulse was set to 80ms, corresponding to an excitation bandwidth of 9.2 Hz. The integral ratio of NOE peak to inverted peak was plotted against the mixing time and its slope was calculated using a linear fit.

We performed 1D PFGSE NOE experiments[2,3,4] with suppression of zero-quantum artifacts,[5,6,7] at mixing times ranging from 50 to 400 ms (in 25 ms steps). During the period of validity of the initial-rate-approximation[8], these mixing time series were evaluated using the PANIC[9,10] approach (for the corresponding plots see Figure SI- 1, Figure SI- 2 and Figure SI- 3):

$$r_{IS} = r_{ref}\left(\frac{\sigma_{IS}}{\sigma_{ref}}\right)^{-\frac{1}{6}}$$

r_{IS} is the distance between nuclei and S that is to be determined; σ_{IS} is equal to the slope of the corresponding PANIC plot. r_{ref} stands for a reference distance with σ_{ref} being equal to the slope of the PANIC plot for the reference distance.

As reference distance, the distance between the protons from the methyl group located at the cyclopentene ring (H60-62/H63-65, numbering scheme see Figure 6 of the main text) and the proton next to this methyl group (H34/H37) was chosen. All six distances were extracted from the calculated geometry of conformer A (see Table SI- 1). An averaged distance was then determined using Tropp averaging,[11] leading to a calibration distance of 2.646 Å.

With this method, an interproton distance between the cyclopentene (H34/H37) and thiophene rings (H38/H39) of 2.62 ± 0.1 Å was determined (see Table SI- 2).

PANIC plots

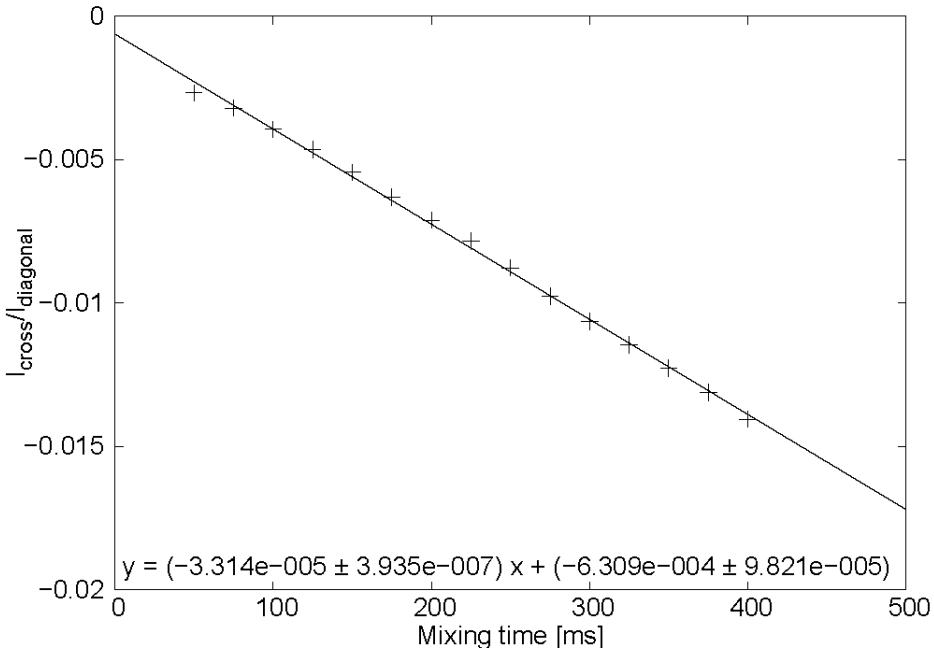


Figure SI- 1: H60-62/H63-65 - H34/H37 (calibration distance)

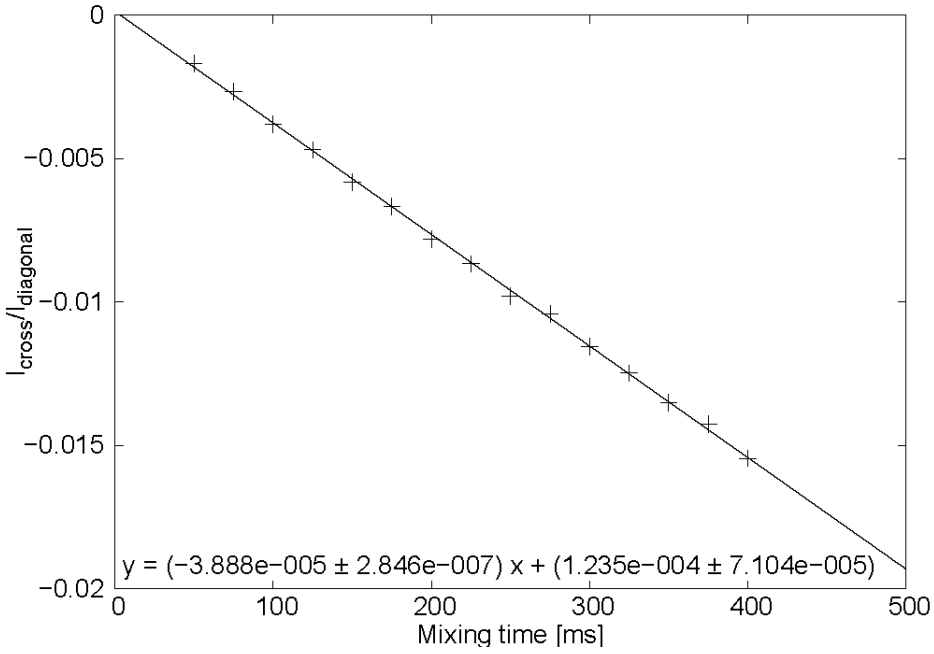


Figure SI- 2: H34/H37 - H38/H39

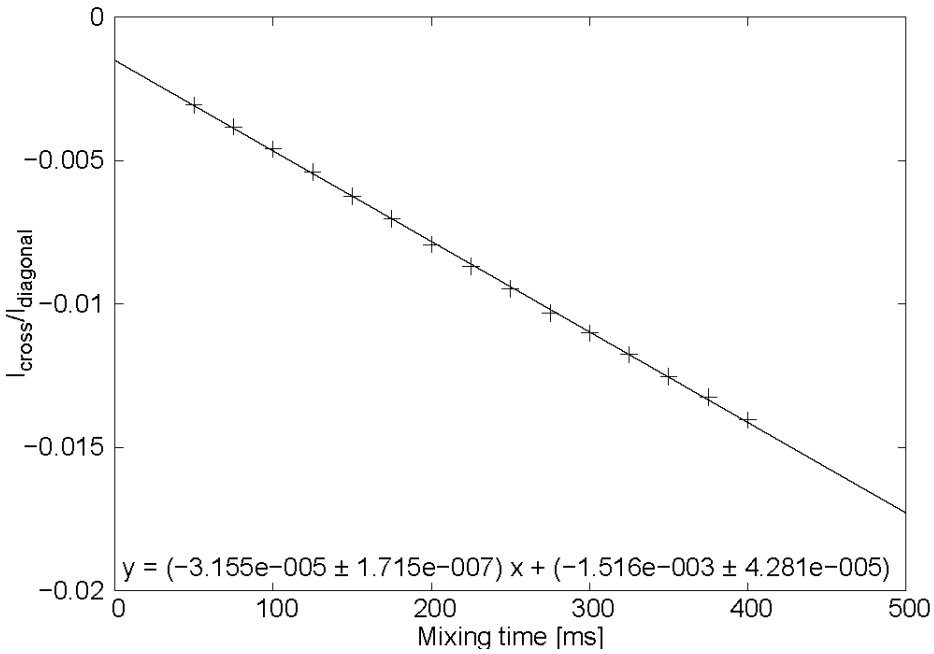


Figure SI- 3: H38/H39 - H34/H37

Table SI- 1: Determination of the calibration distance

Atom 1	Atom 2	Distance from conformer A [Å]
H34	H60	2.475
H34	H61	3.066
H34	H62	2.522
H37	H63	2.511
H37	H64	2.509
H37	H65	3.075
H34/H37	H60-62/H63-65	2.646

Table SI- 2: Determination of the distances via the NOE

	H60-62/H63-65 - H34/H37 (cal)	H34/H37 - H38/H39	H38/H39 - H34/H37
slope	$-3.314*10^{-5}$	$-3.888*10^{-5}$	$-3.155*10^{-5}$
distance	2.646	2.577	2.668
distance (avg)		2.622	

To evaluate whether other conformers are present in solution, we performed a conformation analysis using the software *WEEDHEAD*[12]. To create the symmetry of the molecule, the populations of A and A' (and B-B', C-C', D-D' respectively) were always set equal. The sums of their populations were varied in 1%-steps. Averaged distances were calculated using the formula[13]

$$r_{averaged} = \left(\sum_{\mu=1}^{N} p_\mu r_{IS,\mu}^{-6} \right)^{-\frac{1}{6}}$$

with N being the number of conformers, p the population of the conformer μ (half of the population step size of 1%) and $r_{IS,\mu}$ the distance of the protons I and S in the conformer μ.

Due to the unsymmetric conformers D (see figure 5 in the main text), the population scan was performed twice, once for the "left" side (as shown in figure 5 in the main text), and once for the "right" side of the molecule. Since there are four sets of conformers, this population scan essentially leads to a 5D plot, which is challenging to represent. We therefore chose to represent only the sum of A-A' on the x-axis, and the y-axis contains the difference between the experimentally derived distance and the distance averaged from the calculated structures (see figures S-22, S-23, S-24 and S-25).

Since there are many possible combinations of B-B', C-C' and D-D' to reach a specific population of A-A', the values on the y-axis show a range of differences. Nevertheless, it is possible to extract the information, that the smallest difference can be reached for a sum of A-A' of 83-89% on the "left side" of the molecule, and for a sum of A-A' of 86-91% on the "right" side of the molecule. This leads to the best agreement being possible for 83-91% of A-A', as mentioned in the main text.

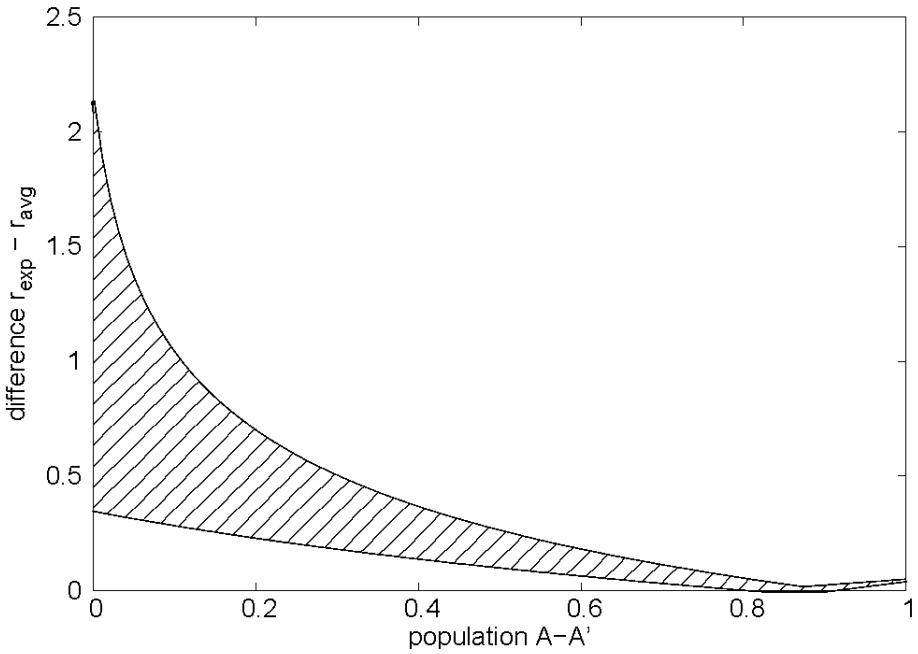


Figure SI- 4: Population scan, "left" side of the molecule

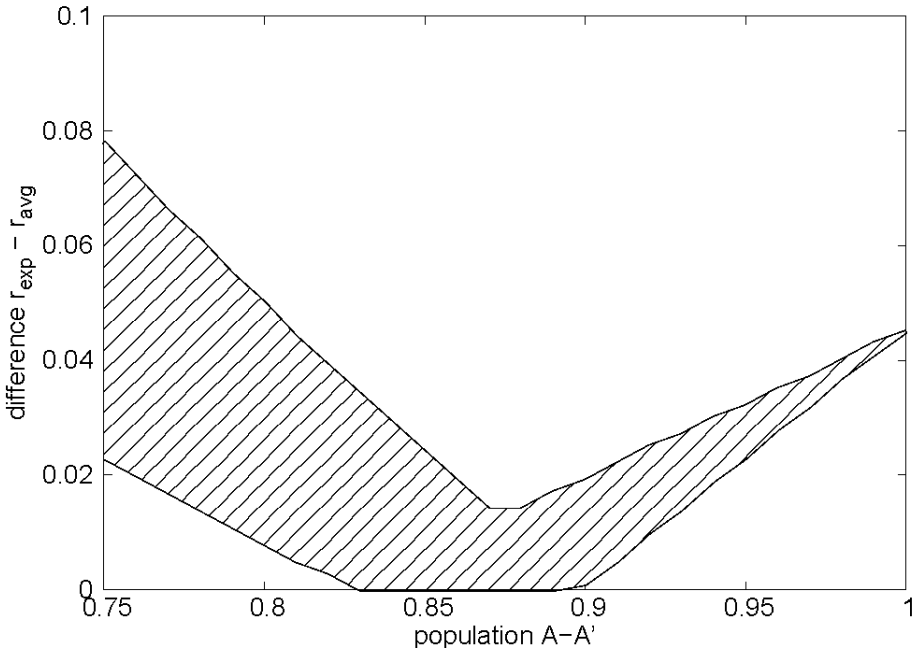


Figure SI- 5: Population scan, "left" side of the molecule, detail

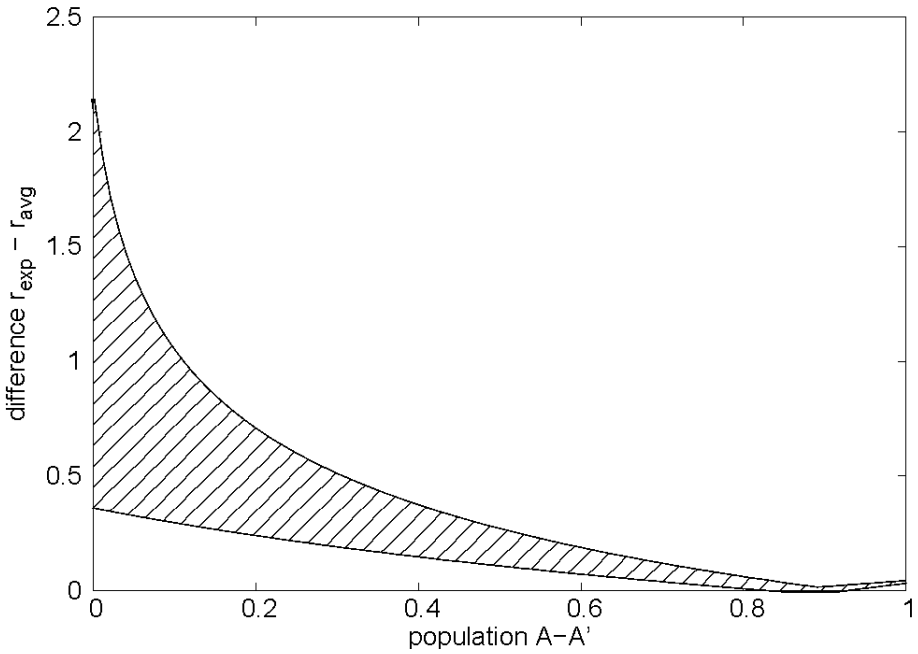


Figure SI- 6: Population scan, "right" side of the molecule

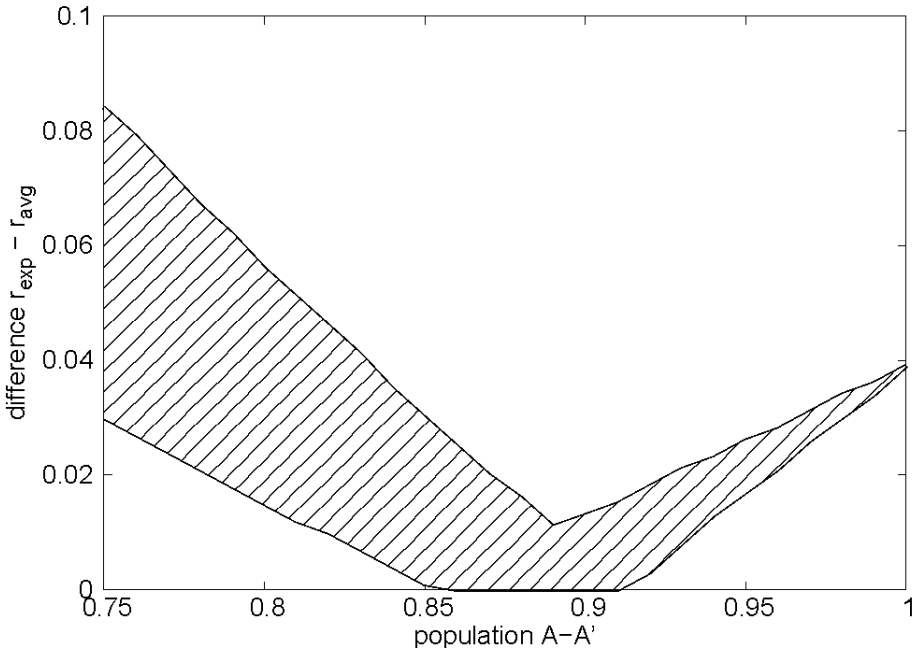


Figure SI- 7: Population scan, "right" side of the molecule, detail

Preparation of the anisotropic NMR samples

For the isotropic and NOE-measurements 3.3 mg of the dithienylcyclopentene derivative **1** were diluted in 600 µl $CDCl_3$ and transferred in an NMR tube. In addition, two anisotropic samples were prepared as followed.

a) Poly-γ-benzyl-L-glutamate stick (cross-linked PBLG gel)[14]

A dried PBLG stick with the given dimensions (length=16mm and diameter 2.3mm) was allowed to swell several weeks in a 5mm NMR tube at 40°C in $CDCl_3$ until a constant quadrupolar splitting was observed in the ^{2}H-NMR spectra. Thereafter 20 mg of compound were added to the tube and the sample was stored again at 40°C until the quadrupolar splitting was sharp and the line widths constant again. It was ensured that the sample was covered with solvent during that period.

b) Polyacetylene[15]

The LC phase was prepared directly in the 5mm NMR tube. A total amount of 130 mg of the Valin-Polyacetylen-Derivative (PA) and 11 mg of compound were weighted directly into the NMR tube, which contained a DMSO-*d*6 capillary to provide the lock signal. After adding 550 mg $CDCl_3$ in the tube, the sample was centrifuged back and forth until the ^{2}H-signal was sharp and the line widths constant.

