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Supporting Information

Bright Luminescence by Combining Chiral [2.2]Paracyclophane with a Boron–Nitrogen-Doped Polyaromatic Hydrocarbon Building Block

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Table of Contents

1. Materials and Synthesis

General. Unless otherwise indicated, all reactions were carried out under dry and inert conditions by heating all glassware with a heat gun under vacuum and purging with argon. All chemicals and solvents were purchased from commercial suppliers in anhydrous form or were dried by known methods or, in the cases of CH_2Cl_2, THF and toluene taken from a MBRAUN SPS 800 solvent purification system. Solvents were degassed by the freeze-pump-thaw method. TLC was done using precoated polyester sheets (40 × 80 mm) from Machery-Nagel (POLYGAM® SIL G/UV254) with 0.2 mm silica gel 60 with fluorescent indicator. A UV light source from Köhler (254 nm and 366 nm) was used for visualization. NMR spectroscopy was done on a Bruker Avance III 400 spectrometer (equipped with a dual ($^1H/^{13}C$) probe head. Chemical shifts δ are given in ppm, coupling constants *J* in hertz (Hz) and standard abbreviations are designated to the multiplicities of the signals. The spectra were calibrated with the solvent residual signals. High resolution mass spectrometry was done with electron spray ionization time of flight mass spectrometry (ESI-TOF-MS) on a maXis 4G Bruker system. UV/Vis absorption spectra were recorded on a PerkinElmer Lambda 1050 spectrometer with a PerkinElmer 3D WB Det Module in 1.0 cm quartz cuvettes, and samples were analyzed in CH_2Cl_2 at room temperature. Agglomeration experiments of higher concentrated samples up to $c = 1.00 \cdot 10^{-3}$ M were measured in a measuring cell with 100-1000 µm optical path. Steady-state excitation and emission spectra were recorded on a Horiba Fluorolog-3 DF spectrofluorimeter equipped with a 450 W Xe lamp, and samples were analysed in CH_2Cl_2 at room temperature. Emission was monitored at a 90° angle using a Hamamatsu R2658P PMT (UV/Vis/NIR, 200 nm < λ_{em} < 1000 nm) detector. Spectral selection was achieved by the double grating monochromator 320DFX for excitation (1200 grooves/nm, blazed at 330 nm) and the single grating emission monochromator iHR550 for the visible path (1200 grooves/nm, blazed at 500 nm). To avoid higher order excitation light, long pass filter plates were used when needed. For the lifetime measurements, a pulsed LED (Horiba DeltaDiode-310, λ_{em} = 308±10 nm, pulse width ~1 ns FWHM, P_{avg} = 5 µW) was used. Lifetime data analysis (least square fitting, statistical parameters, etc.) was performed using the software package DAS from Horiba. Lifetimes were determined from the decay curves by an iterative reconvolution fitting method using appropriate multi-exponential functions and taking into account the instruments response function. The instrument used for determination of fluorescence quantum yields of **6**, ***7m*** and ***7p*** was a PTI Quantamaster QM4 equipped with a 75 W continuous Xe short arc lamp as excitation source. Spectral selection was achieved by single grating monochromators (excitation:1200 grooves/mm, 300 nm blaze; UV-Vis emission: 1200 grooves/mm, 500 nm blaze). Samples of **6**, ***7m*** and ***7p*** in CH_2Cl_2 were measured with an excitation wavelength λ_{ex} = 345 nm (quinine sulfate in 0.1 M aqueous H_2SO_4 as reference with a fluorescence quantum yield of Φ = 0.546[1]). All measurements were done in spectroscopy grade solvents. Circular dichroism (CD) spectra were recorded on a JASCO J-710 spectropolarimeter with CH_2Cl_2 as a solvent at room temperature. Circular polarized luminescence (CPL) spectra were recorded on a home-build spectrofluorimeter, which is a converted decommissioned circular dichroism spectropolarimeter (Jasco J500-C spectropolarimeter, 1981).[2] A 365 nm LED was used as the excitation source, employing a 90° geometry and the excitation light was linearly polarized parallel to the detection direction. Luminescence dissymmetry factor (g_{lum}) was calculated as $2(I_L-I_R)/(I_L+I_R)$, where I_L and I_R are left and right circularly polarized components of the emission. Specific rotations ($[\alpha]_D^{20}$) were measured with a Polarimeter 341 from Perkin-Elmer.

Materials. The synthesis and full characterization of compounds **1**, **2**, 4,7,12,15-tetrabromo[2.2]paracyclophane, and rac-**5** have been reported previously.[3–5] 4,7,12,15-tetra(trimethylsilylethynyl)[2.2]paracyclophane was prepared following a modified literature procedure,[5] using CuI/$Pd_2(dba)_3$ with (*t*-Bu)$_3$PH·BF_4 as catalysts instead of CuI/Pd(PPh_3)$_4$, resulting in the formation of fewer side-products and higher yield. Enantiopure (R)-**5** and (S)-**5** were prepared according to a procedure by Morisaki et al.[6]

Synthetic Procedures.

4,7,12,15-Tetra(trimethylsilylethynyl)[2.2]paracyclophane

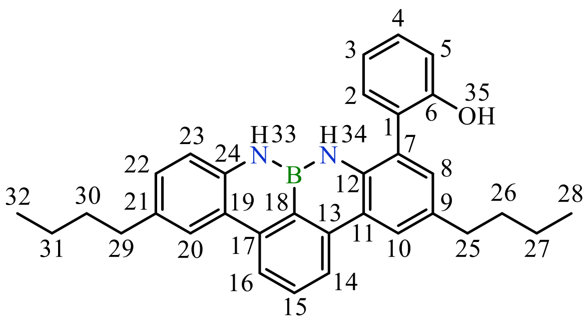
4,7,12,15-Tetrabromo[2.2]paracyclophane (2.50 g, 4.77 mmol, 1.00 eq), CuI (182 mg, 0.95 mmol 0.20 eq), $Pd_2(dba)_3$ (440 mg, 0.48 mmol 0.10 eq.) and (*t*-Bu)$_3$PH·BF_4 (554 mg, 1.91 mmol, 0.40 eq) are suspended in dry, degassed THF/Et_3N (100 ml, 1:1 v/v). Trimethylsilylacetylene (8.15 ml, 57.3 mmol, 12.00 eq) is added and the reaction mixture is heated to 50 °C. After stirring for 18 h, the mixture is allowed to cool to r.t. and all volatiles are removed under reduced pressure. The residue is suspended in CH_2Cl_2 and filtered through a Celite plug. The filtrate is evaporated to dryness and the crude product is purified by silica column chromatography ($CHCl_3$/pentane 1:20) yielding the product as a yellow solid (2.42 g, 4.08 mmol, 86 %).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.98 (s, 4H), 3.43-3.33 (m, 4H), 2.96-2.86 (m, 4H), 0.31 (s, 36H) ppm.

^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 142.3, 134.6, 125.3, 104.9, 99.6, 32.3, 0.2 ppm.