NMR experiments for coupling extraction

All measurements used for coupling extraction were recorded at 300K without sample spinning on a Bruker AVANCE III 600US spectrometer equipped with a SEI 600 MHz SB 5mm probe with Z-gradient. As shown by Samulski et. al.,[16,17] the quadrupolar splitting of the deuterated solvent can be used as qualitative indicator for the alignment in the liquid crystalline (LC) phase. To ensure constant alignment conditions during NMR measurements, the stability of the LC phase was confirmed by ^{2}H NMR spectra before and after each anisotropic measurement. The quadrupolar splitting of the solvent signal was almost constant at 85 Hz (±1 Hz) in poly-γ-benzyl-L-glutamate stick and 45 Hz (±1 Hz) in the polyacetylene LC.

The total couplings (^{1}T) and scalar coupling constants (^{1}J) were recorded by clean in-phase (CLIP)-HSQC[18] experiments using an INEPT delay of 145 Hz. In the ω_2 dimension a total of 16384 (isotropic) and 4096 data points (anisotropic PBLG gel and PA) were sampled over a spectral width of 10 ppm to give an FID resolution of 0.73 Hz and 2.93 Hz respectively. In the ω_1 dimension 512 (isotropic), 2048 (PBLG gel) and 256 (PA) data points with a spectral width of 180 ppm were recorded, giving a spectral resolution of 106.09, 26.52 and 212.19 Hz respectively. The isotropic sample was measured with four scans, while the anisotropic samples required 64 scans per increment. The spectra were processed using sine squared window functions with zero filling by a factor of 2 in the ω_2 dimension.

The sign and the magnitude of long-range coupling ^{n}T and ^{n}J were recorded by using the heteronuclear long-range coupling (HETLOC) experiment. [19,20] In the ω_2 dimension a total of 4096 data points were recorded, leading to an FID resolution of 2.93 Hz. In the ω_1 dimension a total of 512 (isotropic) and 1024 data points in the anisotropic measurements were recorded, leading to a resolution of 23.43 and

11.71 Hz respectively. The isotropic and the anisotropic PBLG gel sample were measured with 16, the anisotropic PA sample with 32 scans per increment. The spectra were processed using sine squared window functions with zero filling by a factor of 2 in the ω_2 dimension of the isotropic sample.

The carbon-carbon total couplings (^{1}T) and scalar coupling constants (^{1}J) were recorded by 1,1-ADEQUATE[21,22] experiment. In the ω2 dimension a total of 1536 data points in the isotropic as well as in the anisotropic phases were recorded, leading to an FID resolution of 7.82 Hz. In the ω_1 dimension a total of 400 data points in the isotropic as well as in the anisotropic measurement PBLG-gel-phase (350 data points in the PA phase) were recorded, leading to a resolution of 113.17 and 129.3 Hz respectively. The isotropic sample was measured with 128 scans and both anisotropic samples with 512 scans per increment. The spectra were processed using sine squared window functions with zero filling by a factor of 3 in the ω_2 dimension of the isotropic sample.

Couplings were measured by extracting the relevant rows of the 2D spectra, superimposing them, and shifting one of the subspectra onto the other, such that the multiplet components show maximum overlap. By repeating this procedure manually a standard deviation is estimated and used as an experimental error for T and J. RDCs and their estimated uncertainties are then calculated from T = J + 2D.

Assignment and Temperature Dependence of NMR Chemical Shifts of 1o

Spectra were recorded at 300K without sample spinning on a Bruker AVANCE III 600US spectrometer equipped with a SEI 600 MHz SB 5mm probe with Z-gradient. Relevant delays and durations are given, where appropriate.

Assignment of Chemical Shifts

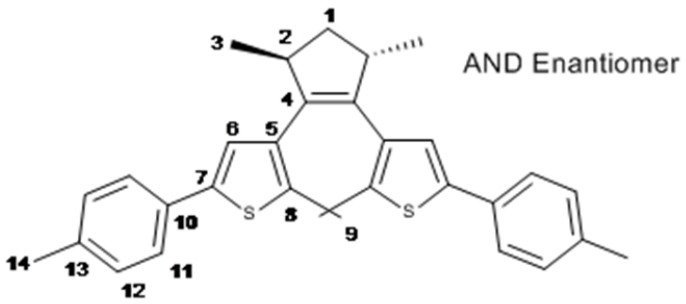


Figure SI- 8: Atom numbering of investigated DAE (1o)

Table SI- 3: Assignment of ^{1}H and ^{13}C chemical shifts of Dithienylcyclopentenes in isotropic solution ($CDCl_3$). Numbering scheme above.

Position	^{1}H(ppm)	^{13}C(ppm)
1	1.93(d)	40.67
2	3.25 (m)	42.31
3	1.00 (d)	19.95
4	-	139.54
5	-	135.73
6	6.94 (s)	123.34
7	-	139.61
8		134.45
9	1.93 (s)	14.10
10	-	131.88
11	7.40 (d)	125.17
12	7.13 (d)	129.42
13	-	136.66
14	2.34 (s)	21.09

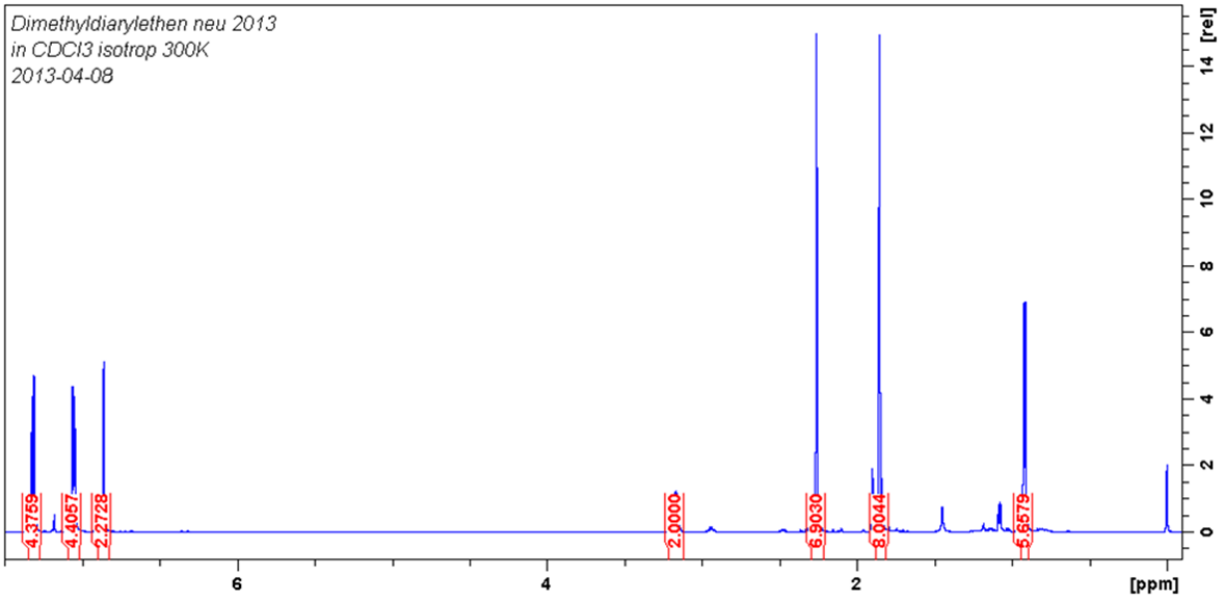


Figure SI- 9: ^{1}H, 300K, isotropic

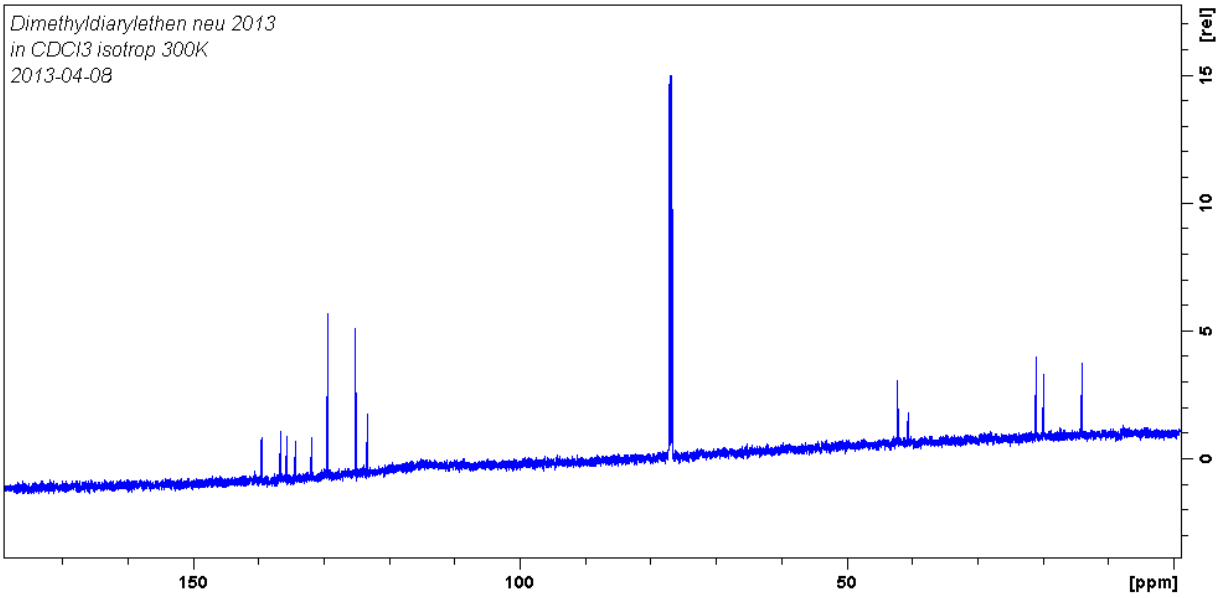


Figure SI- 10: ^{13}C, 300K, isotropic

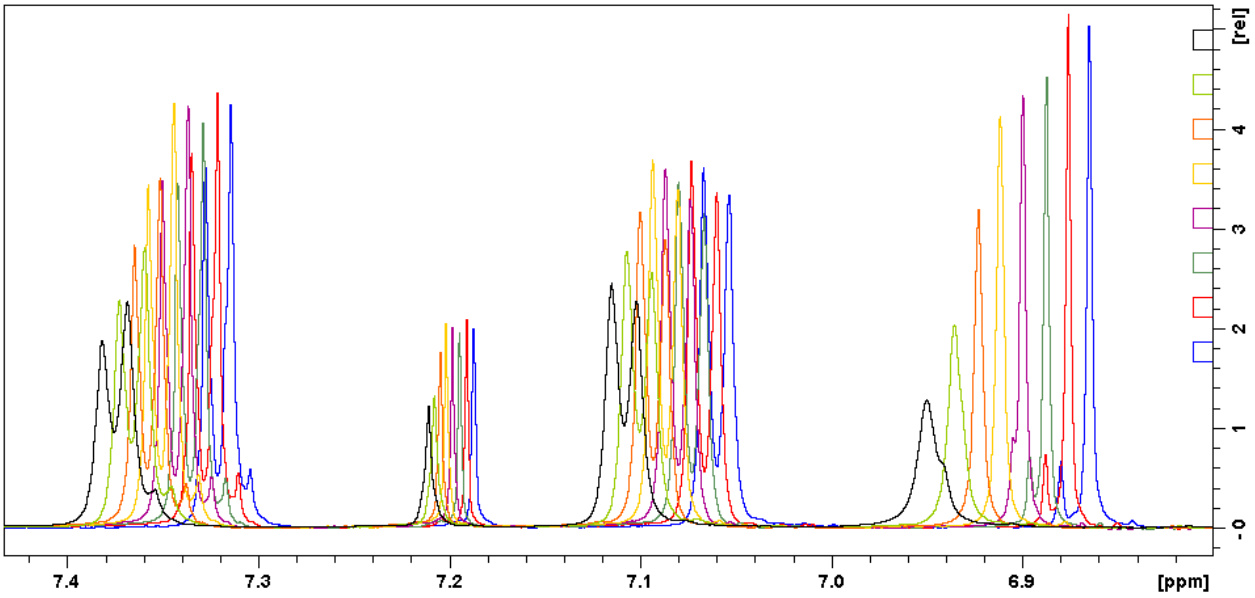


Figure SI- 11: ^{1}H, temperature-shift, from left: 230K (black), 240K (green), 250K (orange), 260K (yellow), 270K (purple), 280K (mint), 290K (red), 300K (blue), isotropic

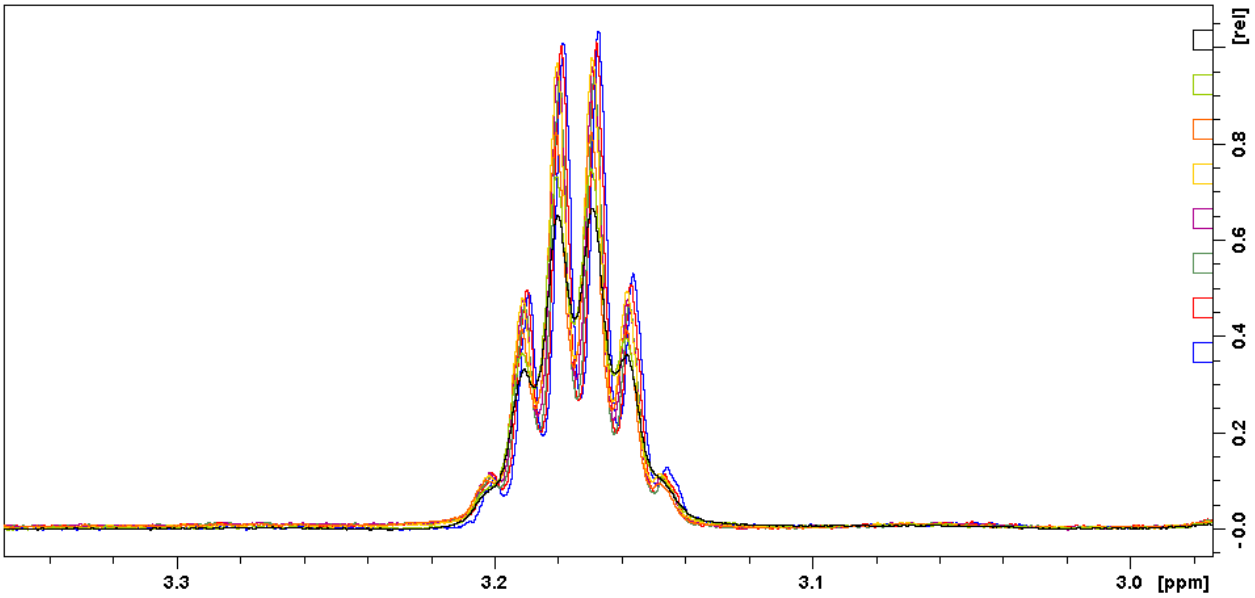


Figure SI- 12: ^{1}H, temperature-shift, aliphatic region

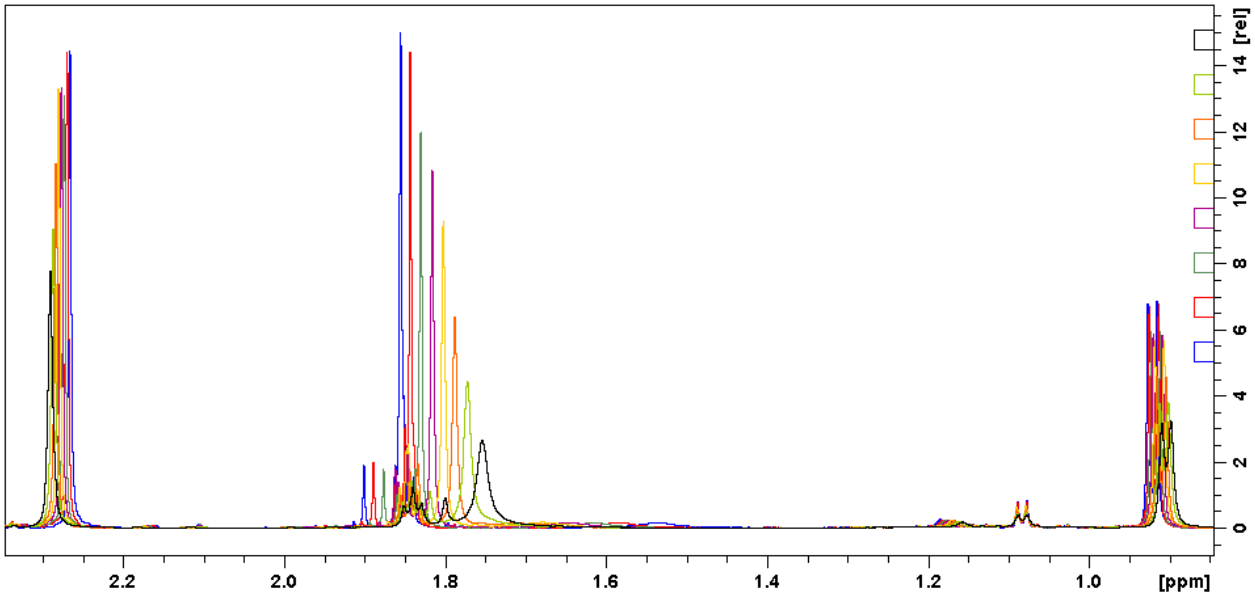


Figure SI- 13: ^{1}H, temperature-shift, aliphatic region

Table SI- 4: Evolution of the ^{1}H chemical shifts of 1o with varying temperature

Position ^{1}H (ppm)	300K	290K	280K	270K	260K	250K	240K	230K
1	1.85	1.85	1.84	1.84	1.85	1.84	1.84	1.84
2	3.17	3.17	3.18	3.17	3.18	3.18	3.18	3.18
3	0.92	0.92	0.92	0.91	0.91	0.91	0.91	0.90
6	6.86	6.88	6.89	6.90	6.91	6.92	6.94	6.95
9	1.85	1.84	1.83	1.82	1.80	1.79	1.77	1.75
11	7.32	7.33	7.34	7.34	7.35	7.36	7.37	7.37
12	7.06	7.07	7.07	7.08	7.09	7.09	7.10	7.11
14	2.27	2.27	2.27	2.28	2.28	2.28	2.29	2.29

Temperature Dependence of NMR Chemical Shifts of 4o

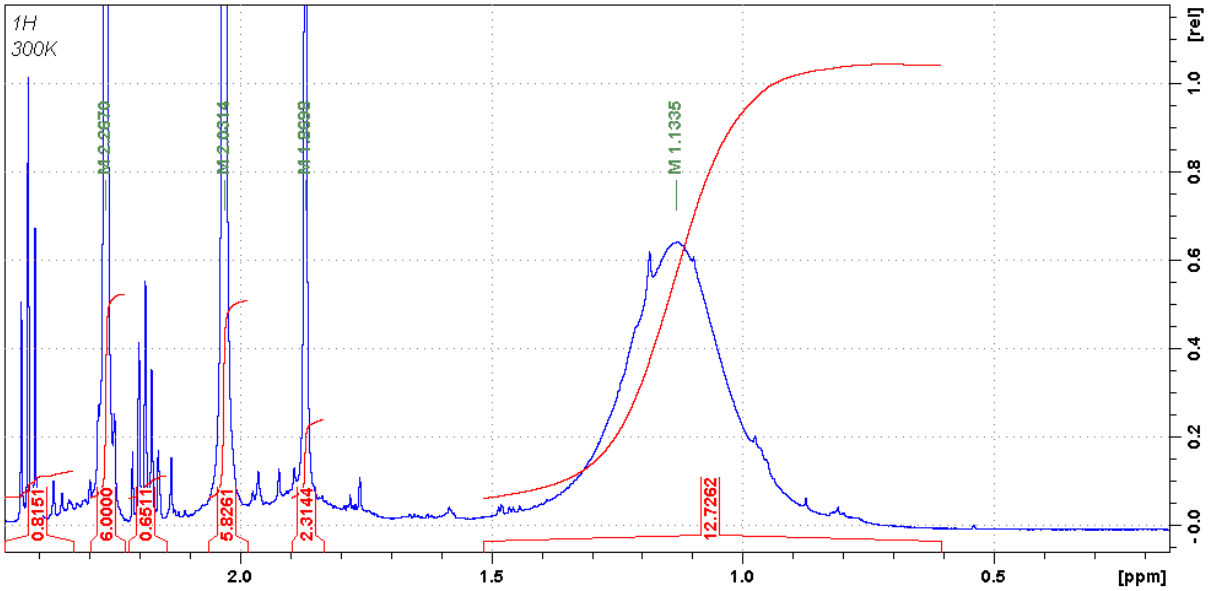
Details for the synthesis and assignment of NMR resonances of the tetramethyl derivative **4o** were previously published in Ref. 1. The ^{1}H signals of the methyl groups at the cyclopentene core show a broad temperature range in which coalescence is observed. Only below 270K are the resonances split into two distinct signal sets (see Table SI- 5 and spectra below).