The signals are according to the literature.[5]

1-(2-Hydroxyphenyl)-NBN-benzo[*f,g*]tetracene, 3*o*



1-Bromo-NBN-benzo[*f,g*]tetracene (**2**) (500 mg, 1.09 mmol, 1.00 eq), 2-hydroxyphenylboronic acid pinacol ester (335 mg, 1.52 mmol, 1.40 eq) and Pd(PPh_3)$_4$ (126 mg, 0.11 mmol, 0.10 eq) are suspended in deoxygenated THF (5 mL) and aqueous, deoxygenated 2M K_2CO_3 (2.18 mL, 4.36 mmol, 4.00 eq). The mixture is heated to 75 °C for 40-48 h and is allowed to cool to r.t.. The suspension is poured into water (25 mL) and the aqueous phase is extracted with CH_2Cl_2 (3 x 20 mL). The combined organic phases are washed with brine (20 mL), dried over $MgSO_4$ and filtered. The solvent is evaporated under reduced pressure and the crude product is purified by silica gel column chromatography (EA/hexane 2:7, R_f = 0.61 in EA/hexane 1:2) yielding **3*o*** as a colorless, foam-like solid (509 mg, 1.08 mmol, 99 %); mp 67-68 °C. Small impurities remain in the isolated product that are related to the starting material hydroxyphenylboronic acid pinacol ester or compounds with a similar substitution pattern on the benzene ring and are best removed in the following synthesis step by triflation of the hydroxyl group of **3*o*** and subsequent column chromatography.

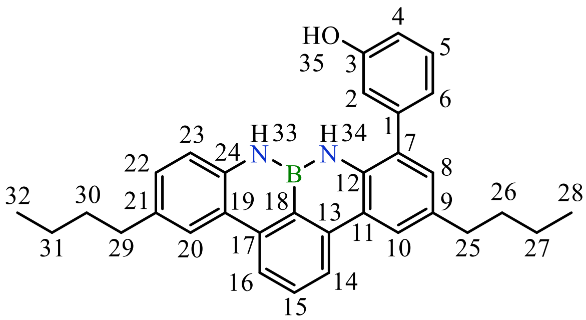
^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.24 (d, ^3J = 8.0 Hz, 1H, H-14), 8.20 (d, ^3J = 8.0 Hz, 1H, H-16), 8.17 (d, ^4J = 1.9 Hz, 1H, H-10), 8.04 (d, ^4J = 1.9 Hz, 1H, H-20), 7.83 (vt, ^3J = 8.0 Hz, 1H, H-15), 7.41 (ddd, ^3J = 8.2 Hz, ^3J = 7.4 Hz, ^4J = 1.7 Hz, 1H, H-4), 7.33 (dd, ^3J = 7.8 Hz, ^4J = 1.7 Hz, 1H, H-2), 7.18-7-06 (m, 4H, H-3, H-5, H-8, H-22), 6.91 (d, ^3J = 8.1 Hz, 1H, H-23), 6.31 (s, 1H, NH-34), 6.28 (s, 1H, NH-33), 5.13 (s, 1H, OH-35), 2.77-2.65 (m, 4H, H-25, H-29), 1.75-1.60 (m, 4H, H-26, H-30), 1.49-1.35 (m, 4H, H-27, H-31), 1.01-0.92 (m, 6H, H-28, H-32) ppm.

$^{13}C\{^1H\}$ NMR (101 MHz, CD_2Cl_2): δ 154.1 (C-6), 139.6 (C-17), 139.5 (C-13), 139.0 (C-24), 137.3 (C-12), 134.9 (C-9), 134.8 (C-21), 131.9 (C-2), 131.5 (C-15), 131.2 (C-8), 130.6 (C-4), 129.4 (C-22), 127.6 (C-18, determined via 2D spectra), 125.2 (C-10), 125.0 (C-1), 124.4 (C-20), 124.3 (C-7), 123.2 (C-11), 122.2 (C-19), 121.7 (C-3), 119.6 (C-16), 119.5 (C-14), 118.6 (C-23), 116.5 (C-5), 35.8 (C-29), 35.8 (C-25), 34.8 (C-30), 34.7 (C-26), 23.0 (C-31), 23.0 (C-27), 14.4 (C-28, C-32) ppm.

$^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2): δ 26.9 ppm.

HRMS (ESI): *m/z* $[M\text{-}H]^-$ calculated for $C_{32}H_{32}BN_2O$: 471.26187; found: 471.26209 (Δ: 0.45 ppm).

1-(3-Hydroxyphenyl)-NBN-benzo[*f,g*]tetracene, 3*m*



1-Bromo-NBN-benzo[*f,g*]tetracene (**2**) (565 mg, 1.23 mmol, 1.00 eq), 3-hydroxyphenylboronic acid pinacol ester (379 mg, 1.72 mmol, 1.40 eq) and $Pd(PPh_3)_4$ (142 mg, 0.12 mmol, 0.10 eq) are suspended in deoxygenated THF (6 mL) and aqueous, deoxygenated 2M K_2CO_3 (2.46 mL, 4.92 mmol, 4.00 eq). The mixture is heated to 75 °C for 40-48 h and is allowed to cool to r.t.. The suspension is poured into water (25 mL) and the aqueous phase is extracted with CH_2Cl_2 (3 x 20 mL). The combined organic phases are washed with brine (20 mL), dried over $MgSO_4$ and filtered. The solvent is evaporated under reduced pressure and the crude product is purified by silica gel column chromatography (EA/hexane 2:7, R_f = 0.65 in EA/hexane 1:2) yielding **3*m*** as a colorless, highly viscous oil (575 mg, 1.22 mmol, 99 %). Small impurities remain in the isolated product that are related to the starting material hydroxyphenylboronic acid pinacol ester or compounds with a similar substitution pattern on the benzene ring and are best removed in the following synthesis step by triflation of the hydroxyl group of **3*m*** and subsequent column chromatography.

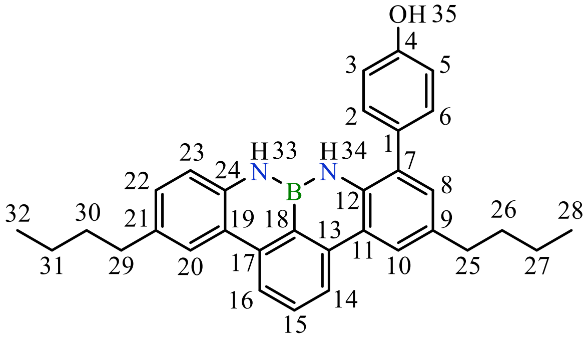
^1H NMR (400 MHz, CD_2Cl_2): δ 8.23 (d, ^3J = 8.0 Hz, 1H, H-14), 8.18 (d, ^3J = 8.0 Hz, 1H, H-16), 8.10 (d, ^4J = 1.3 Hz, 1H, H-10), 8.04 (d, ^4J = 1.1 Hz, 1H, H-20), 7.82 (vt, ^3J = 8.0 Hz, 1H, H-15), 7.42 (vt, ^3J = 7.8 Hz, 1H, H-5), 7.12 (m, 2H, H-8 + H-22), 7.08 (dvt, ^3J = 7.8 Hz, ^4J = 1.0 Hz, 1H, H-6), 6.99 (dd, ^4J = 2.5 Hz, ^4J = 1.0 Hz, 1H, H-2), 6.95 (ddd, ^3J = 7.8 Hz, ^4J = 2.5 Hz, ^4J = 1.0 Hz, 1H, H-4), 6.90 (d, ^3J = 8.1 Hz, 1H, H-23), 6.69 (s, 1H, NH-34), 6.26 (s, 1H, NH-33), 5.63 (s, 1H, OH-35), 2.78-2.65 (m, 4H, H-25 + H-29), 1.76-1.61 (m, 4H, H-26 + H-30), 1.50-1.36 (m, 4H, H-27 + H-31), 1.03-0.93 (m, 6H, H-28 + H-32) ppm.

$^{13}C\{^1H\}$ NMR (101 MHz, CD_2Cl_2): δ 157.0 (C-3), 141.6 (C-1), 139.8 (C-13), 139.6 (C-17), 139.2 (C-24), 136.3 (C-12), 134.7 (C-21), 134.1 (C-9), 131.4 (C-15), 131.0 (C-5), 130.7 (C-7), 130.4 (C-8), 129.3 (C-22), 127.4 (C-18), 124.4 (C-20), 124.1 (C-10), 122.5 (C-11), 122.5 (C-6), 122.2 (C-19), 119.6 (C-14), 119.3 (C-16), 118.5 (C-23), 117.1 (C-2), 115.1 (C-4), 35.8 (C-29 + C-25), 34.8 (C-30), 34.7 (C-26), 23.0 (C-31), 23.0 (C-27), 14.4 (C-32), 14.4 (C-28) ppm.

$^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2): δ 26.7 ppm.

HRMS (ESI): *m/z* $[M\text{-}H]^-$ calculated for $C_{32}H_{32}BN_2O$: 471.26187; found: 471.26254 (Δ: 1.41 ppm).

1-(4-Hydroxyphenyl)-NBN-benzo[*f*,*g*]tetracene, 3*p*



1-Bromo-NBN-benzo[*f*,*g*]tetracene (**2**) (500 mg, 1.09 mmol, 1.00 eq), 4-hydroxyphenylboronic acid pinacol ester (335 mg, 1.52 mmol, 1.40 eq) and $Pd(PPh_3)_4$ (126 mg, 0.11 mmol, 0.10 eq) are suspended in deoxygenated THF (5 mL) and aqueous, deoxygenated 2M K_2CO_3 (2.18 mL, 4.36 mmol, 4.00 eq). The mixture is heated to 75 °C for 40-48 h and is allowed to cool to r.t.. The suspension is poured into water (25 mL) and the aqueous phase is extracted with CH_2Cl_2 (3 x 20 mL). The combined organic phases are washed with brine (20 mL), dried over $MgSO_4$ and filtered. The solvent is evaporated under reduced pressure and the crude product is purified by silica gel column chromatography (EA/hexane 2:7, R_f = 0.58 in EA/hexane 1:2) yielding **3*p*** as a colorless, foam-like solid (444 mg, 0.940 mmol, 86 %); mp 159-162 °C (decomposition). Small impurities remain in the isolated product that are related to the starting material hydroxyphenylboronic acid pinacol ester or compounds with a similar substitution pattern on the benzene ring and are best removed in the following synthesis step by triflation of the hydroxyl group of **3*p*** and subsequent column chromatography.

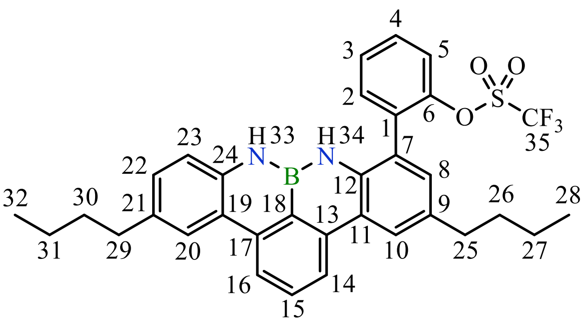
^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.23 (d, ^3J = 8.0 Hz, 1H, H-14), 8.18 (d, ^3J = 8.0 Hz, 1H, H-16), 8.08 (d, ^4J = 1.8 Hz, 1H, H-10), 8.04 (d, ^4J = 1.8 Hz, 1H, H-20), 7.82 (vt, ^3J = 8.0 Hz, 1H, H-15), 7.42-7.36 (m, 2H, H-2 + H-6), 7.13 (dd, ^3J = 8.1 Hz, ^4J = 1.8 Hz, 1H, H-22), 7.09 (d, ^4J = 1.8 Hz, 1H, H-6), 7.04-6.99 (m, 2H, H-3 + H-5), 6.92 (d, ^3J = 8.1 Hz, 1H, H-23), 6.62 (s, 1H, NH-34), 6.24 (s, 1H, NH-33), 5.18 (s, 1H, OH-35), 2.77-2.64 (m, 4H, H-25 + H-29), 1.75-1.60 (m, 4H, H-26 + H-30), 1.50-1.35 (m, 4H, H-27 + H-31), 1.02-0.92 (m, 6H, H-28 + H-32) ppm.

^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2): δ 155.9 (C-4), 139.9 (C-13), 139.6 (C-17), 139.2 (C-24), 136.4 (C-12), 134.7 (C-9), 134.1 (C-21), 132.1 (C-1), 131.6 (C-6), 131.4 (C-15), 130.7 (C-8), 130.7 (C-7), 129.3 (C-22), 127.4 (C-18, determined via 2D spectra), 124.4 (C-20), 123.7 (C-10), 122.4 (C-11), 122.2 (C-19), 119.5 (C-14), 119.2 (C-16), 118.5 (C-23), 116.5 (C-3 + C-5), 35.8 (C-29), 35.8 (C-25), 34.8 (C-30), 34.8 (C-26), 23.0 (C-31), 23.0 (C-27), 14.4 (C-32), 14.4 (C-28) ppm.

^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2): δ 26.8 ppm.

HRMS (ESI): *m/z* $[M-H]^-$ calculated for $C_{32}H_{32}BN_2O$: 471.26187; found: 471.26231 (Δ: 0.92 ppm).

1-(2-(Trifluoromethylsulfonyl)phenyl)-NBN-benzo[*f*,*g*]tetracene, 4*o*



1-(2-Hydroxyphenyl)-NBN-benzo[*f*,*g*]tetracene (**3*o***) (507 mg, 1.07 mmol, 1.00 eq) is dissolved in anhydrous CH_2Cl_2 (35 mL). Anhydrous pyridine (0.89 mL, 11.1 mmol, 10.3 eq) is added and the solution is cooled to 0 °C. Trifluoromethanesulfonic anhydride (0.44 mL, 2.61 mmol, 2.43 eq) is added drop-wise under stirring and the mixture is allowed to warm to r.t.. The reaction is stopped after 2 h by addition of aqueous HCl (3N, 30 mL) and is extracted with CH_2Cl_2 (1 x 20 mL, 2 x 10 mL). The combined org. phases are washed with aqueous HCl (1N, 20 mL), sat. aqueous $NaHCO_3$ (20 mL) and brine (20 mL), dried over $MgSO_4$ and filtered. The solvent is evaporated under reduced pressure and the crude product is purified by silica gel column chromatography ($CHCl_3$/hexane 2:3, R_f = 0.27) yielding **4*o*** as a colorless, foam-like solid (587 mg, 0.97 mmol, 90 %); mp 61-62 °C.