Table SI- 5: Evolution of the ^{1}H chemical shifts of 4o with varying temperature. Atom numbering is consistent with the scheme given for the dimethylated compound 1o in Figure SI- 8.

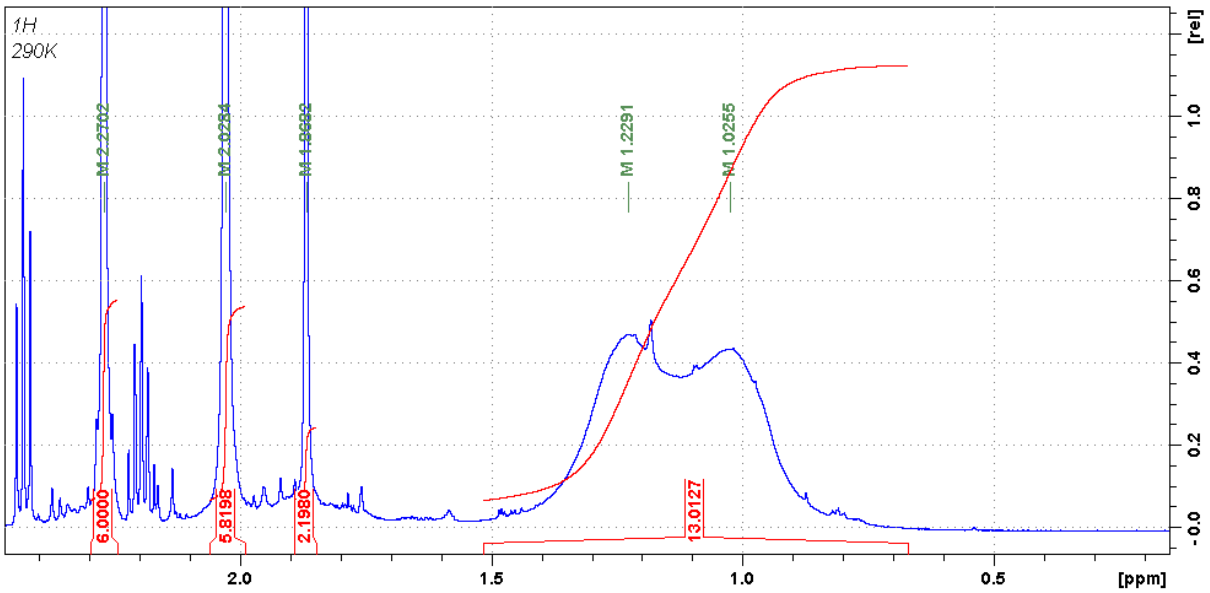
Position ^{1}H (ppm)	300K	290	280	270	260	250	240	230
1	1.87	1.87	1.87	1.86	1.86	1.86	1.86	1.85
3	1.13[a]	1.03[a]	0.98[a]	0.97[a]	0.96	0.96	0.96	0.95
3′	1.13[a]	1.23[a]	1.28[a]	1.29[a]	1.29	1.29	1.29	1.29
6	6.93	6.94	6.94	6.95	6.95	6.96	6.97	6.98
9	2.03	2.03	2.03	2.02	2.02	2.01	2.00	2.00
11	7.32	7.33	7.33	7.34	7.34	7.35	7.36	7.36
12	7.06	7.07	7.07	7.08	7.08	7.09	7.10	7.10
14	2.27	2.27	2.27	2.28	2.28	2.28	2.29	2.29

[a] Peak positions cannot be determined exactly due to coalescence.

300K:



290K: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290K
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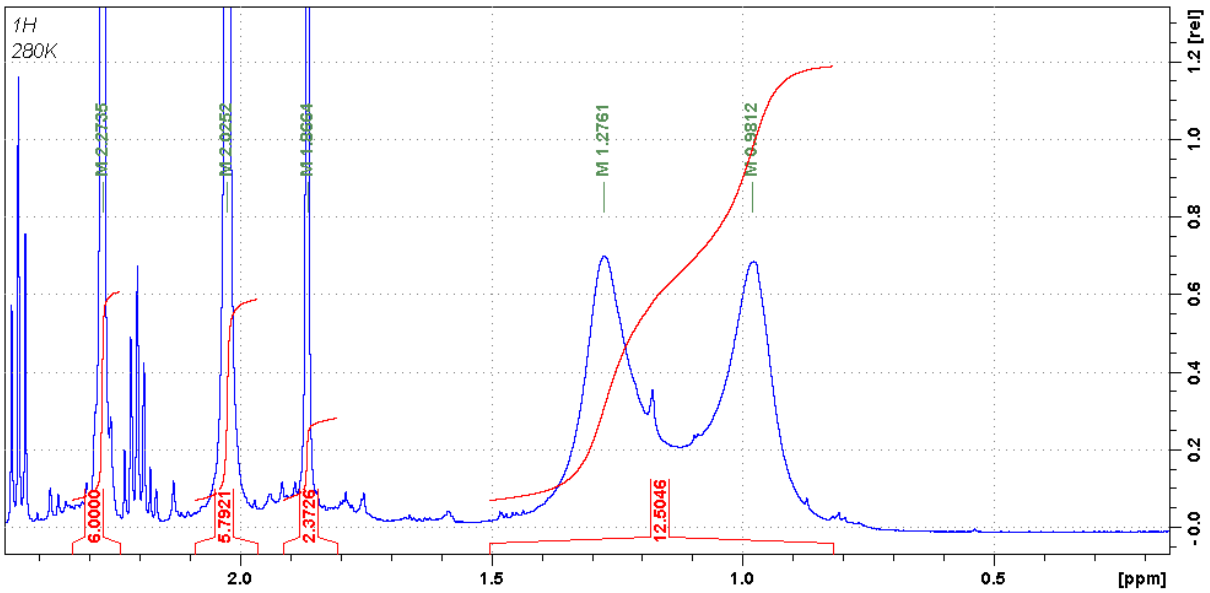
M 2.0284
M 1.8682
M 1.2291
M 1.0255
6.0000
5.8198
2.1980
13.0127
2.0
1.5
1.0
0.5
[ppm]
[rel]
1.0
0.8
0.6
0.4
0.2
-0.0

280K: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M 1.8661
M 1.2761
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12.5046
2.0
1.5
1.0
0.5
[ppm]
[rel]
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1.0
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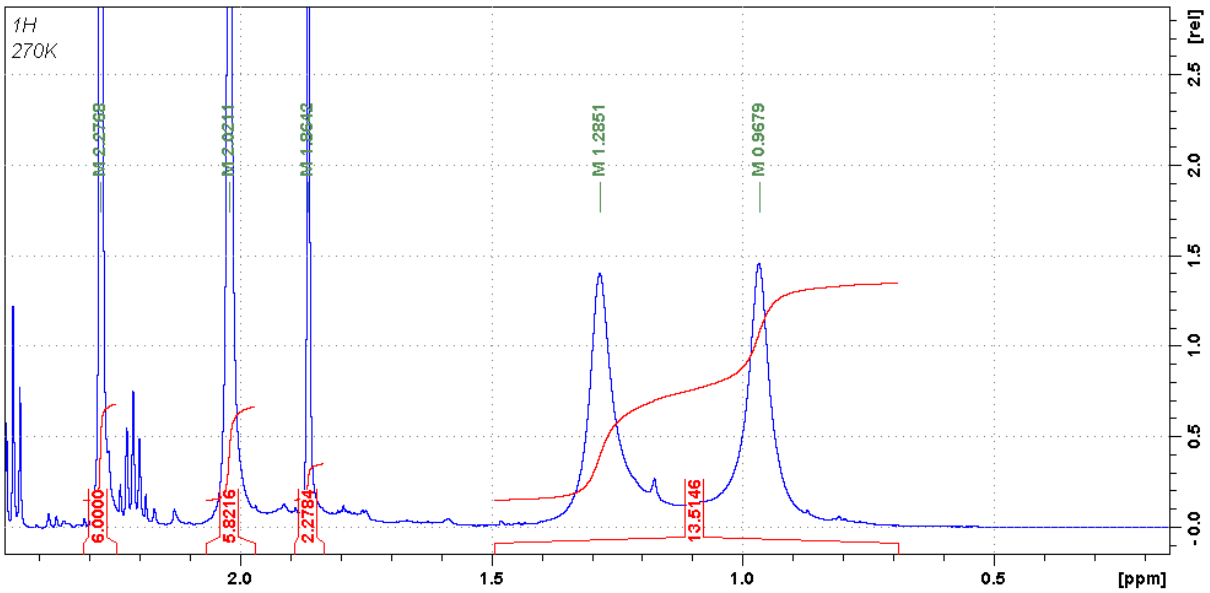
0.6
0.4
0.2
-0.0

270K: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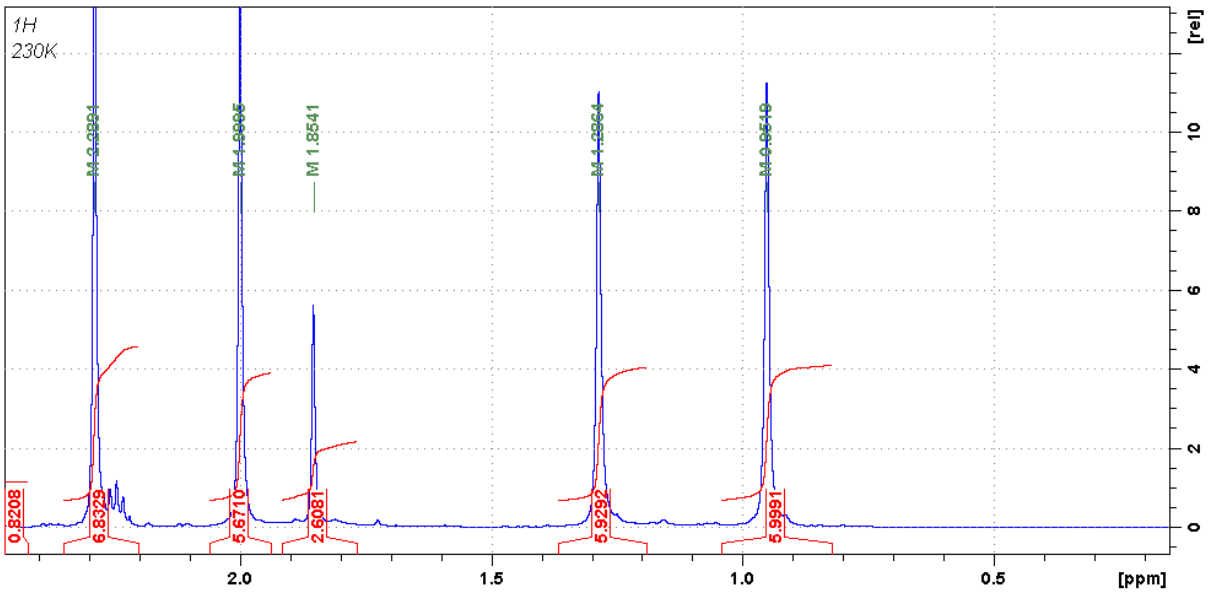
270K
M 2.2768
M 2.0211
M 1.8642
M 1.2851
M 0.9679
6.0000
5.8216
2.2784
13.5146
[rel]
[ppm]

230K:


1H
230K
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M 1.9865
M 1.8541
M 1.2864
M 0.8518
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5.6710
2.6081
5.9292
5.9991
[rel]
[ppm]

Isotropic measurements.

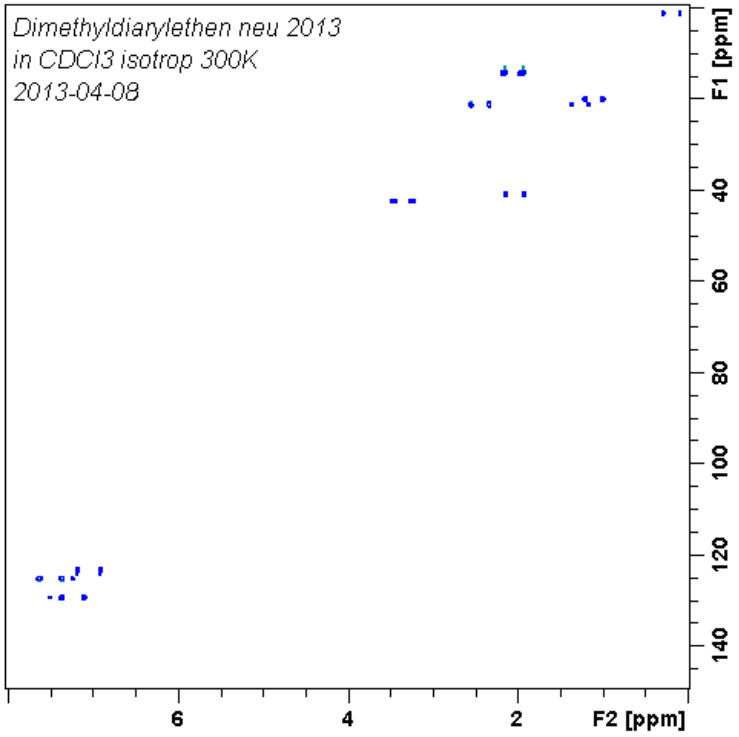

Figure SI- 14: ^{1}H-^{13}C CLIP-HSQC,[18] 300K, INEPT delay optimized for 145 Hz, isotropic

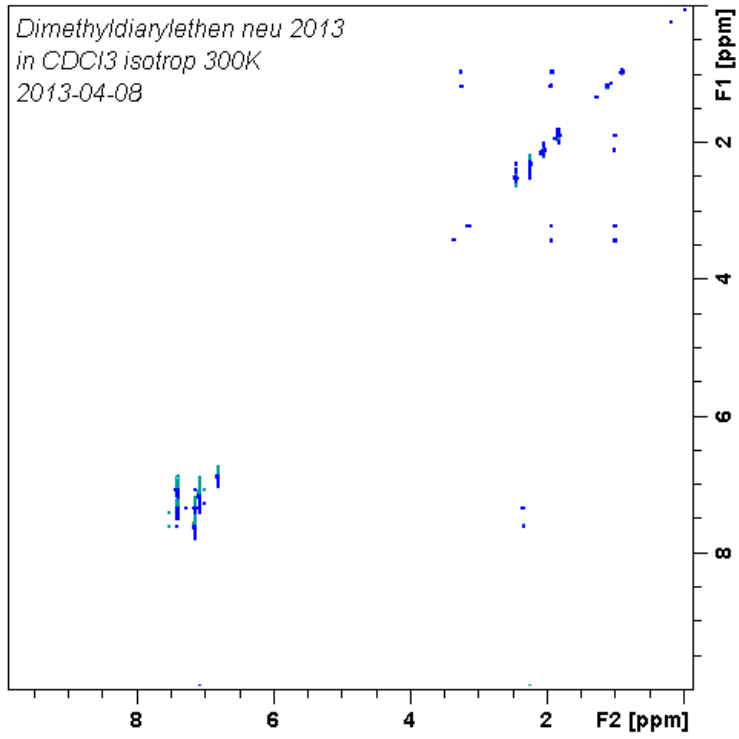

Figure SI- 15: ^{1}H-^{13}C HETLOC,[19,20] 300K, INEPT delay optimized for 145 Hz, TOCSY mixing 60ms, isotropic

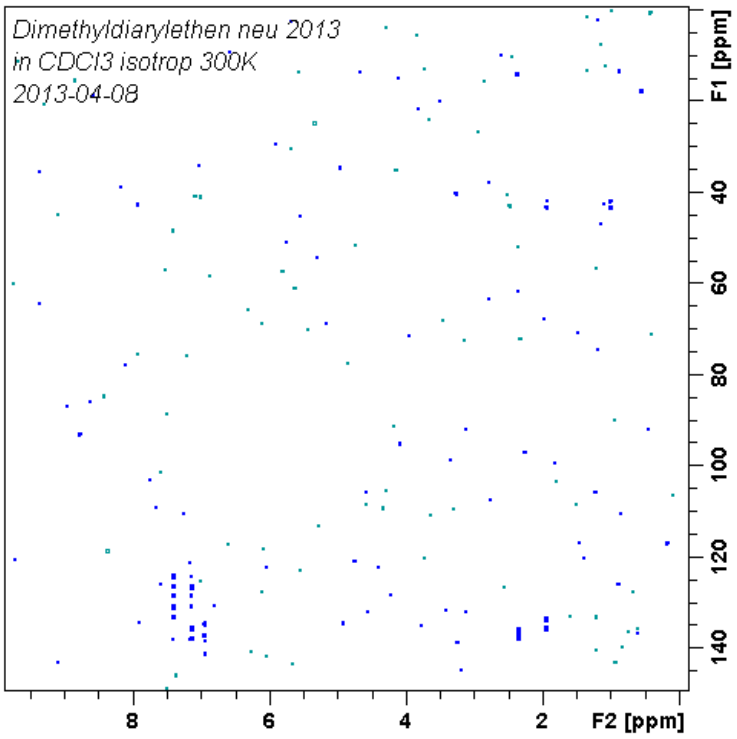

Figure SI- 16: 1,1-ADEQUATE: 2D-HSQC-$^{1}J_{(CC)}$-ADEQUATE,[22] 300K, J(scale) factor = 6 + 1, $J_{(CH)}$ = 155HZ, $J_{(CC)}$ = 55Hz, isotropic

Anisotropic measurements (PBLG-Stick)[14]

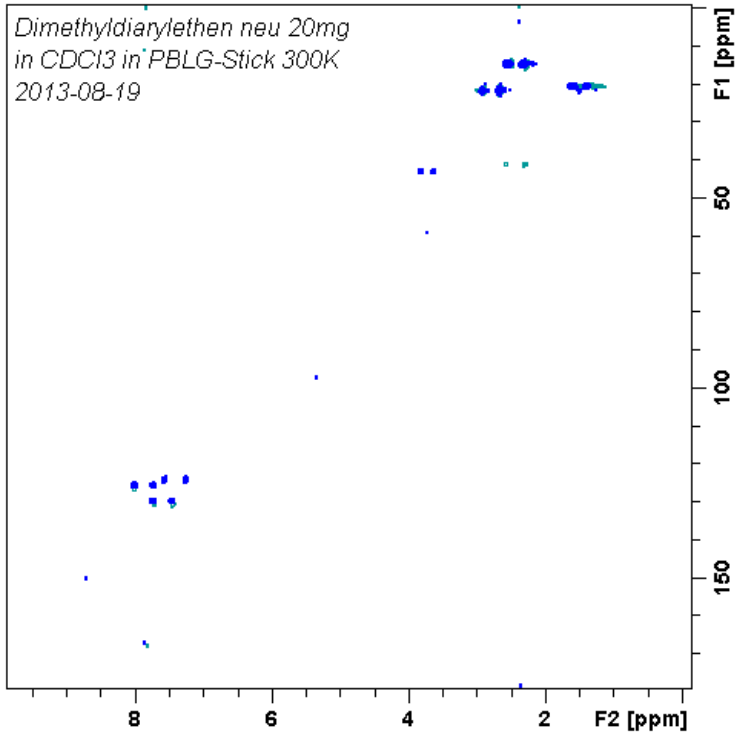

Figure SI- 17: ^{1}H-^{13}C CLIP-HSQC,[18] 300K, INEPT delay optimized for 145 Hz, anisotropic

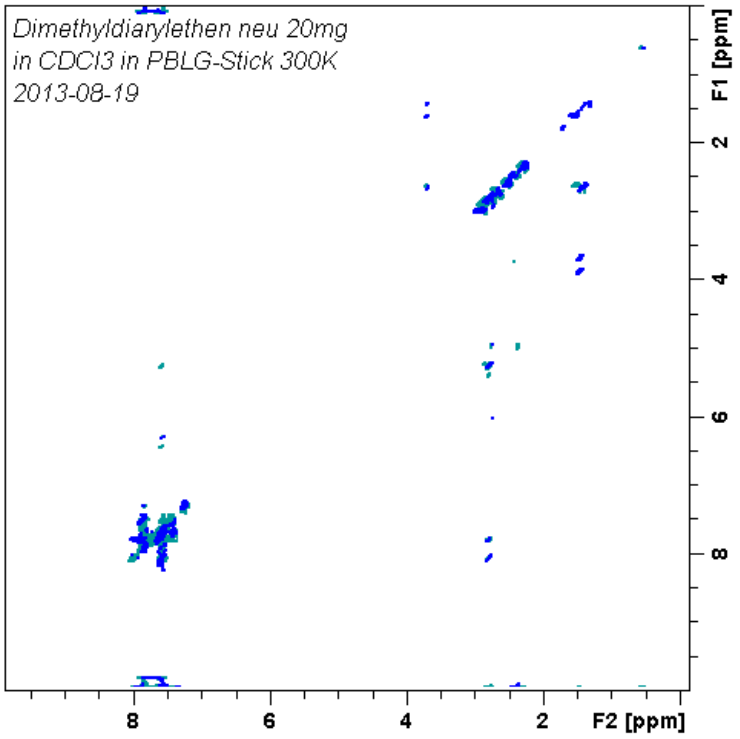

Figure SI- 18: ^{1}H-^{13}C HETLOC,[19,20] 300K, INEPT delay optimized for 145 Hz, TOCSY mixing 60ms, anisotropic

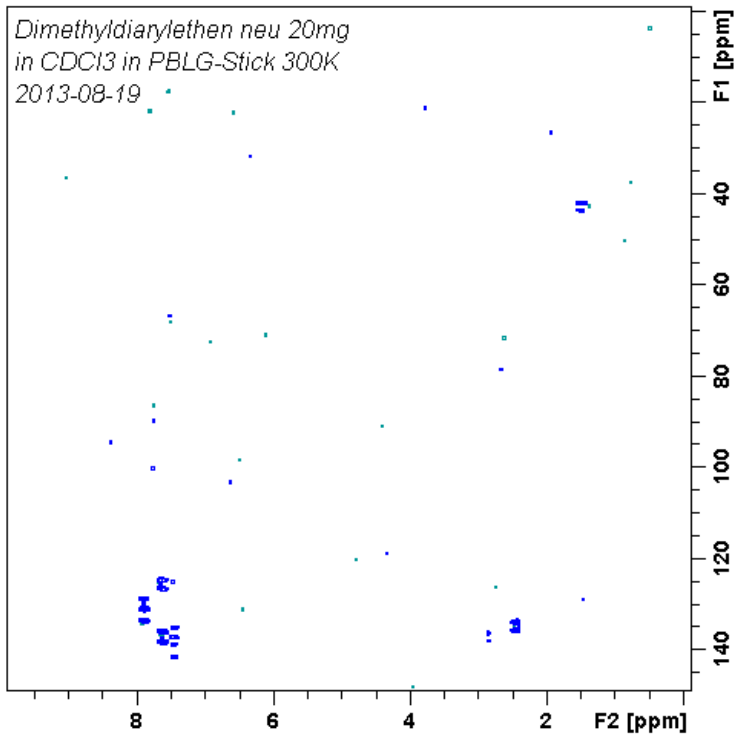

Figure SI- 19: 1,1-ADEQUATE: 2D-HSQC-$^{1}J_{(CC)}$-ADEQUATE,[22,21] 300K, J(scale) factor = 6 + 1, $J_{(CH)}$ = 155HZ, $J_{(CC)}$ = 55Hz, anisotropic

Anisotropic measurements (Polyacetylene)[15]

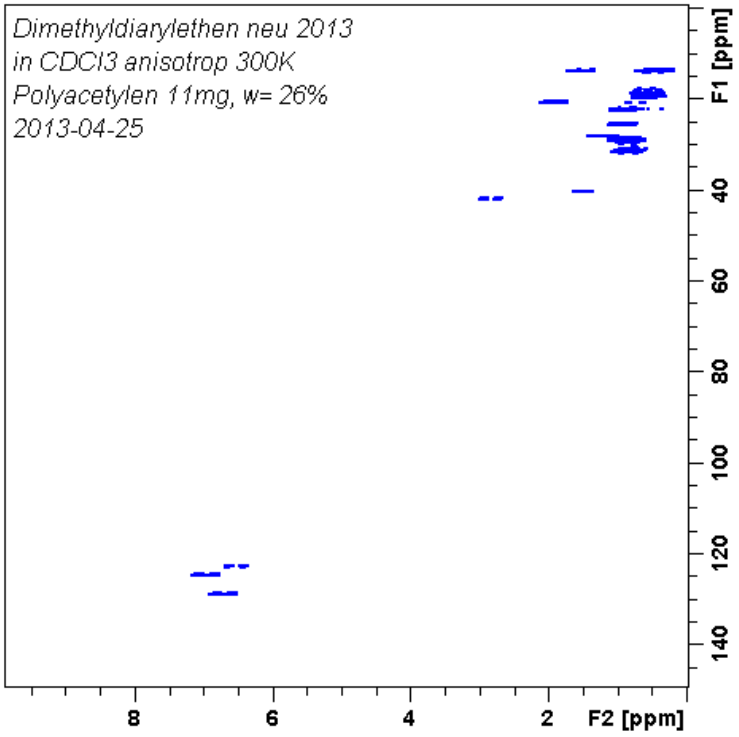

Figure SI- 20: ^{1}H-^{13}C CLIP-HSQC,[18] 300K, INEPT delay optimized for 145 Hz, anisotropic

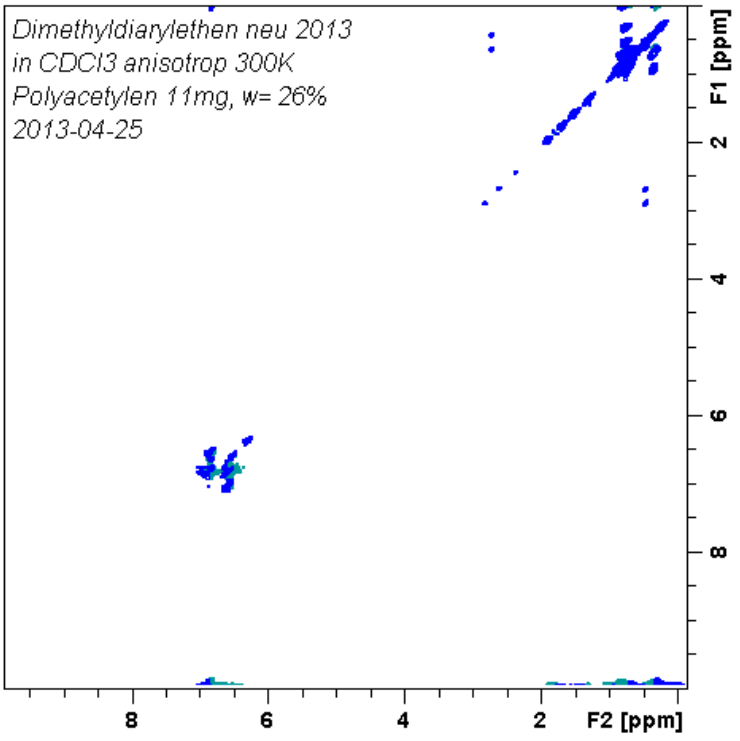

Figure SI- 21: ^{1}H-^{13}C HETLOC,[19,20] 300K, INEPT delay optimized for 145 Hz, TOCSY mixing 60ms, anisotropic

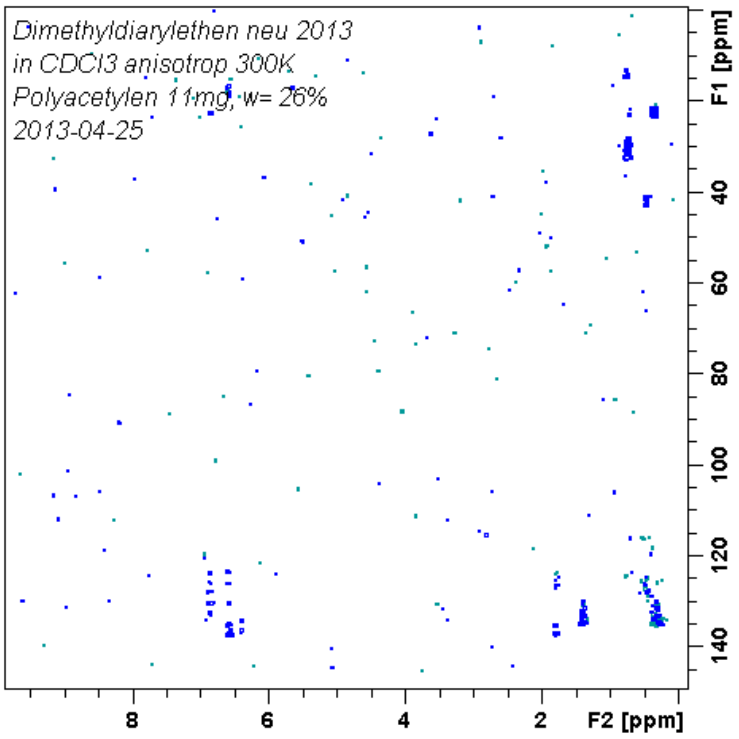

Figure SI- 22: 1,1-ADEQUATE: 2D-HSQC-$^{1}J_{(CC)}$-ADEQUATE,[22,21] 300K, J(scale) factor = 6 + 1, $J_{(CH)}$ = 155HZ, $J_{(CC)}$ = 55Hz, anisotropic

Structure Generation, Resulting Geometries and Molecular Order Tensor Calculation.

The Macromodel module (MacroModel, version 9.9, Schrödinger, LLC, New York, NY, 2012) of the program package Maestro (Maestro, version 9.3, Schrödinger, LLC, New York, NY, 2012) was used for conformational analysis. The OPLS_2005 force field[23] with chloroform as implicit solvent was applied for a "Mixed Torsional/Low mode sampling" approach. Entirely 700 calculation steps were carried out in this method followed by a Polak-Ribiere-type conjugate gradient (PRCG) energy minimization with up to 2000 iteration steps. After RMSD-based clustering (cutoff = 0.5 Ångström) to remove duplicate conformations, 31 unique conformations were obtained in a relative potential OPLS-2005 energy window <20 kJ/mol.

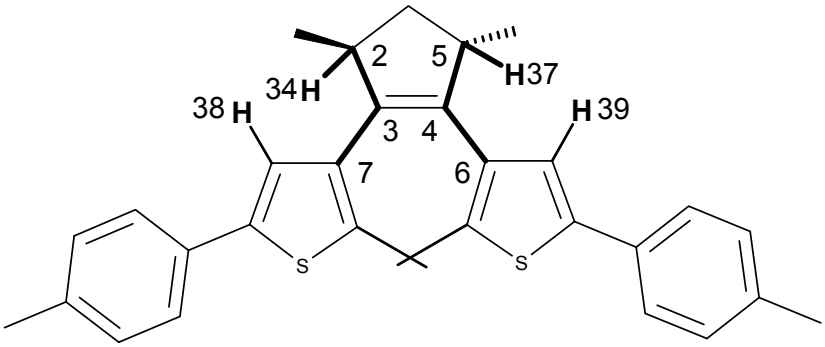

Figure SI- 23: Graphical display of determined torsion angles [°] and inter-proton-distances [Å] (bold) of 1o conformers, open form

Table SI- 6: Results of the conformational analysis of 1o. Blue: geometries used in the RDC and NOE analysis. Red: convergence criteria not fulfilled. Black: conformations redundant to Conf01/05/12/17/19/21/25/26

Conformer	Potential Energy [kJ/ mol]	Minimization Converged	Times Found	Torsion-angle [°] 34/2/3/7 and 37/5/4/6	Interproton distance [Å] 34/38 and 37/39
Conf01 a-p mixed (C)	36.6	True	56	54.8; 79.0	4.71; 4.82
Conf02	37.4	True	69	51.4; 81.3	2.52; 4,82
Conf03	37.5	True	39	51.6; 81.3	2.51; 4.82
Conf04	37.8	True	31	54.4; 79.7	4.67; 4.81
Conf05 a-p mixed (C´)	38.0	True	38	79.1; 55.6	4.80; 4.72
Conf06	38.2	True	36	51.5; 81.6	2.51; 4.81
Conf07	38.3	False	1	--	--
Conf08	38.4	True	35	54.9; 79.8	4.68; 4.80
Conf09	38.5	True	49	51.6; 81.4	2.49; 4.81

Conf10	39.2	False	1	--	--
Conf11	39.2	False	2	--	--
Conf12 parallel (D)	39.3	True	29	75.1; 58.8	2.66; 4.75
Conf13	39.3	True	31	75.7; 58.1	2.67; 4.74
Conf14	39.3	False	2	--	--
Conf15	39.4	False	1	--	--
Conf16	40.0	True	21	75.7; 58.0	2.68; 4.73
Conf17 parallel (D´)	40.4	True	49	57.1; 76.5	4.72; 2.68
Conf18	41.3	False	2	--	--
Conf19 a-p(P*,S*,S*) (A)	41.7	True	26	79.2; 53.1	2.71; 2.49
Conf20	41.9	True	24	79.2; 53.2	2.71; 2.49
Conf21 a-p(P*,S*,S*) (A´)	41.9	True	33	53.1; 79.3	2.48; 2.71
Conf22	42.2	True	21	53.0; 79.2	2.48; 2.70
Conf23	48.6	True	25	75.8; 45.6	4.10; 3.77
Conf24	48.9	True	16	75.7; 45.8	4.11; 3.80
Conf25 a-p(M*,S*,S*) (B)	49.0	True	24	75.7; 45.8	4.10; 3.78
Conf26 a-p(M*,S*,S*) (B´)	49.3	True	21	45.7; 75.7	3.77; 4.10
Conf27	51.8	False	5	--	--
Conf28	52.2	False	3	--	--
Conf29	53.2	False	1	--	--
Conf30	53.6	False	2	--	--
Conf31	54.3	False	1	--	--

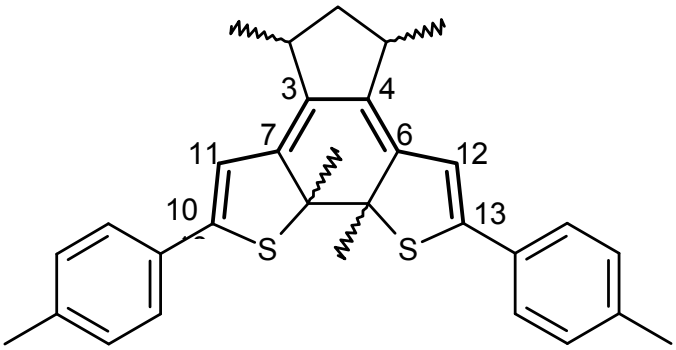

Figure SI- 24: Graphical display of determined torsion angles [°] (bold) of conformers, ring closed form (1c1 and 1c2)

Table SI- 7: Measured torsion angles [°] of computed conformers, closed forms. Configuration SSSS (1c2) corresponds to conformers 25 and 26 (a-p(M*,S*,S*) in Table SI- 6, configuration RRSS (1c1) to conformers 19 and 21 (a-p(P*,S*,S*).

Torsion	*SSSS [°]* **1c2**	*RRSS [°]* **1c1**
10-11-7-3	-162.8	-163.9
11-7-3-4	175.0	173.0
7-3-4-6	-21.2	-15.4
3-4-6-12	175.9	171.3
4-6-12-13	-162.7	-164.5

RDC fits with hotFCHT

Experimental RDCs are fitted using the SVD-based approach outlined by Losonczi et al.,[24] as implemented in a self-written module of the software hotFCHT.[25,26] Based on proposed geometries, an alignment tensor is calculated, and used to back calculate the RDCs. The comparison of the experimental and back calculated RDCs give quality factors, showing the goodness-of-fit.[27] Derived parameters describing the magnitude, eigenvalues and orientation of the alignment tensor[28] are also given below.