^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.24 (d, ^3J = 8.0 Hz, 1H, H-14), 8.20 (d, ^3J = 8.0 Hz, 1H, H-16), 8.17 (d, ^4J = 1.7 Hz, 1H, H-10), 8.04 (d, ^4J = 1.6 Hz, 1H, H-20), 7.83 (vt, ^3J = 8.0 Hz, 1H, H-15), 7.65-7.57 (m, 3H, H-2, H-3, H-4), 7.56-7.49 (m, 1H, H-5), 7.13 (dd, ^3J = 8.1 Hz, ^4J = 1.6 Hz, 1H, H-22), 7.11 (d, ^4J = 1.7 Hz, 1H, H-8), 6.92 (d, ^3J = 8.1 Hz, 1H, H-23), 6.26 (s, 1H, NH-34), 6.15 (s, 1H, NH-33), 2.80-2.62 (m, 4H, H-25, H-29), 1.76-1.61 (m, 4H, H-26, H-30), 1.49-1.34 (m, 4H, H-27, H-31), 1.00-0.92 (m, 6H, H-28, H-32) ppm.

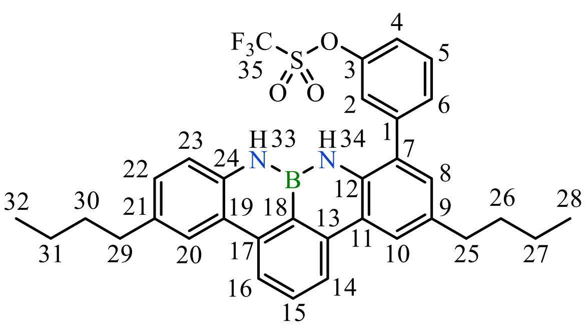
^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2): δ 148.5 (C-6), 139.6 (C-17), 139.5 (C-13), 139.0 (C-24), 136.9 (C-12), 134.9 (C-21), 134.1 (C-9), 133.8 (C-2), 133.3 (C-1), 131.5 (C-15), 131.2 (C-8), 130.7 (C-4), 129.7 (C-3), 129.3 (C-22), 127.5 (C-18, determined via 2D spectra), 125.3 (C-10), 124.4 (C-20), 123.8 (C-7), 123.1 (C-11), 122.2 (C-19), 119.6 (C-16), 119.5 (C-14), 118.9 (q, $^1J_{CF}$ = 320 Hz, C-35), 118.6 (C-23), 35.8 (C-29), 35.7 (C-25), 34.8 (C-30), 34.6 (C-26), 23.0 (C-31), 22.8 (C-27), 14.4 (C-32), 14.3 (C-28) ppm.

^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2): δ 26.8 ppm.

^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2): δ -74.6 ppm.

HRMS (ESI): *m/z* $[M+Na]^+$ calculated for $C_{33}H_{32}BF_3N_2NaO_3S$: 627.20767; found: 627.20835 (Δ: 1.07 ppm).

1-(3-(Trifluoromethylsulfonyl)phenyl)-NBN-benzo[*f*,*g*]tetracene, 4*m*



1-(3-Hydroxyphenyl)-NBN-benzo[*f*,*g*]tetracene (**3*m***) (525 mg, 1.11 mmol, 1.00 eq) is dissolved in anhydrous CH_2Cl_2 (35 mL). Anhydrous pyridine (0.98 mL, 11.4 mmol, 10.3 eq) is added and the solution is cooled to 0 °C. Trifluoromethanesulfonic anhydride (0.45 mL, 2.70 mmol, 2.43 eq) is added drop-wise under stirring and the mixture is allowed to warm to r.t.. The reaction is stopped after 2 h by addition of aqueous HCl (3N, 40 mL) and is extracted with CH_2Cl_2 (1 x 30 mL, 2 x 20 mL). The combined org. phases are washed with aqueous HCl (1N, 30 mL), sat. aqueous $NaHCO_3$ (30 mL) and brine (30 mL), dried over $MgSO_4$ and filtered. The solvent is evaporated under reduced pressure and the crude product is purified by silica gel column chromatography ($CHCl_3$/hexane 2:3, R_f = 0.58 in $CHCl_3$/hexane 1:1) yielding **4*m*** as a yellow, highly viscous oil (598 mg, 0.99 mmol, 89 %).

^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.24 (d, ^3J = 8.0 Hz, 1H, H-14), 8.20 (d, ^3J = 8.0 Hz, 1H, H-16), 8.14 (d, ^4J = 1.6 Hz, 1H, H-10), 8.05 (d, ^4J = 1.4 Hz, 1H, H-20), 7.83 (vt, ^3J = 8.0 Hz, 1H, H-15), 7.67 (vt, ^3J = 7.9 Hz, 1H, H-5), 7.61 (ddd, ^3J = 7.9 Hz, ^4J = 1.6 Hz, ^4J = 1.0 Hz, 1H, H-6), 7.50 (dd, ^4J = 2.6 Hz, ^4J = 1.6 Hz, 1H, H-2), 7.40 (ddd, ^3J = 7.9 Hz, ^4J = 2.6 Hz, ^4J = 1.0 Hz, 1H, H-4), 7.14 (dd, ^3J = 8.1 Hz, ^4J = 1.8 Hz, 1H, H-22), 7.12 (d, ^4J = 1.8 Hz, 1H, H-8), 6.95 (d, ^3J = 8.1 Hz, 1H, H-23), 6.50 (s, 1H, NH-34), 6.26 (s, 1H, NH-33), 2.78-2.65 (m, 4H, H-25, H-29), 1.76-1.61 (m, 4H, H-26, H-30), 1.50-1.35 (m, 4H, H-27, H-31), 1.02-0.93 (m, 6H, H-28, H-32) ppm.

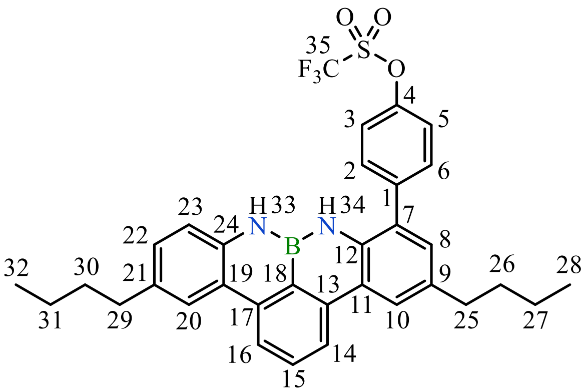
$^{13}C\{^1H\}$ NMR (101 MHz, CD_2Cl_2): δ 150.6 (C-3), 142.7 (C-1), 139.6 (C-17), 139.5 (C-13), 139.0 (C-24), 136.1 (C-12), 134.9 (C-21), 134.5 (C-9), 131.7 (C-5), 131.5 (C-15), 130.6 (C-6), 130.4 (C-8), 129.4 (C-22), 128.7 (C-7), 127.4 (C-18, determined via 2D spectra), 124.9 (C-10), 124.4 (C-20), 123.4 (C-2), 123.0 (C-11), 122.2 (C-19), 120.9 (C-4), 119.6 (C-14), 119.6 (C-16), 119.4 (q, $^1J_{CF}$ = 321 Hz, C-35), 118.6 (C-23), 35.8 (C-29), 35.8 (C-25), 34.8 (C-30), 34.7 (C-26), 23.0 (C-31), 23.0 (C-27), 14.4 (C-28, C-32) ppm.