Through a user controlled flag an automated normalization of RDCs before SVD can be performed within hotFCHT. The weighting factor is determined by normalizing the magnetogyric ratios γ and distances r of each coupling to the respective values of the largest coupling. Each row of the coefficient matrix is multiplied by the weighing factor w_i of the respective coupling before SVD, and then renormalized after the alignment tensor is calculated.

$$w_i = \left| \frac{max\left(\frac{\gamma_j \gamma_k}{r^3}\right)}{\frac{\gamma_{i,j}\gamma_{i,k}}{r_i^3}} \right|$$

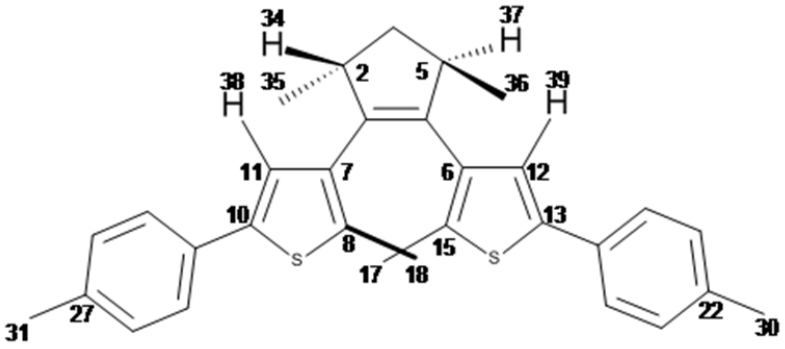

Figure SI- 25: Atom numbering of 1o. Atom numbers are corresponding to the atom id's of the cartesian coordinates of calculated structure models (see p34).

Table SI- 8: Single-Conformer-Single-Tensor fits of experimental RDCs to the calculated models in PBLG-Stick. Weighting-factor of each shown coupling is 1.00.

Conformer:		01 C	05 C′	12 D	17 D′	19 A	21 A′	25 B	26 B′
RDC	D_{exp} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]
C2-H34	-8.44	0.56	-8.24	-3.43	-7.64	-1.61	-15.64	-1.88	-11.09
(C5-H37)		-7.98	1.11	-8.27	-2.76	-15.63	-1.60	-11.14	-1.93
C11-H38	10.98	8.05	6.56	8.82	5.85	7.49	9.89	9.62	7.30
(C12-H39)		7.82	9.14	6.46	8.84	9.90	7.47	7.34	9.63
C35-H34	3.18	-1.16	0.75	-0.48	-1.14	2.05	1.42	-0.37	0.20
(C36-H37)		0.68	-1.12	-1.17	-0.35	1.43	2.03	0.20	-0.36
C2-C35	1.64	0.82	2.99	1.30	0.66	0.19	1.53	-1.48	-0.03
(C5-C36)		2.98	0.87	0.79	1.45	1.52	0.17	-0.03	-1.46
C8-C18	-1.56	-2.43	-1.13	-0.26	-3.55	-1.33	-1.16	-0.36	-0.47
(C15-C17)		-0.98	-2.28	-3.44	-0.21	-1.15	-1.32	-0.47	-0.34
C27-C31	-2.70	-2.90	-2.24	-1.09	-3.24	-1.30	-2.24	0.00	-0.78
(C22-C30)		-2.39	-2.86	-3.42	-1.18	-2.25	-1.29	-0.79	0.06

C11-C7 (C12-C6)	-3.05	-3.47 -2.05	-2.12 -3.36	-0.74 -4.51	-4.52 -0.74	-1.92 -2.31	-2.33 -1.91	-0.41 -0.94	-0.94 -0.40
C11-C10 (C12-C13)	-1.29	0.81 -1.85	-1.47 0.67	-0.70 1.64	2.21 -1.11	1.73 -0.56	-0.57 1.74	2.39 0.45	0.44 2.35
Quality Factor Q		0.54	0.57	0.49	0.52	0.54	0.54	0.55	0.55
Condition Number		7.74	6.91	7.33	7.18	5.96	5.99	4.56	4.54
Tensor Magnitude GDO ($*10^{-3}$)		2.25	2.22	1.82	1.85	1.31	1.31	1.40	1.39
Axial Component Da ($*10^{-3}$)		-1.06	-1.05	0.86	0.87	0.64	0.64	0.62	0.62
Rhombic Component Dr ($*10^{-3}$)		-0.41	-0.41	0.33	0.37	0.10	0.10	0.37	0.37
Tensor	α(°)	170.8	172.0	22.3	17.5	-129.7	49.0	0.9	0.9
	β(°)	67.4	66.9	52.0	54.2	95.1	95.0	79.6	79.6
Euler-Angles	γ(°)	170.7	172.1	66.0	63.9	165.6	165.7	169.5	169.6

Table SI- 9: Single-Conformer-Single-Tensor fits of experimental RDCs to the calculated models in Polyacetylene. Weighting-factor of each shown coupling is 1.00.

Conformer:		01 C	05 C′	12 D	17 D′	19 A	21 A′	25 B	26 B′
RDC	D_{exp} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]
C2-H34	-2.85	-6.00	-2.52	-4.13	-3.14	-4.91	-1.01	-6.64	-0.43
(C5-H37)		-2.58	-6.52	-2.84	-4.18	-1.01	-4.89	-0.41	-6.60
C11-H38	-13.70	-13.05	-10.64	-13.06	-12.21	-12.39	-13.41	-12.81	-11.00
(C12-H39)		-11.58	-13.54	-12.51	-13.08	-13.41	-12.39	-10.97	-12.82
C35-H34	-0.99	0.52	0.10	1.48	0.90	1.24	-0.26	-0.02	-1.21
(C36-H37)		0.17	0.44	0.93	1.47	-0.28	1.26	-1.21	-0.02
C2-C35	0.19	-0.18	-1.09	0.50	0.26	2.32	0.77	1.89	0.36
(C5-C36)		-1.11	-0.23	0.18	0.41	0.77	2.32	-0.37	1.88
C8-C18	0.04	1.74	-0.24	-0.60	2.04	-0.15	-0.28	0.06	0.36
(C15-C17)		-0.38	1.55	1.85	-0.62	-0.28	-0.15	0.35	0.05
C27-C31	0.94	2.34	0.87	-0.07	2.46	-0.21	0.55	-0.44	1.79
(C22-C30)		0.93	2.27	2.42	-0.01	0.59	-0.22	1.79	-0.49
C11-C7	1.63	2.73	0.39	-0.46	2.99	-0.02	0.30	0.00	1.46
(C12-C6)		0.31	2.56	2.86	-0.44	0.31	-0.03	1.45	-0.01
C11-C10	-0.36	-1.02	1.09	-0.48	-1.18	-2.18	-0.08	-3.10	1.52
(C12-C13)		1.38	-0.78	-0.76	-0.21	-0.10	-2.17	1.53	-3.08
Quality Factor Q		0.28	0.30	0.25	0.26	0.27	0.27	0.35	0.34
Condition Number		11.39	11.26	7.13	8.55	8.96	8.81	6.76	6.86
Tensor Magnitude GDO($*10^{-3}$)		1.41	1.35	1.27	1.27	1.43	1.41	1.56	1.56
Axial Component Da($*10^{-3}$)		0.63	0.60	-0.62	-0.61	-0.66	-0.65	-0.75	-0.75
Rhombic Component Dr($*10^{-3}$)		0.36	0.35	-0.13	-0.18	-0.30	-0.30	-0.23	-0.23
Tensor	α(°)	160.3	20.8	-17.2	7.1	2.6	-177.5	-5.8	-167.9
	β(°)	81.0	81.1	41.6	92.3	59.9	58.8	74.4	72.2
Euler-Angles	γ(°)	168.0	-174.0	83.1	-124.4	166.3	-172.8	155.5	-157.9

Table SI- 10: Multi-Conformer-Single-Tensor fits of experimental RDCs to the calculated models in PBLG-Stick. Dcalc values are shown at 50% of each conformer. Weighting-factor of each shown coupling is 1.00.

Conformer ensemble (50:50):		01-05 C/C′	12-17 D/D′	19-21 A/A′	25-26 B/B′
RDC	D_{exp} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]
C2-H34 (C5-H37)	-8.44	-6.39	-4.11	-8.73	-7.44
		-6.12	-4.08	-8.72	-7.48
C11-H38 (C12-H39)	10.98	9.16	8.97	11.16	10.69
		10.48	8.67	11.16	10.71
C35-H34 (C36-H37)	3.18	-1.16	0.14	3.34	0.07
		-1.23	0.21	3.34	0.06
C2-C35 (C5-C36)	1.64	1.68	2.10	1.82	-0.81
		1.72	2.22	1.82	-0.80
C8-C18 (C15-C17)	-1.56	-2.18	-2.18	-1.45	-0.40
		-2.00	-2.22	-1.44	-0.39
C27-C31 (C22-C30)	-2.70	-2.87	-2.93	-2.44	-0.40
		-2.92	-3.13	-2.44	-0.39
C11-C7 (C12-C6)	-3.05	-3.27	-3.27	-2.73	-0.72
		-3.18	-3.38	-2.71	-0.71
C11-C10 (C12-C13)	-1.29	0.14	-0.00	0.08	1.69
		-0.26	-0.35	0.07	1.64
Quality Factor Q		0.35	0.39	0.10	0.40
Condition Number		7.29	5.84	5.57	4.44
Tensor Magnitude GDO(*10^{-3})		2.50	2.59	1.69	1.63
Axial Component Da(*10^{-3})		-1.23	1.19	0.79	0.73
Rhombic Component Dr(*10^{-3})		-0.28	0.58	0.32	0.41
Tensor α(°)		0.4	22.1	-87.8	3.2
β(°)		70.2	62.0	97.0	79.9
Euler-Angles γ(°)		176.5	65.0	178.4	179.0

Table SI- 11: Multi-Conformer-Single-Tensor fits of experimental RDCs to the calculated models in Polyacetylen. DCalc values are shown at 50% of each Conformer. Weighting-factor of each shown coupling is 1.00.

Conformer ensemble (50:50):		01-05 C/C′	12-17 D/D′	19-21 A/A′	25-26 B/B′
RDC	D_{exp} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]	D_{calc} [Hz]
C2-H34 (C5-H37)	-2.85	-3.26	-3.69	-2.70	-2.94
		-3.45	-3.77	-2.71	-2.88
C11-H38 (C12-H39)	-13.70	-12.96	-13.10	-13.74	-13.69
		-13.65	-13.03	-13.74	-13.68
C35-H34 (C36-H37)	-0.99	0.73	-0.24	-1.34	-0.83
		0.77	-0.25	-1.34	-0.82
C2-C35 (C5-C36)	0.19	-0.42	-0.89	0.27	0.74
		-0.45	-0.93	0.27	0.73
C8-C18 (C15-C17)	0.04	0.79	1.04	-0.00	0.12
		0.70	1.07	-0.01	0.11
C27-C31 (C22-C30)	0.94	1.64	1.97	0.84	0.63
		1.71	2.09	0.84	0.61
C11-C7 (C12-C6)	1.63	1.61	1.97	0.73	0.67
		1.59	2.04	0.72	0.66
C11-C10 (C12-C13)	-0.36	-0.10	-0.02	-0.38	-0.96
		0.15	0.14	-0.39	-0.90
Quality Factor Q		0.16	0.16	0.07	0.09
Condition Number		11.13	6.59	7.45	6.68
Tensor Magnitude GDO(*10^{-3})		1.34	1.66	1.21	1.38
Axial Component Da(*10^{-3})		0.64	-0.79	-0.60	-0.68
Rhombic Component Dr(*10^{-3})		0.21	-0.27	-0.01	-0.13
Tensor α(°)		1.8	-1.2	176.6	3.1
β(°)		80.2	62.6	103.2	72.8
Euler-Angles γ(°)		176.6	65.4	-2.4	178.5

Cartesian coordinates of conformers after Eckart transformation:

File name: DMDAE_conf01-conf05.fcht.sp.rdc
Calculations for Structure: **conf1 (C)** (single conformer, single tensor fit)
Coordinates /(AA): (origin shifted to center of mass, reference structure of the Eckart frame)

1	C1	-0.253	5.296	0.197
2	C2	-1.363	4.361	-0.313
3	C3	-0.769	2.975	-0.162
4	C4Ring	0.559	3.027	0.052
5	C5Ring	1.038	4.460	0.183
6	C6	1.421	1.856	0.317
7	C7	-1.552	1.738	-0.359
8	C8	-2.714	1.452	0.316
9	S	-3.319	-0.111	-0.173
10	C10	-1.977	-0.358	-1.270
11	C11	-1.127	0.718	-1.260
12	C12	1.043	0.825	1.226
13	C13	1.973	-0.181	1.289
14	S	3.333	0.149	0.237
15	C15	2.626	1.649	-0.309
16	C16	1.925	-1.416	2.068
17	C17	3.319	2.489	-1.331
18	C18	-3.437	2.250	1.351
19	C19	-1.862	-1.602	-2.028
20	C20	0.680	-2.001	2.389
21	C21	0.612	-3.188	3.144
22	C22	1.794	-3.806	3.598
23	C23	3.042	-3.230	3.286
24	C24	3.105	-2.044	2.528
25	C25	-3.006	-2.336	-2.419
26	C26	-2.880	-3.529	-3.158
27	C27	-1.604	-4.007	-3.517
28	C28	-0.458	-3.281	-3.137
29	C29	-0.589	-2.088	-2.400
30	C30	1.723	-5.084	4.409
31	C31	-1.466	-5.290	-4.313
32	H1	-0.159	6.209	-0.392
33	H2	-0.490	5.600	1.218
34	H3	-2.237	4.466	0.328
35	C4Methyl	-1.767	4.652	-1.767
36	C5Methyl	1.930	4.704	1.412
37	H6	1.611	4.692	-0.714
38	H7	-0.226	0.806	-1.849
39	H8	0.117	0.852	1.781
40	H9	2.619	2.836	-2.091
41	H10	4.104	1.925	-1.836
42	H11	3.781	3.362	-0.868
43	H12	-4.074	1.611	1.963
44	H13	-4.071	3.003	0.884
45	H14	-2.738	2.754	2.018
46	H15	-0.236	-1.545	2.042
47	H16	-0.352	-3.620	3.371
48	H17	3.957	-3.694	3.627
49	H18	4.071	-1.615	2.309
50	H19	-3.993	-1.984	-2.162
51	H20	-3.768	-4.072	-3.447
52	H21	0.527	-3.635	-3.406
53	H22	0.301	-1.549	-2.109
54	H23	1.722	-5.950	3.746
55	H24	0.816	-5.112	5.013
56	H25	2.577	-5.168	5.081
57	H26	-1.472	-5.072	-5.381
58	H27	-2.287	-5.973	-4.097
59	H28	-0.533	-5.799	-4.071
60	H27	-2.537	3.958	-2.106
61	H28	-0.915	4.559	-2.442
62	H29	-2.166	5.661	-1.869
63	H30	2.215	5.754	1.485
64	H31	2.848	4.118	1.363
65	H32	1.416	4.433	2.335

File name: DMDAE_conf01-conf05.fcht.sp.rdc

Calculations for Structure: **conf5 (C´)** (single conformer, single tensor fit)
Coordinates /(AA): (origin shifted to center of mass, and transformed to Eckart frame)

1	C1	-0.077	5.252	-0.350
2	C2	-1.306	4.330	-0.285
3	C3	-0.726	2.940	-0.117
4	C4Ring	0.605	2.986	0.078
5	C5Ring	1.103	4.414	0.171
6	C6	1.472	1.814	0.316
7	C7	-1.510	1.706	-0.330
8	C8	-2.670	1.427	0.349
9	S	-3.303	-0.117	-0.160
10	C10	-1.975	-0.366	-1.278
11	C11	-1.106	0.696	-1.252
12	C12	1.120	0.802	1.258
13	C13	2.051	-0.202	1.320
14	S	3.377	0.100	0.217
15	C15	2.656	1.589	-0.343
16	C16	2.031	-1.414	2.138
17	C17	3.325	2.396	-1.406
18	C18	-3.372	2.231	1.394
19	C19	-1.910	-1.581	-2.092
20	C20	0.798	-1.967	2.552
21	C21	0.757	-3.129	3.347
22	C22	1.954	-3.756	3.745
23	C23	3.190	-3.210	3.344
24	C24	3.226	-2.049	2.548
25	C25	-1.168	-1.589	-3.295
26	C26	-1.087	-2.750	-4.089
27	C27	-1.749	-3.928	-3.689
28	C28	-2.487	-3.935	-2.489
29	C29	-2.565	-2.771	-1.699
30	C30	1.914	-5.004	4.602
31	C31	-1.660	-5.179	-4.539
32	H1	0.122	5.535	-1.385
33	H2	-0.224	6.177	0.209
34	H3	-1.878	4.550	0.617
35	C4Methyl	-2.237	4.471	-1.501
36	C5Methyl	1.510	4.782	1.606
37	H6	1.957	4.557	-0.490
38	H7	-0.207	0.783	-1.843
39	H8	0.212	0.847	1.841
40	H9	2.595	2.818	-2.097
41	H10	4.013	1.782	-1.988
42	H11	3.897	3.214	-0.968
43	H12	-2.663	2.641	2.114
44	H13	-4.088	1.621	1.945
45	H14	-3.917	3.061	0.943
46	H15	-0.130	-1.504	2.249
47	H16	-0.198	-3.534	3.648
48	H17	4.116	-3.677	3.646
49	H18	4.184	-1.644	2.260
50	H19	-0.657	-0.697	-3.622
51	H20	-0.513	-2.730	-5.004
52	H21	-2.993	-4.833	-2.166
53	H22	-3.129	-2.808	-0.780
54	H23	2.768	-5.649	4.393
55	H24	1.006	-5.579	4.413
56	H25	1.937	-4.736	5.659
57	H26	-2.563	-5.783	-4.439
58	H27	-0.807	-5.783	-4.231
59	H28	-1.540	-4.927	-5.593
60	H27	-3.112	3.826	-1.409
61	H28	-1.725	4.203	-2.425
62	H29	-2.596	5.495	-1.601
63	H30	1.840	5.819	1.667
64	H31	2.332	4.155	1.953
65	H32	0.678	4.654	2.300

File name: DMDAE_conf12-conf17.fcht.sp
Calculations for Structure: **conf12 (D)** (single conformer, single tensor fit)
Coordinates /(AA): (origin shifted to center of mass, reference structure of the Eckart frame)