$^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2): δ 26.8 ppm.

$^{19}F\{^1H\}$ NMR (376 MHz, CD_2Cl_2): δ -73.1 ppm.

HRMS (ESI): *m/z* $[M+Na]^+$ calculated for $C_{33}H_{32}BF_3N_2NaO_3S$: 627.20767; found: 627.20855 (Δ: 1.39 ppm).

1-(4-(Trifluoromethylsulfonyl)phenyl)-NBN-benzo[*f,g*]tetracene, 4*p*



1-(4-Hydroxyphenyl)-NBN-benzo[*f,g*]tetracene (**3*p***) (405 mg, 0.86 mmol, 1.00 eq) is dissolved in anhydrous CH_2Cl_2 (30 mL). Anhydrous pyridine (0.71 mL, 8.83 mmol, 10.3 eq) is added and the solution is cooled to 0 °C. Trifluoromethanesulfonic anhydride (0.35 mL, 2.08 mmol, 2.43 eq) is added drop-wise under stirring and the mixture is allowed to warm to r.t.. The reaction is stopped after 2 h by addition of aqueous HCl (3N, 30 mL) and is extracted with CH_2Cl_2 (1 x 25 mL, 2 x 15 mL). The combined org. phases are washed with aqueous HCl (1N, 25 mL), sat. aqueous $NaHCO_3$ (25 mL) and brine (25 mL), dried over $MgSO_4$ and filtered. The solvent is evaporated under reduced pressure and the crude product is purified by silica gel column chromatography ($CHCl_3$/hexane 1:2, R_f = 0.28) yielding **4*p*** as a colorless, crystalline solid (463 mg, 0.77 mmol, 89 %); mp 161-162 °C.

^1H NMR (400 MHz, CD_2Cl_2): δ 8.24 (d, ^3J = 8.0 Hz, 1H, H-14), 8.20 (d, ^3J = 8.0 Hz, 1H, H-16), 8.14 (d, ^4J = 1.6 Hz, 1H, H-10), 8.05 (d, ^4J = 1.4 Hz, 1H, H-20), 7.83 (vt, ^3J = 8.0 Hz, 1H, H-15), 7.67 (vt, ^3J = 7.9 Hz, 1H, H-5), 7.61 (ddd, ^3J = 7.9 Hz, ^4J = 1.6 Hz, ^4J = 1.0 Hz, 1H, H-6), 7.50 (dd, ^4J = 2.6 Hz, ^4J = 1.6 Hz, 1H, H-2), 7.40 (ddd, ^3J = 7.9 Hz, ^4J = 2.6 Hz, ^4J = 1.0 Hz, 1H, H-4), 7.14 (dd, ^3J = 8.1 Hz, ^4J = 1.8 Hz, 1H, H-22), 7.12 (d, ^4J = 1.8 Hz, 1H, H-8), 6.95 (d, ^3J = 8.1 Hz, 1H, H-23), 6.50 (s, 1H, NH-34), 6.26 (s, 1H, NH-33), 2.78-2.65 (m, 4H, H-25, H-29), 1.76-1.61 (m, 4H, H-26, H-30), 1.50-1.35 (m, 4H, H-27, H-31), 1.02-0.93 (m, 6H, H-28, H-32) ppm.

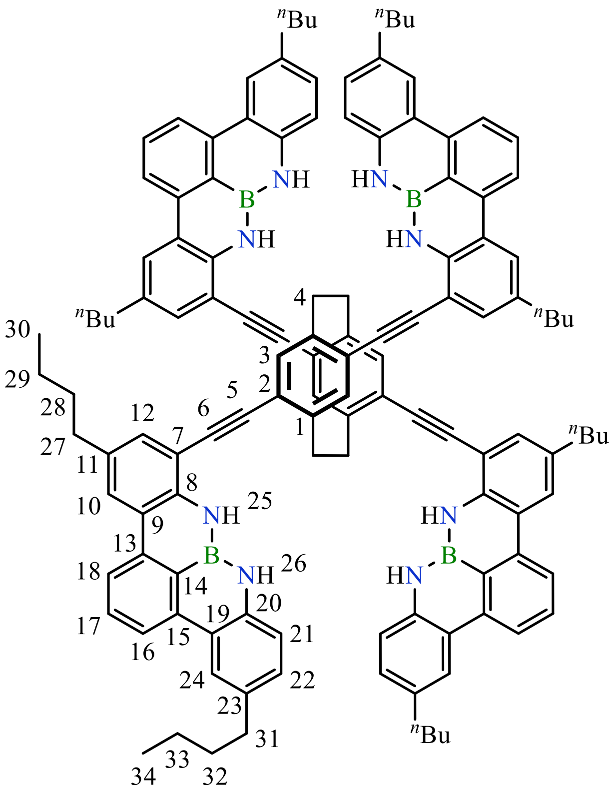
$^{13}C\{^1H\}$ NMR (101 MHz, CD_2Cl_2): δ 150.6 (C-3), 142.7 (C-1), 139.6 (C-17), 139.5 (C-13), 139.0 (C-24), 136.1 (C-12), 134.9 (C-21), 134.5 (C-9), 131.7 (C-5), 131.5 (C-15), 130.6 (C-6), 130.4 (C-8), 129.4 (C-22), 128.7 (C-7), 127.4 (C-18, determined via 2D spectra), 124.9 (C-10), 124.4 (C-20), 123.4 (C-2), 123.0 (C-11), 122.2 (C-19), 120.9 (C-4), 119.6 (C-14), 119.6 (C-16), 119.4 (q, $^1J_{CF}$ = 321 Hz, C-35), 118.6 (C-23), 35.8 (C-29), 35.8 (C-25), 34.8 (C-30), 34.7 (C-26), 23.0 (C-31), 23.0 (C-27), 14.4 (C-28, C-32) ppm.

$^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2): δ 26.8 ppm.

$^{19}F\{^1H\}$ NMR (376 MHz, CD_2Cl_2): δ -73.1 ppm.

HRMS (ESI): *m/z* $[M+Na]^+$ calculated for $C_{33}H_{32}BF_3N_2NaO_3S$: 627.20767; found: 627.20855 (Δ: 1.39 ppm).

4,7,12,15-Tetra[NBN-benzo[*f*,*g*]tetracen-1-ylethynyl][2.2]paracyclophane, rac-6, (R)-6, (S)-6.