1	C1	-1.186	4.794	1.182

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2   C2           0.098      3.947      1.202
3   C3          -0.389      2.520      1.073
4   C4Ring      -1.714      2.466      0.840
5   C5Ring      -2.306      3.854      0.700
6   C6          -2.484      1.231      0.583
7   C7           0.498      1.362      1.293
8   C8           0.294      0.389      2.242
9   S            1.559     -0.808      2.146
10  C10          2.363      0.050      0.845
11  C11          1.673      1.188      0.509
12  C12         -2.003      0.214     -0.295
13  C13         -2.855     -0.856     -0.376
14  S           -4.270     -0.610      0.625
15  C15         -3.692      0.944      1.172
16  C16         -2.693     -2.094     -1.137
17  C17         -4.483      1.734      2.162
18  C18         -0.793      0.260      3.259
19  C19          3.596     -0.479      0.260
20  C20         -3.809     -2.826     -1.602
21  C21         -3.636     -4.013     -2.342
22  C22         -2.340     -4.485     -2.630
23  C23         -1.220     -3.760     -2.176
24  C24         -1.399     -2.574     -1.437
25  C25          3.982     -0.097     -1.045
26  C26          5.168     -0.589     -1.624
27  C27          5.993     -1.475     -0.902
28  C28          5.623     -1.859      0.402
29  C29          4.436     -1.364      0.976
30  C30         -2.151     -5.759     -3.428
31  C31          7.271     -2.003     -1.521
32  H1          -1.423      5.139      2.189
33  H2          -1.080      5.684      0.560
34  H3           0.693      4.161      0.313
35  C4Methyl     0.970      4.190      2.445
36  C5Methyl    -2.750      4.142     -0.743
37  H6          -3.164      3.960      1.362
38  H7           1.959      1.889     -0.261
39  H8          -1.063      0.301     -0.820
40  H9          -3.831      2.200      2.901
41  H10         -5.186      1.096      2.699
42  H11         -5.056      2.516      1.664
43  H12         -0.412     -0.173      4.183
44  H13         -1.590     -0.386      2.890
45  H14         -1.228      1.230      3.502
46  H15         -4.811     -2.479     -1.400
47  H16         -4.504     -4.555     -2.689
48  H17         -0.220     -4.108     -2.390
49  H18         -0.529     -2.035     -1.090
50  H19          3.363      0.576     -1.619
51  H20          5.441     -0.284     -2.624
52  H21          6.249     -2.532      0.970
53  H22          4.182     -1.668      1.980
54  H23         -2.095     -5.531     -4.492
55  H24         -2.982     -6.447     -3.267
56  H25         -1.233     -6.269     -3.136
57  H26          7.521     -2.987     -1.122
58  H27          8.099     -1.327     -1.310
59  H28          7.170     -2.097     -2.603
60  H27          1.885      3.598      2.411
61  H28          0.438      3.924      3.360
62  H29          1.261      5.238      2.520
63  H30         -3.149      5.153     -0.836
64  H31         -3.531      3.450     -1.059
65  H32         -1.918      4.046     -1.441

File name:  DMDAE_conf12-conf17.fcht.sp
Calculations for Structure: conf17 (D´) (single conformer, single tensor fit)
Coordinates /(AA): (origin shifted to center of mass, and transformed to Eckart frame)
1   C1          -2.542      3.171      2.987
2   C2          -1.003      3.182      3.022
3   C3          -0.601      2.455      1.755
4   C4Ring      -1.651      1.823      1.198
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5   C5Ring       -2.931      2.095      1.959
6   C6           -1.632      1.055     -0.061
7   C7            0.801      2.346      1.303
8   C8            1.624      3.428      1.108
9   S             3.197      2.892      0.573
10  C10           2.709      1.210      0.608
11  C11           1.405      1.086      1.019
12  C12          -2.117     -0.283     -0.102
13  C13          -2.023     -0.836     -1.354
14  S            -1.333      0.305     -2.492
15  C15          -1.190      1.540     -1.268
16  C16          -2.401     -2.182     -1.791
17  C17          -0.660      2.892     -1.618
18  C18           1.339      4.885      1.266
19  C19           3.656      0.158      0.239
20  C20          -2.505     -3.230     -0.848
21  C21          -2.874     -4.530     -1.245
22  C22          -3.148     -4.804     -2.599
23  C23          -3.055     -3.768     -3.549
24  C24          -2.685     -2.470     -3.146
25  C25           3.497     -1.150      0.749
26  C26           4.394     -2.178      0.399
27  C27           5.468     -1.913     -0.473
28  C28           5.634     -0.614     -0.994
29  C29           4.734      0.410     -0.640
30  C30          -3.547     -6.201     -3.030
31  C31           6.432     -3.017     -0.856
32  H1           -2.991      2.988      3.965
33  H2           -2.894      4.150      2.655
34  H3           -0.656      4.213      2.987
35  C4Methyl     -0.431      2.503      4.276
36  C5Methyl     -4.109      2.508      1.061
37  H6           -3.195      1.171      2.476
38  H7            0.870      0.153      1.118
39  H8           -2.510     -0.779      0.774
40  H9           -1.032      3.654     -0.933
41  H10          -0.959      3.179     -2.626
42  H11           0.430      2.901     -1.576
43  H12           0.327      5.125      0.937
44  H13           2.029      5.486      0.673
45  H14           1.443      5.189      2.307
46  H15          -2.293     -3.045      0.194
47  H16          -2.944     -5.315     -0.505
48  H17          -3.268     -3.962     -4.590
49  H18          -2.630     -1.693     -3.894
50  H19           2.683     -1.373      1.422
51  H20           4.251     -3.170      0.803
52  H21           6.449     -0.398     -1.670
53  H22           4.878      1.394     -1.061
54  H23          -4.631     -6.313     -2.987
55  H24          -3.097     -6.953     -2.381
56  H25          -3.222     -6.402     -4.051
57  H26           7.432     -2.618     -1.032
58  H27           6.095     -3.512     -1.767
59  H28           6.505     -3.764     -0.065
60  H27           0.660      2.508      4.260
61  H28          -0.757      1.465      4.349
62  H29          -0.749      3.018      5.182
63  H30          -4.993      2.737      1.656
64  H31          -4.379      1.711      0.367
65  H32          -3.866      3.392      0.470

File name: DMDAE_conf19-conf21.fcht.sp
Calculations for Structure: conf19 (A) (single conformer, single tensor fit)
Coordinates /(AA): (origin shifted to center of mass, reference structure of the Eckart frame)
1   C1           -0.233      4.298      0.171
2   C2            1.060      3.465      0.147
3   C3            0.580      2.033      0.033
4   C4Ring       -0.742      1.981     -0.213
5   C5Ring       -1.339      3.364     -0.355
6   C6           -1.553      0.763     -0.398
7   C7            1.460      0.881      0.309
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8	C8	1.238	-0.064	1.281
9	S	2.517	-1.251	1.257
10	C10	3.347	-0.428	-0.049
11	C11	2.660	0.696	-0.435
12	C12	-2.736	0.553	0.368
13	C13	-3.349	-0.637	0.065
14	S	-2.475	-1.492	-1.190
15	C15	-1.276	-0.230	-1.306
16	C16	-4.571	-1.206	0.636
17	C17	-0.168	-0.335	-2.303
18	C18	0.132	-0.172	2.279
19	C19	4.610	-0.951	-0.571
20	C20	-4.813	-2.599	0.625
21	C21	-5.989	-3.134	1.187
22	C22	-6.945	-2.280	1.771
23	C23	-6.713	-0.891	1.794
24	C24	-5.535	-0.362	1.232
25	C25	4.956	-2.317	-0.441
26	C26	6.172	-2.807	-0.957
27	C27	7.063	-1.938	-1.617
28	C28	6.729	-0.577	-1.754
29	C29	5.512	-0.091	-1.237
30	C30	-8.210	-2.853	2.378
31	C31	8.373	-2.463	-2.169
32	H1	-0.473	4.585	1.196
33	H2	-0.142	5.220	-0.405
34	H3	1.624	3.682	-0.761
35	C4Methyl	1.971	3.720	1.360
36	C5Methyl	-1.733	3.668	-1.809
37	H6	-2.218	3.449	0.286
38	H7	2.959	1.374	-1.220
39	H8	-3.075	1.259	1.110
40	H9	0.219	0.648	-2.572
41	H10	-0.514	-0.815	-3.218
42	H11	0.654	-0.928	-1.903
43	H12	-0.324	0.799	2.474
44	H13	0.502	-0.560	3.228
45	H14	-0.645	-0.848	1.921
46	H15	-4.092	-3.276	0.191
47	H16	-6.150	-4.202	1.168
48	H17	-7.436	-0.224	2.242
49	H18	-5.380	0.706	1.254
50	H19	4.288	-3.006	0.052
51	H20	6.414	-3.854	-0.844
52	H21	7.404	0.102	-2.255
53	H22	5.279	0.957	-1.349
54	H23	-9.033	-2.141	2.311
55	H24	-8.048	-3.093	3.429
56	H25	-8.513	-3.764	1.861
57	H26	9.156	-2.389	-1.415
58	H27	8.684	-1.892	-3.045
59	H28	8.280	-3.508	-2.467
60	H27	2.893	3.143	1.294
61	H28	1.476	3.446	2.292
62	H29	2.249	4.773	1.425
63	H30	-2.137	4.676	-1.904
64	H31	-2.495	2.973	-2.162
65	H32	-0.875	3.587	-2.477

File name: DMDAE_conf19-conf21.fcht.sp
Calculations for Structure: **conf21 (A´)** (single conformer, single tensor fit)
Coordinates /(AA): (origin shifted to center of mass, and transformed to Eckart frame)

1	C1	-0.045	4.276	-0.526
2	C2	1.117	3.461	0.070
3	C3	0.610	2.035	0.044
4	C4Ring	-0.712	1.983	-0.199
5	C5Ring	-1.283	3.367	-0.428
6	C6	-1.516	0.759	-0.376
7	C7	1.497	0.891	0.324
8	C8	1.282	-0.044	1.308
9	S	2.563	-1.229	1.292
10	C10	3.388	-0.416	-0.023

11	C11	2.695	0.700	-0.422
12	C12	-2.702	0.559	0.387
13	C13	-3.313	-0.636	0.100
14	S	-2.431	-1.510	-1.137
15	C15	-1.233	-0.248	-1.267
16	C16	-4.538	-1.197	0.672
17	C17	-0.122	-0.367	-2.258
18	C18	0.179	-0.143	2.311
19	C19	4.641	-0.954	-0.557
20	C20	-4.781	-2.590	0.678
21	C21	-5.960	-3.116	1.241
22	C22	-6.917	-2.255	1.812
23	C23	-6.686	-0.865	1.815
24	C24	-5.504	-0.344	1.251
25	C25	5.046	-0.635	-1.873
26	C26	6.251	-1.137	-2.402
27	C27	7.075	-1.967	-1.619
28	C28	6.687	-2.288	-0.303
29	C29	5.481	-1.784	0.222
30	C30	-8.189	-2.818	2.414
31	C31	8.374	-2.505	-2.185
32	H1	-0.196	5.235	-0.028
33	H2	0.177	4.492	-1.572
34	H3	1.989	3.549	-0.578
35	C4Methyl	1.488	3.908	1.493
36	C5Methyl	-2.208	3.464	-1.653
37	H6	-1.859	3.622	0.462
38	H7	2.994	1.370	-1.214
39	H8	-3.046	1.278	1.114
40	H9	0.270	0.612	-2.536
41	H10	-0.465	-0.856	-3.170
42	H11	0.697	-0.959	-1.849
43	H12	0.551	-0.525	3.261
44	H13	-0.600	-0.820	1.960
45	H14	-0.275	0.829	2.501
46	H15	-4.059	-3.273	0.256
47	H16	-6.124	-4.184	1.232
48	H17	-7.413	-0.192	2.246
49	H18	-5.349	0.724	1.259
50	H19	4.426	-0.005	-2.493
51	H20	6.537	-0.880	-3.412
52	H21	7.313	-2.918	0.312
53	H22	5.212	-2.038	1.236
54	H23	-8.538	-2.196	3.239
55	H24	-8.026	-3.825	2.799
56	H25	-8.975	-2.861	1.660
57	H26	8.646	-3.450	-1.713
58	H27	9.182	-1.793	-2.017
59	H28	8.287	-2.680	-3.258
60	H27	2.293	3.293	1.899
61	H28	0.636	3.827	2.169
62	H29	1.827	4.944	1.504
63	H30	-2.552	4.488	-1.803
64	H31	-3.092	2.837	-1.536
65	H32	-1.696	3.147	-2.562

File name: DMDAE_conf25-conf26.fcht.sp
Calculations for Structure: **conf25 (B)** (single conformer, single tensor fit)
Coordinates /(AA): (origin shifted to center of mass, reference structure of the Eckart frame)

1	C1	-0.202	4.557	0.136
2	C2	1.095	3.730	0.095
3	C3	0.602	2.299	0.030
4	C4Ring	-0.700	2.250	-0.299
5	C5Ring	-1.302	3.634	-0.424
6	C6	-1.509	1.020	-0.349
7	C7	1.464	1.117	0.217
8	C8	1.798	0.257	-0.800
9	S	2.821	-1.018	-0.191
10	C10	2.791	-0.354	1.431
11	C11	2.031	0.788	1.481
12	C12	-2.091	0.562	-1.565

13	C13	-2.806	-0.598	-1.398
14	S	-2.767	-1.122	0.274
15	C15	-1.787	0.241	0.747
16	C16	-3.522	-1.383	-2.404
17	C17	-1.380	0.422	2.173
18	C18	1.410	0.295	-2.242
19	C19	3.528	-1.009	2.512
20	C20	-3.167	-1.281	-3.768
21	C21	-3.850	-2.022	-4.753
22	C22	-4.905	-2.880	-4.387
23	C23	-5.274	-2.986	-3.031
24	C24	-4.588	-2.243	-2.051
25	C25	3.957	-0.262	3.632
26	C26	4.659	-0.876	4.688
27	C27	4.942	-2.256	4.640
28	C28	4.514	-3.013	3.532
29	C29	3.813	-2.394	2.479
30	C30	-5.643	-3.676	-5.444
31	C31	5.694	-2.921	5.775
32	H1	-0.449	4.809	1.169
33	H2	-0.110	5.499	-0.408
34	H3	1.624	3.918	-0.840
35	C4Methyl	2.045	4.042	1.263
36	C5Methyl	-1.670	3.990	-1.873
37	H6	-2.186	3.700	0.213
38	H7	1.850	1.378	2.367
39	H8	-1.957	1.083	-2.501
40	H9	-1.084	1.452	2.377
41	H10	-0.539	-0.227	2.416
42	H11	-2.201	0.174	2.845
43	H12	0.562	-0.364	-2.428
44	H13	2.235	-0.032	-2.875
45	H14	1.131	1.302	-2.554
46	H15	-2.357	-0.634	-4.070
47	H16	-3.557	-1.928	-5.789
48	H17	-6.086	-3.635	-2.736
49	H18	-4.896	-2.337	-1.020
50	H19	3.756	0.798	3.685
51	H20	4.979	-0.283	5.532
52	H21	4.717	-4.074	3.485
53	H22	3.487	-2.999	1.646
54	H23	-6.028	-4.610	-5.032
55	H24	-4.984	-3.924	-6.276
56	H25	-6.484	-3.100	-5.831
57	H26	6.371	-2.218	6.260
58	H27	6.287	-3.760	5.410
59	H28	4.993	-3.295	6.522
60	H27	2.970	3.469	1.184
61	H28	1.586	3.813	2.224
62	H29	2.318	5.097	1.268
63	H30	-2.012	5.023	-1.946
64	H31	-2.477	3.359	-2.243
65	H32	-0.816	3.873	-2.541

File name: DMDAE_conf25-conf26.fcht.sp
Calculations for Structure: **conf26 (B´)** (single conformer, single tensor fit)
Coordinates /(AA): (origin shifted to center of mass, and transformed to Eckart frame)

1	C1	0.144	4.519	-0.640
2	C2	1.256	3.674	0.011
3	C3	0.667	2.279	0.047
4	C4Ring	-0.637	2.279	-0.277
5	C5Ring	-1.145	3.689	-0.500
6	C6	-1.488	1.076	-0.326
7	C7	1.488	1.070	0.227
8	C8	1.766	0.176	-0.777
9	S	2.765	-1.116	-0.163
10	C10	2.811	-0.406	1.439
11	C11	2.085	0.757	1.482
12	C12	-2.053	0.599	-1.543
13	C13	-2.807	-0.533	-1.362
14	S	-2.825	-1.010	0.325
15	C15	-1.813	0.335	0.783

16	C16	-3.522	-1.324	-2.364
17	C17	-1.423	0.541	2.210
18	C18	1.346	0.191	-2.211
19	C19	3.545	-1.065	2.521
20	C20	-3.127	-1.275	-3.720
21	C21	-3.808	-2.023	-4.701
22	C22	-4.902	-2.832	-4.339
23	C23	-5.308	-2.889	-2.991
24	C24	-4.624	-2.140	-2.014
25	C25	3.197	-0.817	3.868
26	C26	3.896	-1.434	4.923
27	C27	4.963	-2.311	4.647
28	C28	5.323	-2.566	3.309
29	C29	4.620	-1.946	2.257
30	C30	-5.634	-3.641	-5.391
31	C31	5.716	-2.980	5.779
32	H1	0.045	5.514	-0.203
33	H2	0.382	4.658	-1.696
34	H3	2.135	3.676	-0.635
35	C4Methyl	1.630	4.193	1.409
36	C5Methyl	-2.103	3.858	-1.690
37	H6	-1.672	3.976	0.411
38	H7	1.953	1.379	2.354
39	H8	-1.882	1.090	-2.489
40	H9	-0.562	-0.077	2.465
41	H10	-2.240	0.271	2.879
42	H11	-1.163	1.581	2.407
43	H12	1.033	1.186	-2.526
44	H13	0.514	-0.495	-2.373
45	H14	2.167	-0.119	-2.858
46	H15	-2.288	-0.665	-4.018
47	H16	-3.483	-1.972	-5.730
48	H17	-6.146	-3.506	-2.699
49	H18	-4.961	-2.194	-0.990
50	H19	2.379	-0.152	4.102
51	H20	3.607	-1.232	5.945
52	H21	6.139	-3.236	3.081
53	H22	4.922	-2.151	1.241
54	H23	-5.186	-4.630	-5.485
55	H24	-5.588	-3.149	-6.364
56	H25	-6.685	-3.763	-5.127
57	H26	6.755	-3.162	5.503
58	H27	5.253	-3.935	6.026
59	H28	5.712	-2.355	6.673
60	H27	2.447	3.615	1.840
61	H28	0.782	4.143	2.093
62	H29	1.961	5.231	1.364
63	H30	-2.387	4.904	-1.813
64	H31	-3.021	3.289	-1.544
65	H32	-1.645	3.528	-2.623

DFT calulations

High-level DFT calculations were used to determine relative energies at the B3LYP/6-311+G(d,p) level of theory,[29,30] as implemented in the Gaussian 09 program suite.[31] Solvation effects were treated by the integral equation formalism variant of the polarizable continuum model (IEFPCM),[32] using the SMD solvation model by Truhlar and coworkers[33] (default parameters for Chloroform). The identified stationary points were subsequently characterized by thermal frequency analysis. Initial geometries were derived from the MM calculations (see above) and input files for the calculation prepared using the MolArch+ utility.[34]

All calculations were performed at the FUCHS cluster of the Frankfurt Center for Scientific Computing.

Table SI- 12: Results of the DFT calculations for the respective conformers of the dimethyl substituted 1o. Relative (electronic) energies, energies including zero-point corrections and relative Gibbs free energies are given in kJ/mol. Fractional populations and the respective sum over the "envelope flip" in the cyclopentene core are calculated based on a Boltzmann distribution.

Conformer (1o)		ΔE (kJ/mol)	ΔE(SCF+ZPE) (kJ/mol)	ΔG (kJ/mol)	fractional population (%)	population sum over envelope flip (%)
a-p (P*,S*,S*)	A	0.000	0.063	1.016	28.75	**72.07**
	A'	0.004	0.000	0.000	43.32	
a-p (M*,S*,S*)	B	8.965	9.864	8.746	1.27	**7.21**
	B'	8.991	9.042	4.925	5.94	
a-p mixed	C	2.878	4.505	5.170	5.38	**10.43**
	C'	2.984	4.616	5.327	5.05	
p	D	1.351	2.408	5.487	4.74	**10.29**
	D'	2.441	3.067	5.093	5.55	

Table SI- 13: Results of the DFT calculations for the respective conformers of the tetramethyl substituted 4o. Relative (electronic) energies, energies including zero-point corrections and relative Gibbs free energies are given in kJ/mol. Fractional populations and the respective sum over the "envelope flip" in the cyclopentene core are calculated based on a Boltzmann distribution.

Conformer (4o)		ΔE (kJ/mol)	ΔE(SCF+ZPE) (kJ/mol)	ΔG (kJ/mol)	fractional population (%)	population sum over envelope flip (%)
a-p	E	0.000	0.066	0.323	42.90	**91.76**
	E'	0.015	0.000	0.000	48.86	
p	F	3.111	5.275	7.112	2.77	**8.24**
	F'	5.383	6.036	5.430	5.47	

Cartesian Coordinates of DFT-Optimized Geometries

Conformer A, a-p (P^*,S^*,S^*), ΔE = 0 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	0.10925	4.28671	-0.28556
C	-1.16322	3.41772	-0.41472
C	-0.61553	1.99505	-0.26799
C	0.64420	1.99934	0.21644
C	1.15064	3.42064	0.45804
C	1.50089	0.85071	0.57866
C	-1.46405	0.83410	-0.60586
C	-1.13147	-0.18051	-1.47619
S	-2.44520	-1.32524	-1.62387
C	-3.46285	-0.42746	-0.50971
C	-2.79243	0.68565	-0.07828
C	2.83524	0.71174	0.06369
C	3.51411	-0.38976	0.51125
S	2.49806	-1.28625	1.62776
C	1.17297	-0.15788	1.45796
C	4.87651	-0.82878	0.18355
C	-0.07720	-0.37578	2.25217
C	0.11576	-0.39221	-2.27650
C	-4.82003	-0.87582	-0.17274
C	5.26988	-2.17251	0.28930
C	6.56713	-2.56937	-0.02282
C	7.52413	-1.64894	-0.46376
C	7.13239	-0.30788	-0.56861
C	5.84188	0.09816	-0.24801
C	-5.20120	-2.22511	-0.26684
C	-6.49234	-2.63172	0.05255
C	-7.45836	-1.71611	0.48766
C	-7.07693	-0.37306	0.58932
C	-5.79054	0.04333	0.26035
C	8.91938	-2.08509	-0.83419
C	-8.86432	-2.16033	0.80309
H	0.47681	4.52003	-1.29050
H	-0.08230	5.23750	0.21932
H	-1.83727	3.61503	0.43147
C	-1.94677	3.68510	-1.70422
C	1.25968	3.74319	1.95868
H	2.14687	3.54987	0.02007
H	-3.21855	1.38163	0.63341
H	3.25809	1.40344	-0.65405
H	-0.65136	0.54936	2.31693
H	0.15010	-0.70429	3.27066
H	-0.72072	-1.13600	1.79752
H	0.67619	0.54025	-2.35779
H	-0.11394	-0.73863	-3.28850
H	0.77388	-1.13628	-1.81592
H	4.55393	-2.92228	0.60847
H	6.83665	-3.61653	0.07319
H	7.85488	0.43500	-0.89267
H	5.58627	1.14967	-0.31215
H	-4.47766	-2.97073	-0.57838
H	-6.75073	-3.68308	-0.02988
H	-7.80198	0.36403	0.92040
H	-5.54279	1.09665	0.32523
H	9.65324	-1.30718	-0.60808
H	8.99285	-2.29937	-1.90680
H	9.20888	-2.99327	-0.29985
H	-9.44323	-2.31246	-0.11513
H	-9.39197	-1.41699	1.40505
H	-8.87131	-3.10793	1.34886
H	-2.85163	3.07489	-1.76750
H	-1.33520	3.47179	-2.58713
H	-2.25108	4.73569	-1.75361
H	1.64197	4.75800	2.10773
H	1.94021	3.05304	2.46577
H	0.28424	3.67437	2.45153

Conformer A', a-p (P^*,S^*,S^*) flip, ΔE = 0.004 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	0.10415	4.29096	-0.25874
C	1.14414	3.41839	0.47919
C	0.64018	1.99905	0.22155
C	-0.61795	1.99815	-0.26689
C	-1.16654	3.42152	-0.40219
C	-1.46548	0.83946	-0.61490
C	1.49680	0.84789	0.57605
C	1.16812	-0.16695	1.44782
S	2.49350	-1.29573	1.61172
C	3.51070	-0.39111	0.50270
C	2.83177	0.71301	0.06164
C	-2.79397	0.68690	-0.08886
C	-3.46292	-0.42468	-0.52631
S	-2.44438	-1.31506	-1.64536
C	-1.13174	-0.16975	-1.49099
C	-4.81804	-0.87734	-0.18684
C	0.11627	-0.37611	-2.29148
C	-0.08288	-0.39048	2.23917
C	4.87447	-0.82702	0.17642
C	-5.19630	-2.22640	-0.28046
C	-6.48641	-2.63627	0.04374
C	-7.45106	-1.72404	0.48539
C	-7.07478	-0.37777	0.57724
C	-5.79141	0.04120	0.24436
C	5.26787	-2.17241	0.27603
C	6.56438	-2.56760	-0.03579
C	7.52387	-1.64394	-0.46842
C	7.13042	-0.30474	-0.57490
C	5.83847	0.10033	-0.25358
C	-8.83728	-2.17477	0.87163
C	8.93521	-2.07575	-0.77702
H	-0.09083	5.23582	0.25591
H	0.47518	4.53599	-1.25959
H	2.14173	3.55328	0.04609
C	1.24732	3.72471	1.98363
C	-1.94462	3.70006	-1.69264
H	-1.84486	3.60941	0.44274
H	3.25492	1.40999	-0.65077
H	-3.22109	1.37804	0.62695
H	0.67600	0.55723	-2.36753
H	-0.11239	-0.71735	-3.30548
H	0.77466	-1.12207	-1.83434
H	-0.65898	0.53326	2.30639
H	0.14343	-0.72233	3.25680
H	-0.72406	-1.15039	1.78071
H	-4.47378	-2.96981	-0.59959
H	-6.74414	-3.68722	-0.04279
H	-7.80385	0.35870	0.90113
H	-5.54786	1.09606	0.29913
H	4.54964	-2.92416	0.58525
H	6.83215	-3.61634	0.05025
H	7.85018	0.43838	-0.90408
H	5.58109	1.15114	-0.32209
H	-9.57975	-1.39891	0.66804
H	-8.89144	-2.40435	1.94224
H	-9.12929	-3.07776	0.32982
H	9.50961	-2.22788	0.14401
H	9.46069	-1.32545	-1.37217
H	8.95313	-3.02063	-1.32732
H	1.92652	3.02956	2.48568
H	0.26998	3.64952	2.47181
H	1.62797	4.73815	2.14540
H	-2.25166	4.75024	-1.73295
H	-2.84737	3.08791	-1.76629
H	-1.32818	3.49741	-2.57467

Conformer B, a-p (M^*,S^*,S^*), ΔE = 8.965 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	-0.18377	4.84889	-0.40730
C	-1.00961	4.01872	0.60354
C	-0.56956	2.58587	0.29764
C	0.52672	2.55886	-0.47988
C	1.01777	3.96551	-0.82237
C	1.24358	1.34947	-0.96030
C	-1.27294	1.41202	0.87600
C	-0.85790	0.73179	1.99737
S	-1.96191	-0.57132	2.37588
C	-2.99769	-0.19642	1.00965
C	-2.49071	0.88135	0.33315
C	2.44979	0.85243	-0.36275
C	2.97638	-0.25661	-0.97158
S	1.96603	-0.71266	-2.33217
C	0.85517	0.60895	-2.05273
C	4.17976	-1.01772	-0.61280
C	-0.31754	0.79786	-2.96475
C	0.33201	0.97239	2.87446
C	-4.21394	-0.96934	0.72624
C	4.67432	-0.99869	0.70246
C	5.82904	-1.69537	1.04450
C	6.53351	-2.45150	0.09985
C	6.03518	-2.47872	-1.20820
C	4.88757	-1.77595	-1.56051
C	-5.30830	-0.36669	0.08533
C	-6.46140	-1.09328	-0.19984
C	-6.57923	-2.44209	0.15264
C	-5.48985	-3.04106	0.79885
C	-4.33127	-2.32524	1.07813
C	7.76572	-3.23225	0.48177
C	-7.83110	-3.22880	-0.14459
H	-0.80665	5.05308	-1.28459
H	0.12848	5.81406	0.00088
H	-0.69464	4.25111	1.63166
C	-2.51546	4.28863	0.52054
C	2.32480	4.34024	-0.10197
H	1.20272	4.04209	-1.89991
H	-2.95634	1.27731	-0.55988
H	2.91421	1.32174	0.49425
H	-0.82945	1.73256	-2.73040
H	-1.04376	-0.01575	-2.86687
H	-0.00930	0.83632	-4.01442
H	1.04462	0.14247	2.82938
H	0.04113	1.09718	3.92251
H	0.85245	1.87861	2.56191
H	4.14463	-0.44372	1.46833
H	6.18475	-1.65771	2.06954
H	6.55884	-3.04991	-1.96865
H	4.55028	-1.80348	-2.59104
H	-5.26407	0.68427	-0.17702
H	-7.29082	-0.59686	-0.69392
H	-5.54625	-4.08787	1.08216
H	-3.50167	-2.83118	1.56012
H	7.51779	-4.27779	0.69902
H	8.24070	-2.81703	1.37395
H	8.50282	-3.23559	-0.32573
H	-8.57399	-2.61486	-0.65829
H	-8.28881	-3.60982	0.77430
H	-7.61499	-4.09498	-0.77853
H	-3.07708	3.69352	1.24567
H	-2.90456	4.06631	-0.47851
H	-2.72122	5.34359	0.72969
H	2.62262	5.36092	-0.36261
H	3.14653	3.67715	-0.38501
H	2.20829	4.29258	0.98579

Conformer B', a-p (M^*,S^*,S^*) flip, ΔE = 8.991 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	0.19493	4.84296	0.15094
C	-1.02442	4.00051	0.59718
C	-0.54084	2.57003	0.35785
C	0.57030	2.53625	-0.39862
C	1.02753	3.94258	-0.79153
C	1.26895	1.31999	-0.88736
C	-1.27480	1.40302	0.91045
C	-0.88363	0.71289	2.03479
S	-2.01003	-0.57528	2.39497
C	-3.02364	-0.18153	1.01810
C	-2.49282	0.89063	0.35026
C	2.50205	0.84412	-0.32797
C	3.00934	-0.27748	-0.92910
S	1.94885	-0.77104	-2.23768
C	0.84177	0.55118	-1.94536
C	4.22971	-1.02504	-0.60066
C	-0.36342	0.71266	-2.81924
C	0.30005	0.93302	2.92548
C	-4.24695	-0.93684	0.71842
C	4.76715	-0.98431	0.69698
C	5.93690	-1.66944	1.01024
C	6.61446	-2.43481	0.05360
C	6.07399	-2.48267	-1.23717
C	4.91091	-1.79174	-1.56101
C	-5.32464	-0.31898	0.06385
C	-6.48495	-1.02887	-0.23406
C	-6.62692	-2.37536	0.11820
C	-5.55386	-2.98978	0.77705
C	-4.38823	-2.29082	1.06912
C	7.86249	-3.20436	0.40602
C	-7.88790	-3.14300	-0.19016
H	-0.09727	5.78496	-0.32105
H	0.80494	5.09302	1.02545
H	-1.22969	4.14909	1.66359
C	-2.31246	4.34191	-0.17200
C	2.53380	4.20997	-0.70626
H	0.72761	4.10855	-1.83674
H	-2.94013	1.29220	-0.54938
H	2.99963	1.33900	0.49555
H	-0.89006	1.63387	-2.56673
H	-1.06561	-0.11868	-2.70035
H	-0.08906	0.76074	-3.87798
H	1.02918	0.12047	2.84056
H	0.00515	0.99869	3.97757
H	0.80285	1.86397	2.65907
H	4.25893	-0.42182	1.47190
H	6.32580	-1.61561	2.02238
H	6.57601	-3.06136	-2.00654
H	4.54002	-1.83523	-2.57941
H	-5.26235	0.73097	-0.19892
H	-7.30114	-0.52075	-0.73818
H	-5.62861	-4.03544	1.06022
H	-3.57188	-2.80868	1.56097
H	7.62946	-4.25309	0.62420
H	8.35195	-2.78734	1.28943
H	8.58245	-3.19763	-0.41691
H	-8.60843	-2.52417	-0.72925
H	-8.37090	-3.49808	0.72625
H	-7.67678	-4.02471	-0.80390
H	-3.14541	3.70245	0.13190
H	-2.17430	4.23046	-1.25243
H	-2.60681	5.37805	0.02294
H	2.74714	5.24900	-0.97815
H	3.10262	3.56874	-1.38477
H	2.90962	4.04986	0.30962

Conformer C, a-p mixed, ΔE = 2.878 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	5.17601	-0.06766	0.22137
C	4.32958	-0.91842	-0.75483
C	2.89786	-0.51870	-0.39183
C	2.87501	0.57825	0.39532
C	4.28162	1.11770	0.64609
C	1.67462	1.30212	0.87178
C	1.72055	-1.28693	-0.85538
C	1.47088	-1.63831	-2.16513
S	-0.00477	-2.56499	-2.28723
C	-0.29645	-2.48430	-0.55861
C	0.70917	-1.77229	0.03943
C	0.63926	1.76698	-0.00748
C	-0.36750	2.46181	0.60740
S	-0.05660	2.53810	2.33285
C	1.43853	1.64765	2.18561
C	-1.56156	3.07429	0.01115
C	2.23874	1.34316	3.41701
C	2.25057	-1.32822	-3.40857
C	-1.46596	-3.12173	0.06037
C	-2.12343	2.54400	-1.16453
C	-3.24430	3.12389	-1.74577
C	-3.86358	4.24720	-1.17932
C	-3.30879	4.76901	-0.00712
C	-2.17925	4.19962	0.57667
C	-1.43811	-3.50831	1.41007
C	-2.54991	-4.09008	2.01270
C	-3.72877	-4.32612	1.29694
C	-3.75307	-3.94971	-0.05218
C	-2.65056	-3.35826	-0.65844
C	-5.08865	4.85811	-1.81275
C	-4.92869	-4.97106	1.94435
H	5.41624	-0.67691	1.09935
H	6.12279	0.25748	-0.21860
H	4.53146	-0.60654	-1.78828
C	4.62831	-2.41831	-0.65648
C	4.55123	2.40499	-0.15323
H	4.42792	1.35268	1.70449
H	0.73426	-1.57727	1.10321
H	0.66999	1.60828	-1.07739
H	2.87119	0.46832	3.25639
H	1.58992	1.12893	4.27096
H	2.88545	2.18042	3.70274
H	1.60222	-1.29086	-4.28763
H	3.02186	-2.08133	-3.60587
H	2.74552	-0.35859	-3.32428
H	-1.68772	1.65939	-1.61477
H	-3.65576	2.68667	-2.65075
H	-3.76039	5.64068	0.45602
H	-1.76705	4.64996	1.47339
H	-0.53540	-3.36304	1.99236
H	-2.49477	-4.37500	3.05876
H	-4.65353	-4.11289	-0.63669
H	-2.72065	-3.05964	-1.69902
H	-5.91605	4.14164	-1.84629
H	-4.89074	5.16841	-2.84389
H	-5.42766	5.73527	-1.25723
H	-4.79134	-5.07350	3.02299
H	-5.11118	-5.97087	1.53545
H	-5.83632	-4.38417	1.77349
H	4.02864	-3.00336	-1.35864
H	4.42398	-2.79361	0.35172
H	5.68289	-2.61188	-0.87846
H	5.55591	2.78428	0.05914
H	3.83665	3.19214	0.10455
H	4.47893	2.22619	-1.23097

Conformer C', a-p mixed flip, ΔE = 2.984 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	5.16560	0.27003	-0.32275
C	4.30624	-0.94714	-0.72937
C	2.88640	-0.45793	-0.45203
C	2.88461	0.63995	0.33402
C	4.30767	1.09150	0.66837
C	1.68936	1.36102	0.82517
C	1.70449	-1.22866	-0.90164
C	1.44280	-1.56981	-2.21142
S	-0.02278	-2.51480	-2.32436
C	-0.29358	-2.45293	-0.59055
C	0.70976	-1.73332	0.00154
C	0.63899	1.80831	-0.04482
C	-0.37022	2.49403	0.57695
S	-0.04009	2.58626	2.29722
C	1.46383	1.71360	2.13923
C	-1.57969	3.08512	-0.00991
C	2.28472	1.43608	3.36358
C	2.20055	-1.23020	-3.46037
C	-1.44689	-3.11093	0.03686
C	-2.14636	2.53980	-1.17640
C	-3.28242	3.09923	-1.74824
C	-3.91270	4.21601	-1.18104
C	-3.35307	4.75277	-0.01795
C	-2.20834	4.20417	0.55606
C	-1.39834	-3.50555	1.38364
C	-2.49510	-4.10631	1.99507
C	-3.67853	-4.35441	1.29094
C	-3.72310	-3.97039	-0.05548
C	-2.63586	-3.35984	-0.67028
C	-5.15520	4.80335	-1.80269
C	-4.86244	-5.01951	1.94730
H	6.13136	-0.02044	0.09994
H	5.36718	0.88592	-1.20575
H	4.44000	-1.17917	-1.79015
C	4.63432	-2.22264	0.06730
C	4.54956	2.60110	0.56283
H	4.54069	0.78859	1.69807
H	0.74434	-1.54546	1.06639
H	0.66038	1.64431	-1.11414
H	2.80338	0.47943	3.27431
H	1.66050	1.38898	4.25963
H	3.03981	2.21171	3.53480
H	1.52421	-1.01527	-4.29236
H	2.85497	-2.05000	-3.77747
H	2.82089	-0.34601	-3.30331
H	-1.70243	1.65915	-1.62640
H	-3.69719	2.65073	-2.64619
H	-3.81297	5.61989	0.44560
H	-1.79330	4.66598	1.44559
H	-0.49121	-3.35113	1.95668
H	-2.42419	-4.39661	3.03870
H	-4.62764	-4.14274	-0.63098
H	-2.72149	-3.05595	-1.70813
H	-5.97385	4.07609	-1.81347
H	-4.97791	5.10266	-2.84078
H	-5.49643	5.68323	-1.25288
H	-4.71399	-5.12285	3.02438
H	-5.03335	-6.02089	1.53718
H	-5.78028	-4.44590	1.78612
H	3.94359	-3.03476	-0.17774
H	4.57287	-2.04403	1.14579
H	5.64802	-2.56765	-0.16004
H	5.59882	2.83447	0.77180
H	3.93703	3.16538	1.27089
H	4.31913	2.96587	-0.44355