Synthesis and purification are performed in the dark or under red light. 4,7,12,15-Tetraethynyl[2.2]paracyclophane rac-**5** (30.4 mg, 0.10 mmol, 1.00 eq), 1-bromo-NBN-benzo[*f*,*g*]tetracene (**2**) (202 mg, 0.44 mmol, 4.40 eq), CuI (4.2 mg, 22 µmol 0.22 eq), $Pd_2(dba)_3$ (12.8 mg, 11 µmol 0.11 eq) and $(t\text{-}Bu)_3PH\cdot BF_4$ (12.8 mg, 44 µmol, 0.44 eq) are suspended in dry, degassed THF/Et_3N (4 ml, 1:1 v/v). The reaction mixture is stirred at 50 °C for 18 h in a flask wrapped with aluminum foil to exclude daylight. The mixture is allowed to cool to r.t. and the solvent is removed under reduced pressure. The residue is suspended in CH_2Cl_2 and filtered through a Celite plug. The orange filtrate is evaporated to dryness and the crude product is purified by silica column chromatography ($CHCl_3$/hexane 2:3→1:1→3:2, $R_f = 0.23$ in $CHCl_3$/hexane 1:1) yielding rac-**6** as a yellow solid (149 mg, 82 µmol, 82 %); mp > 299 °C. Enantiopure (R)-**6** and (S)-**6** are obtained by a similar procedure starting from (R)-**5** and (S)-**5** in 79 % and 80 % yield, respectively. $[\alpha]^{20}_{589}$ (c 0.50, $CHCl_3$) +1192° for (R)-**6** and -1189° for (S)-**6**.

^{1}H NMR ($CDCl_3$, 400 MHz,): δ 7.76 (d, ^3J = 8.0 Hz, 4H, H-16), 7.72-7.69 (m, 8H, H-10, H-24), 7.52 (d, ^4J = 1.6 Hz, 4H, H-12), 7.49 (s, 4H, H–3), 7.42 (d, ^3J = 8.0 Hz, 4H, H-18), 7.34 (vt, ^3J = 8.0 Hz, 4H, H-17), 7.01 (dd, ^3J = 8.0 Hz, ^4J = 1.6 Hz, 4H, H-22), 6.99 (s, 4H, NH-25), 6.41 (d, ^3J = 8.0 Hz, 4H, H-21), 5.59 (s, 4H, NH-26), 3.99-3.83 (m, 4H, H-4a), 3.55-3.41 (m, 4H, H-4b), 2.80-2.67 (m, 16H, H-25, H-27), 1.83-1.72 (m, 16H, H-26, H-28), 1.59-1.48 (m, 16H, H-33, H-29, superimposed with H_2O from solvent), 1.09 (s, 12H, H-34), 1.06 (s, 12H, H-30) ppm.

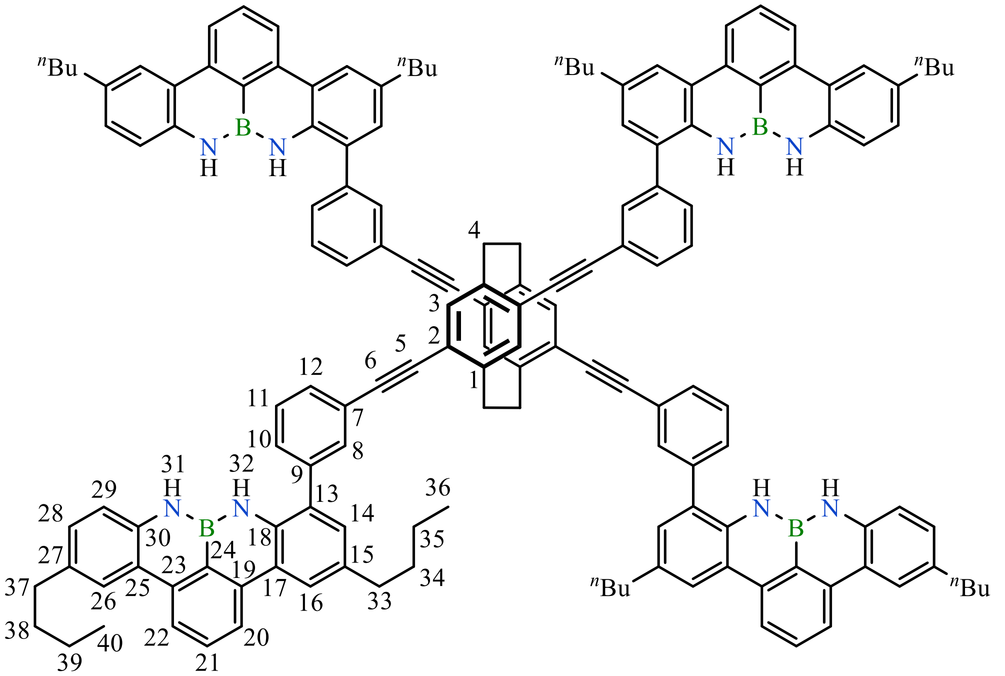
^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz): δ 141.7 (C-2), 139.9 (C-8), 138.3 (C-13), 138.0 (C-20), 137.7 (C-15), 134.5 (C-3), 133.7 (C-23), 133.1 (C-11), 131.0 (C-12), 130.0 (C-17), 127.8 (C-22), 126.6 (C-14), 125.9 (C-10), 125.5 (C-1), 123.5 (C-24), 122.7 (C-9), 121.9 (C-19), 119.0 (C-16), 118.3 (C-18), 118.2 (C-21), 110.2 (C-7), 95.8 (C-5), 92.2 (C-6), 35.6 (C-31), 35.4 (C-27), 34.6 (C-32), 34.2 (C-28), 33.1 (C-4), 22.7 (C-33), 22.7 (C-29), 14.3 (C-34), 14.3 (C-30) ppm.

^{11}B{1H} NMR ($CDCl_3$, 128 MHz): δ 28.3 ppm.

HRMS (ESI): *m/z* $[M+H]^+$ calculated for $C_{128}H_{125}B_4N_8$: 1818.03939; found: 1818.04292 (Δ: 1.09 ppm).

4,7,12,15-Tetra[NBN-benzo[*f*,*g*]tetracen-1-yl-phen-3-yl-ethynyl][2.2]paracyclophane, rac-7m, (R)-7m, (S)-7m.

Synthesis and purification are performed in the dark or under red light. 4,7,12,15-Tetraethynyl[2.2]paracyclophane rac-**5** (22.9 mg, 75.2 µmol, 1.00 eq), 1-(3-(trifluoromethylsulfonyl)phenyl)-NBN-benzo[*f*,*g*]tetracene (**4*m***) (200 mg, 330 µmol, 4.40 eq), CuI (2.9 mg, 15 µmol 0.20 eq) and $PdCl_2$(dppf) (11.0 mg, 15 µmol 0.20 eq) are suspended in dry, degassed THF/Et_3N (2.6 ml, 1:1 v/v). The reaction mixture is stirred at 50 °C for 18 h in a flask wrapped with aluminum foil to exclude daylight. The mixture is allowed to cool to r.t. and the solvent is removed under reduced pressure. The residue is suspended in CH_2Cl_2 and filtered through a Celite plug. The filtrate is evaporated to dryness and the crude product is purified by silica column chromatography (CH_2Cl_2/hexane 7:10, $R_f = 0.60$) yielding rac-**7*m*** as a pale yellow solid (82 mg, 47 µmol, 63 %); mp 169-170 °C. Enantiopure (R)-**7*m*** and (S)-**7*m*** are obtained by a similar procedure starting from (R)-**5** and (S)-**5** in 64 % and 61 % yield, respectively.