Conformer D, p, ΔE = 1.351 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	1.04357	-4.67368	-1.32493
C	2.14363	-3.58941	-1.36786
C	1.55380	-2.47877	-0.49808
C	0.23216	-2.66438	-0.29272
C	-0.27015	-3.94129	-0.96768
C	-0.70856	-1.76240	0.40281
C	2.35188	-1.29118	-0.11940
C	3.57069	-1.33463	0.52338
S	4.21112	0.27460	0.75064
C	2.82440	1.02377	-0.02319
C	1.94336	0.05241	-0.41747
C	-1.90560	-1.28407	-0.23099
C	-2.68022	-0.46435	0.54591
S	-1.93257	-0.28134	2.12455
C	-0.58939	-1.31692	1.70045
C	-3.94167	0.20517	0.20375
C	0.46957	-1.60020	2.71930
C	4.34775	-2.51286	1.03020
C	2.72148	2.47969	-0.18693
C	-4.29699	0.42032	-1.13934
C	-5.49641	1.03932	-1.47395
C	-6.39003	1.48210	-0.49039
C	-6.03083	1.27970	0.84690
C	-4.83737	0.65132	1.18938
C	1.93078	3.02872	-1.21251
C	1.80840	4.40468	-1.36467
C	2.47486	5.29637	-0.51317
C	3.27171	4.75047	0.49808
C	3.39065	3.37293	0.66390
C	-7.70098	2.12893	-0.86056
C	2.32036	6.78774	-0.67358
H	0.97025	-5.23515	-2.26033
H	1.27014	-5.39247	-0.53025
H	3.07712	-3.97099	-0.94393
C	2.45365	-3.08807	-2.79006
C	-1.22605	-4.79057	-0.12294
H	-0.80314	-3.65791	-1.88709
H	1.00588	0.27976	-0.90680
H	-2.17515	-1.55356	-1.24438
H	1.03078	-2.49395	2.44183
H	0.03667	-1.76503	3.71032
H	1.18108	-0.77207	2.80384
H	3.67941	-3.34233	1.26942
H	4.90334	-2.26389	1.93828
H	5.07466	-2.87007	0.29201
H	-3.62108	0.11586	-1.93006
H	-5.73681	1.19355	-2.52141
H	-6.69694	1.61340	1.63652
H	-4.60785	0.49997	2.23866
H	1.41950	2.37113	-1.90613
H	1.19128	4.79426	-2.16873
H	3.80414	5.41154	1.17466
H	4.00233	2.99368	1.47558
H	-8.49711	1.38047	-0.94959
H	-7.63256	2.64720	-1.82030
H	-8.01830	2.85156	-0.10452
H	3.11549	7.32905	-0.15567
H	1.36468	7.13141	-0.26132
H	2.34010	7.08029	-1.72719
H	3.17479	-2.26556	-2.77431
H	1.54842	-2.73045	-3.29151
H	2.88065	-3.89297	-3.39672
H	-1.49339	-5.70903	-0.65567
H	-2.15346	-4.25764	0.10301
H	-0.76247	-5.07724	0.82690

Conformer D', p flip, ΔE = 2.441 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	0.94853	-4.35533	-1.83673
C	2.18340	-3.58601	-1.30864
C	1.55508	-2.42428	-0.53371
C	0.23226	-2.61756	-0.34338
C	-0.24054	-3.94024	-0.94109
C	-0.72931	-1.74406	0.36078
C	2.33900	-1.23624	-0.12839
C	3.54564	-1.27029	0.53728
S	4.16719	0.34431	0.78051
C	2.78817	1.08299	-0.01625
C	1.92393	0.10438	-0.42993
C	-1.94338	-1.30168	-0.26717
C	-2.73935	-0.50629	0.51321
S	-1.99236	-0.30444	2.09003
C	-0.62012	-1.29798	1.65957
C	-4.02138	0.12546	0.17539
C	0.44626	-1.55506	2.67766
C	4.32739	-2.44198	1.05166
C	2.67489	2.53842	-0.17747
C	-4.38932	0.32583	-1.16663
C	-5.60992	0.90402	-1.49734
C	-6.51278	1.32111	-0.51100
C	-6.14023	1.13610	0.82514
C	-4.92524	0.54820	1.16385
C	1.88396	3.08442	-1.20456
C	1.75347	4.45983	-1.35486
C	2.41173	5.35440	-0.50000
C	3.20853	4.81173	0.51297
C	3.33534	3.43472	0.67703
C	-7.84738	1.92053	-0.87656
C	2.24922	6.84507	-0.65899
H	0.75621	-4.04474	-2.86889
H	1.10543	-5.43742	-1.84749
H	2.74329	-4.21988	-0.60841
C	3.14544	-3.16587	-2.42585
C	-0.58435	-4.97537	0.14402
H	-1.14274	-3.78197	-1.54265
H	0.99418	0.32343	-0.93745
H	-2.20873	-1.57821	-1.27961
H	1.02878	-2.43504	2.40092
H	0.01765	-1.73062	3.66866
H	1.13707	-0.70977	2.76240
H	3.66295	-3.26861	1.30996
H	4.89352	-2.18122	1.94966
H	5.04576	-2.81114	0.31081
H	-3.70799	0.04094	-1.95998
H	-5.86012	1.04637	-2.54418
H	-6.81268	1.45158	1.61690
H	-4.68566	0.40886	2.21257
H	1.37867	2.42527	-1.90102
H	1.13649	4.84670	-2.16033
H	3.73496	5.47490	1.19221
H	3.94710	3.05831	1.48998
H	-8.61749	1.14414	-0.95556
H	-7.80355	2.43505	-1.83969
H	-8.18487	2.63632	-0.12266
H	3.04138	7.39009	-0.14042
H	1.29167	7.18338	-0.24661
H	2.26763	7.13868	-1.71232
H	4.01649	-2.63094	-2.03914
H	2.64421	-2.51206	-3.14729
H	3.50811	-4.04599	-2.96682
H	-0.94503	-5.90375	-0.31012
H	-1.36646	-4.60703	0.81446
H	0.29277	-5.21739	0.75342

Conformer E, a-p, ΔE = 0.000 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	-0.10916	4.43258	0.29749
C	1.11325	3.54508	0.66704
C	0.58003	2.13293	0.37205
C	-0.59638	2.15219	-0.27895
C	-1.08484	3.58251	-0.56369
C	-1.35288	0.96008	-0.74513
C	1.32944	0.91716	0.78358
C	0.96002	0.09218	1.82158
S	2.10569	-1.21534	2.01440
C	3.09525	-0.65145	0.67918
C	2.54455	0.48628	0.15131
C	-2.56993	0.51429	-0.12668
C	-3.12219	-0.60710	-0.68585
S	-2.13495	-1.13324	-2.03819
C	-0.98550	0.16493	-1.80689
C	-4.34008	-1.32514	-0.28821
C	0.18498	0.28130	-2.73331
C	-0.20812	0.18929	2.75321
C	4.31424	-1.35799	0.26487
C	-4.50331	-2.69916	-0.52332
C	-5.66268	-3.36350	-0.13078
C	-6.70261	-2.69132	0.51943
C	-6.54052	-1.31885	0.75311
C	-5.39094	-0.64652	0.35518
C	4.47935	-2.73861	0.47069
C	5.63816	-3.39198	0.06627
C	6.68102	-2.70311	-0.56645
C	6.51436	-1.32969	-0.77697
C	5.36158	-0.66641	-0.36591
C	-7.94565	-3.41544	0.97233
C	7.94332	-3.41661	-0.98129
H	-0.61820	4.73769	1.21650
H	0.19358	5.34820	-0.21829
C	2.34382	3.88578	-0.20186
C	1.50081	3.71889	2.14719
C	-0.95379	3.90435	-2.06851
C	-2.54438	3.82459	-0.13945
H	2.97193	0.99264	-0.70332
H	-2.99721	0.99968	0.74021
H	0.75761	1.18011	-2.50470
H	-0.13442	0.34124	-3.77897
H	0.85836	-0.57696	-2.64501
H	-0.77522	1.09803	2.54967
H	0.11326	0.21754	3.79960
H	-0.88765	-0.66139	2.64147
H	-3.71158	-3.26300	-1.00473
H	-5.75459	-4.42673	-0.32915
H	-7.33427	-0.76353	1.24368
H	-5.31323	0.42077	0.52886
H	3.68590	-3.31358	0.93582
H	5.72964	-4.46004	0.23904
H	7.30522	-0.76456	-1.26044
H	5.28090	0.40314	-0.52358
H	-8.84493	-2.82349	0.77987
H	-7.91524	-3.61501	2.04970
H	-8.05559	-4.37583	0.46348
H	8.54028	-3.70121	-0.10759
H	8.56728	-2.78445	-1.61709
H	7.72062	-4.33554	-1.53188
H	2.35333	3.08837	2.41587
H	0.66993	3.46551	2.81211
H	1.78112	4.75914	2.34505
H	-1.29294	4.92669	-2.26693
H	-1.56504	3.22884	-2.67448
H	0.08096	3.82366	-2.41093
H	2.13067	3.78148	-1.26886
H	2.65189	4.92112	-0.02163
H	3.19588	3.24491	0.03973
H	-2.70521	3.56771	0.91175

H	-2.79733	4.88286	-0.26553
H	-3.24478	3.24429	-0.74628

Conformer E', a-p flip, ΔE = 0.015 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	0.13306	4.42963	-0.17481
C	1.10121	3.54698	0.66160
C	0.59845	2.12974	0.33923
C	-0.57942	2.13978	-0.30947
C	-1.09825	3.56458	-0.56712
C	-1.34227	0.94284	-0.75016
C	1.34461	0.91920	0.77363
C	0.97066	0.09806	1.81318
S	2.11471	-1.20987	2.01474
C	3.10877	-0.65232	0.67979
C	2.56173	0.48450	0.14740
C	-2.56195	0.51040	-0.12763
C	-3.12255	-0.61129	-0.67906
S	-2.13847	-1.15539	-2.02621
C	-0.98046	0.13680	-1.80556
C	-4.34514	-1.31778	-0.27545
C	0.18826	0.24250	-2.73544
C	-0.20259	0.19392	2.73854
C	4.32844	-1.36173	0.27227
C	-4.52213	-2.69060	-0.50753
C	-5.68657	-3.34326	-0.11036
C	-6.71831	-2.66022	0.54153
C	-6.54241	-1.28896	0.77250
C	-5.38768	-0.62838	0.37016
C	4.48897	-2.74266	0.47952
C	5.64803	-3.39920	0.08098
C	6.69557	-2.71330	-0.54720
C	6.53351	-1.33953	-0.75901
C	5.38053	-0.67300	-0.35364
C	-7.96741	-3.37145	0.99818
C	7.95779	-3.43037	-0.95613
H	-0.15964	5.33414	0.36582
H	0.64408	4.75427	-1.08602
C	2.56237	3.78795	0.24280
C	0.97445	3.82727	2.17524
C	-1.48249	3.78030	-2.04265
C	-2.32617	3.89596	0.30907
H	2.99358	0.99011	-0.70551
H	-2.98437	1.00228	0.73785
H	0.76158	1.14363	-2.51618
H	-0.13322	0.29131	-3.78104
H	0.86213	-0.61454	-2.63909
H	-0.77172	1.10018	2.53155
H	0.11331	0.22537	3.78650
H	-0.87814	-0.65966	2.62512
H	-3.73741	-3.26294	-0.99036
H	-5.78918	-4.40587	-0.30675
H	-7.32934	-0.72508	1.26431
H	-5.29958	0.43839	0.54193
H	3.69175	-3.31537	0.94100
H	5.73594	-4.46743	0.25455
H	7.32815	-0.77671	-1.23898
H	5.30322	0.39670	-0.51206
H	-8.86181	-2.77365	0.80097
H	-7.93959	-3.56422	2.07684
H	-8.08455	-4.33421	0.49545
H	8.55038	-3.71565	-0.07968
H	8.58592	-2.80034	-1.58994
H	7.73505	-4.34924	-1.50680
H	1.58459	3.13258	2.76033
H	-0.05973	3.73966	2.51782
H	1.31753	4.84234	2.40195
H	-1.75334	4.82779	-2.21387
H	-2.34019	3.16465	-2.32882
H	-0.65272	3.53698	-2.71268
H	2.71952	3.56065	-0.81570

H	2.82529	4.83965	0.39990
H	3.25816	3.18384	0.83131
H	-2.11483	3.76525	1.37346
H	-2.62464	4.93799	0.15286
H	-3.18388	3.26885	0.05198

Conformer F, p, ΔE = 3.111 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	-4.45258	-0.24506	-1.74036
C	-3.68878	1.06642	-1.40403
C	-2.59131	0.55644	-0.45496
C	-2.50476	-0.78429	-0.44669
C	-3.53687	-1.44675	-1.37385
C	-1.47002	-1.58288	0.26581
C	-1.66342	1.48723	0.24477
C	-1.87648	2.04109	1.48548
S	-0.54923	3.08870	1.93382
C	0.30999	2.77514	0.43645
C	-0.42296	1.91474	-0.33785
C	-0.22404	-1.94416	-0.34880
C	0.60318	-2.70706	0.43224
S	-0.16348	-2.99835	1.98351
C	-1.58994	-2.08721	1.53953
C	1.93749	-3.23007	0.11133
C	-2.71866	-1.96151	2.51606
C	-3.02701	1.86929	2.42906
C	1.61043	3.39310	0.14763
C	2.43643	-4.40778	0.69464
C	3.69338	-4.89825	0.35871
C	4.50565	-4.24360	-0.57637
C	4.01089	-3.06888	-1.15321
C	2.75815	-2.56543	-0.81422
C	2.48229	3.80105	1.17230
C	3.71269	4.37851	0.88096
C	4.13444	4.56921	-0.44134
C	3.26845	4.16040	-1.46146
C	2.02958	3.59171	-1.17779
C	5.86574	-4.78593	-0.93748
C	5.46866	5.20350	-0.74450
H	-5.36074	-0.29147	-1.13160
H	-4.76798	-0.27657	-2.78712
C	-3.05618	1.70580	-2.66043
C	-4.62318	2.10135	-0.75373
C	-2.85003	-2.04744	-2.62080
C	-4.33380	-2.56268	-0.67526
H	-0.08009	1.56034	-1.30116
H	0.03682	-1.64963	-1.35685
H	-3.46135	-1.25691	2.14158
H	-2.37281	-1.59869	3.48883
H	-3.21797	-2.92173	2.68465
H	-3.72108	1.12226	2.04415
H	-3.58186	2.80358	2.56594
H	-2.69290	1.54007	3.41783
H	1.82899	-4.95827	1.40512
H	4.04613	-5.81344	0.82469
H	4.61996	-2.53019	-1.87246
H	2.41974	-1.63813	-1.26180
H	2.20467	3.64964	2.20996
H	4.36182	4.67906	1.69797
H	3.56081	4.29993	-2.49761
H	1.37560	3.31182	-1.99578
H	6.54416	-4.76514	-0.07787
H	6.32549	-4.20287	-1.73846
H	5.80347	-5.82644	-1.27177
H	5.49774	6.24494	-0.40623
H	5.67903	5.19496	-1.81624
H	6.28347	4.67772	-0.23678
H	-4.08853	3.01814	-0.48853
H	-5.09361	1.70636	0.15037
H	-5.42210	2.37452	-1.45156
H	-3.60278	-2.46181	-3.29984

H	-2.16899	-2.85894	-2.34928
H	-2.27913	-1.29636	-3.17269
H	-2.39863	1.00763	-3.18451
H	-3.83929	2.01966	-3.35869
H	-2.46986	2.59238	-2.40203
H	-4.84559	-2.19193	0.21689
H	-5.09520	-2.96312	-1.35337
H	-3.68690	-3.39324	-0.37770

Conformer F', p flip, ΔE = 5.383 kJ mol^{-1} (B3LYP/6-311+G(d,p)/SMD(Chloroform))

C	-4.10575	-0.22733	-2.15977
C	-3.68106	1.06973	-1.41254
C	-2.56397	0.55472	-0.48929
C	-2.48087	-0.78594	-0.48022
C	-3.53548	-1.44805	-1.38261
C	-1.46502	-1.58917	0.25506
C	-1.65288	1.48412	0.23569
C	-1.87099	2.02413	1.48188
S	-0.55139	3.07815	1.94068
C	0.31171	2.78492	0.44185
C	-0.41454	1.92708	-0.34088
C	-0.21971	-1.96535	-0.35251
C	0.60019	-2.72705	0.43654
S	-0.17341	-3.00148	1.98742
C	-1.59249	-2.08252	1.53246
C	1.93072	-3.26380	0.12281
C	-2.71362	-1.93414	2.51466
C	-3.01317	1.83640	2.43308
C	1.60582	3.41912	0.15969
C	2.42007	-4.43857	0.71991
C	3.67399	-4.94191	0.39169
C	4.49264	-4.30363	-0.54909
C	4.00718	-3.13203	-1.14009
C	2.75764	-2.61567	-0.80886
C	2.47162	3.82789	1.18915
C	3.69434	4.42478	0.90469
C	4.11416	4.63469	-0.41530
C	3.25466	4.22409	-1.44023
C	2.02346	3.63571	-1.16333
C	5.84960	-4.85955	-0.90112
C	5.43896	5.29192	-0.71074
H	-5.19123	-0.29128	-2.27782
H	-3.67658	-0.21484	-3.16592
C	-3.17249	2.13415	-2.40229
C	-4.84941	1.67337	-0.60505
C	-2.92320	-2.47976	-2.34783
C	-4.62105	-2.15183	-0.54139
H	-0.06972	1.58469	-1.30800
H	0.04386	-1.68192	-1.36309
H	-3.48161	-1.27425	2.11242
H	-2.36573	-1.50816	3.46090
H	-3.18245	-2.89672	2.74487
H	-3.70960	1.09200	2.04897
H	-3.56903	2.76726	2.58770
H	-2.66725	1.49817	3.41473
H	1.80746	-4.97671	1.43539
H	4.01926	-5.85434	0.86851
H	4.62121	-2.60592	-1.86442
H	2.42651	-1.69133	-1.26785
H	2.19502	3.66283	2.22499
H	4.33888	4.72580	1.72513
H	3.54593	4.37782	-2.47468
H	1.37363	3.35541	-1.98445
H	6.52565	-4.83547	-0.03974
H	6.31612	-4.28783	-1.70637
H	5.78060	-5.90278	-1.22551
H	5.44855	6.33292	-0.36988
H	5.65443	5.28977	-1.78150
H	6.26010	4.77873	-0.20045
H	-4.52602	2.54133	-0.02371

H	-5.28534	0.94466	0.08348
H	-5.64167	2.00761	-1.28349
H	-3.69126	-2.85063	-3.03512
H	-2.51393	-3.34128	-1.81259
H	-2.12202	-2.04024	-2.94912
H	-2.32147	1.76624	-2.98276
H	-3.96739	2.39993	-3.10726
H	-2.86388	3.04983	-1.88982
H	-5.12807	-1.45412	0.12981
H	-5.37726	-2.59534	-1.19799
H	-4.19422	-2.95795	0.06204

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