^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.22 (d, ^3J = 8.0 Hz, 4H, H-20), 8.17 (d, ^3J = 8.0 Hz, 4H, H-22), 8.09 (d, ^4J = 1.3 Hz, 4H, H-16), 8.01 (d, ^4J = 1.4 Hz, 4H, H-26), 7.81 (vt, ^3J = 8.0 Hz, 4H, H-21), 7.72 (vt, ^4J = 1.6 Hz, 4H, H-8), 7.62 (dvt, ^3J = 7.6 Hz, ^4J = 1.6 Hz, 4H, H-12), 7.39 (dvt, ^3J = 7.6 Hz, ^4J = 1.6 Hz, 4H, H-10), 7.35 (s, ^3J = 7.6 Hz, 4H, H-3), 7.08 (d, ^4J = 1.8 Hz, 4H, H-14), 7.06 (dd, ^3J = 8.1 Hz, ^4J = 1.4 Hz, 4H, H-28), 6.80 (d, ^3J = 8.1 Hz, 4H, H-29), 6.51 (s, 4H, NH-32), 6.18 (s, 4H, NH-31), 3.65-3.54 (m, 4H, H-4a), 3.21-3.08 (m, 4H, H-4b), 2.75-2.61 (m, 16H, H-33, H-37), 1.74-1.57 (m, 16H, H-34, H-38), 1.48-1.33 (m, 16H, H-35, H-39), 0.99-0.91 (m, 16H, H-36, H-40) ppm.

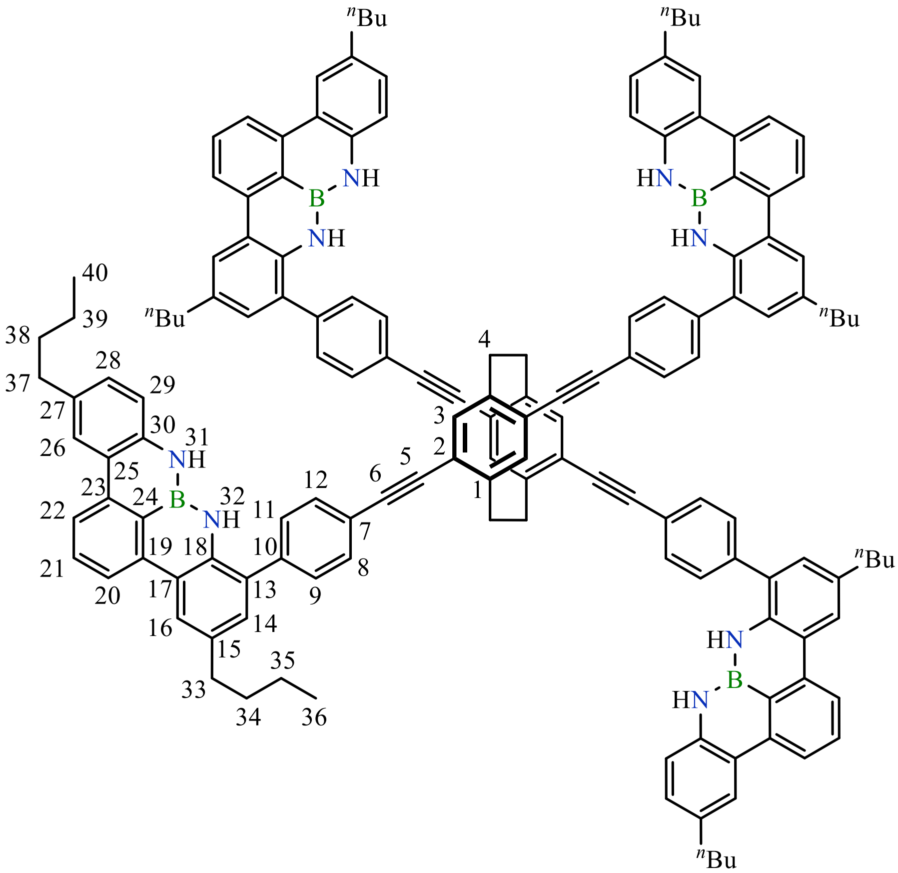
^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2): δ 142.2 (C-2), 139.8 (C-9), 139.1 (C-17), 139.0 (C-23), 138.5 (C-30), 135.7 (C-18), 134.8 (C-3), 134.2 (C-27), 133.7 (C-15), 132.6 (C-8), 130.9 (C-21), 130.6 (C-12), 130.0 (C-10), 129.9 (C-11), 129.5 (C-13), 129.4 (C-14), 128.7 (C-28), 126.9 (C-24), 125.3 (C-1), 124.2 (C-7), 123.8 (C-16, C-26), 122.2 (C-17), 121.6 (C-25), 119.0 (C-20), 118.8 (C-22), 118.0 (C-29), 94.6 (C-6), 89.7 (C-5), 35.2 (C-33, C-37), 34.2 (C-34), 34.1 (C-38), 22.5 (C-35), 22.4 (C-39), 13.8 (C-36), 13.8 (C-40) ppm.

^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2): δ 27.3 ppm.

HRMS (ESI): *m/z* $[M]^+$ calculated for $C_{152}H_{140}B_4N_8$: 2121.16286; found: 2121.16190 (Δ: 0.46 ppm).

4,7,12,15-Tetra[NBN-benzo[*f*,*g*]tetracen-1-yl-phen-4-yl-ethynyl][2.2]paracyclophane, rac-7p, (R)-7p, (S)-7p.

Synthesis and purification are performed in the dark or under red light. 4,7,12,15-Tetraethynyl[2.2]paracyclophane rac-**5** (17.2 mg, 56.4 µmol, 1.00 eq), 1-(4-(trifluoromethylsulfonyl)phenyl)-NBN-benzo[*f*,*g*]tetracene **4*p*** (150 mg, 248 µmol, 4.40 eq), CuI (2.1 mg, 11 µmol 0.20 eq) and $PdCl_2$(dppf) (8.3 mg, 11 µmol 0.20 eq) are suspended in dry, degassed THF/Et_3N (2.0 ml, 1:1 v/v). The reaction mixture is stirred at 50 °C for 18 h in a flask wrapped with aluminum foil to exclude daylight. The mixture is allowed to cool to r.t. and the solvent is removed under reduced pressure. The residue is suspended in CH_2Cl_2 and filtered through a Celite plug. The filtrate is evaporated to dryness and the crude product is purified by silica column chromatography (CH_2Cl_2/hexane 7:10, R_f = 0.64) yielding rac-**7*p*** as a green-yellow solid (73 mg, 34 µmol, 61 %); mp 160-162 °C. Enantiopure (R)-**7*p*** and (S)-**7*p*** are obtained by a similar procedure starting from (R)-**5** and (S)-**5** in 62 % and 61 % yield, respectively.



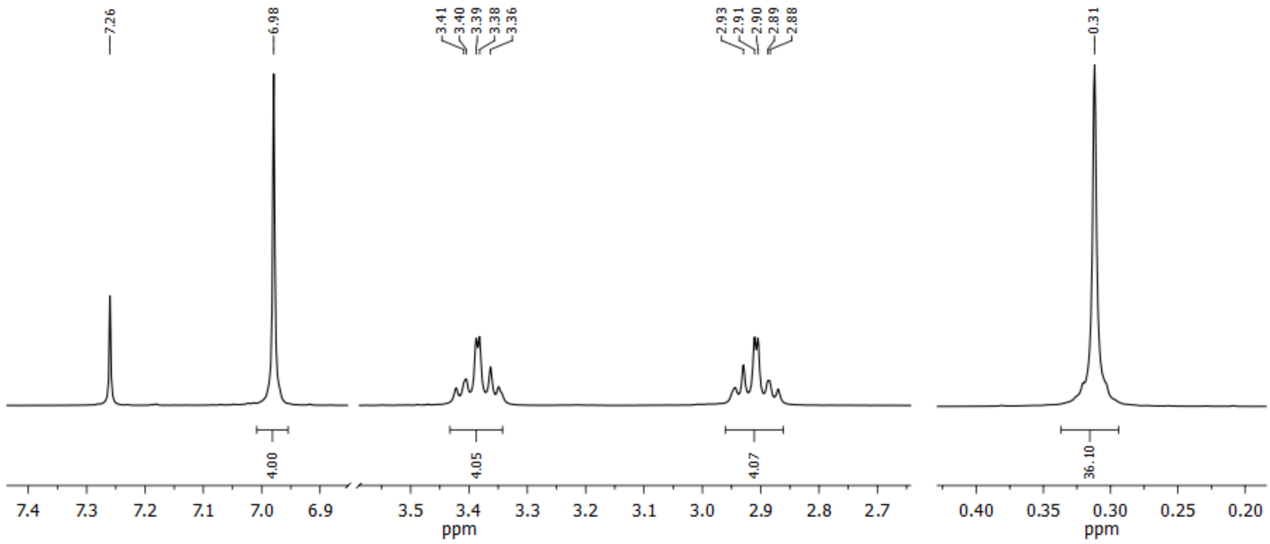
[1]H NMR (400 MHz, CD_2Cl_2): δ 8.23 (d, ^3J = 8.1 Hz, 4H, H-20), 8.18 (d, ^3J = 8.1 Hz, 4H, H-22), 8.11 (d, ^4J = 2.0 Hz, 4H, H-16), 8.02 (d, ^4J = 1.9 Hz, 4H, H-26), 7.93-7.86 (m, 8H, H-8, H-12), 7.82 (vt, ^3J = 8.1 Hz, 4H, H-21), 7.68-7.62 (m, 8H, H-9, H-11), 7.36 (s, 4H, H-3), 7.15 (d, ^4J = 2.0 Hz, 4H, H-14), 7.04 (dd, ^3J = 8.2, ^4J = 1.9 Hz, 4H, H-28), 6.86 (d, ^3J = 8.2 Hz, 4H, H-29), 6.63 (s, 4H, NH-32), 6.24 (s, 4H, NH-31), 3.84-3.70 (m, 4H, H-4a), 3.39-3.24 (m, 4H, H-4b), 2.76-2.61 (m, 16H, H-33, H-37), 1.74-1.57 (m, 16H, H-34, H-38), 1.47-1.34 (m, 16H, H-35, H-39), 0.99-0.91 (m, 24H, H-36, H-40) ppm.

$^{13}C\{^1H\}$ NMR (101 MHz, CD_2Cl_2): δ 142.9 (C-2), 140.4 (C-10), 139.7 (C-19), 139.6 (C-23), 139.0 (C-30), 136.2 (C-18), 135.3 (C-3), 134.8 (C-27), 134.4 (C-15), 132.9 (C-8 + C-12), 131.4 (C-21), 130.7 (C-9, C-11), 130.4 (C-14), 130.3 (C-13), 129.3 (C-28), 127.5 (C-24), 125.8 (C-1), 124.4 (C-16), 124.3 (C-26), 123.3 (C-7), 122.8 (C-17), 122.2 (C-25), 119.6 (C-20), 119.4 (C-22), 118.5 (C-29), 95.2 (C-6), 90.4 (C-5), 35.8 (C-33, C-37), 34.7 (C-38), 34.7 (C-34), 33.4 (C-4), 23.0 (C-39), 23.0 (C-33), 14.4 (C-36, C-40) ppm.

$^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2): δ 26.8 ppm.

HRMS (ESI): *m/z* $[M]^+$ calculated for $C_{152}H_{140}B_4N_8$: 2121.16286; found: 2121.16218 (Δ: 0.33 ppm).

2. Spectra: NMR & mass



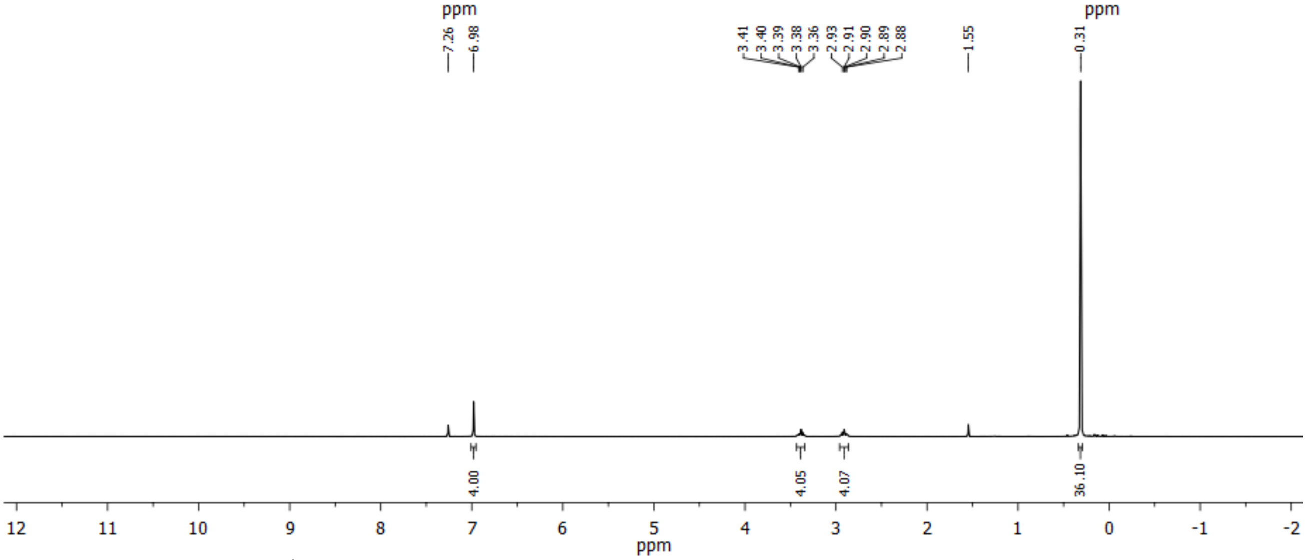


Figure S1. [1]H NMR (400 MHz, $CDCl_3$) of 4,7,12,15-tetra(trimethylsilylethynyl)[2.2]paracyclophane.

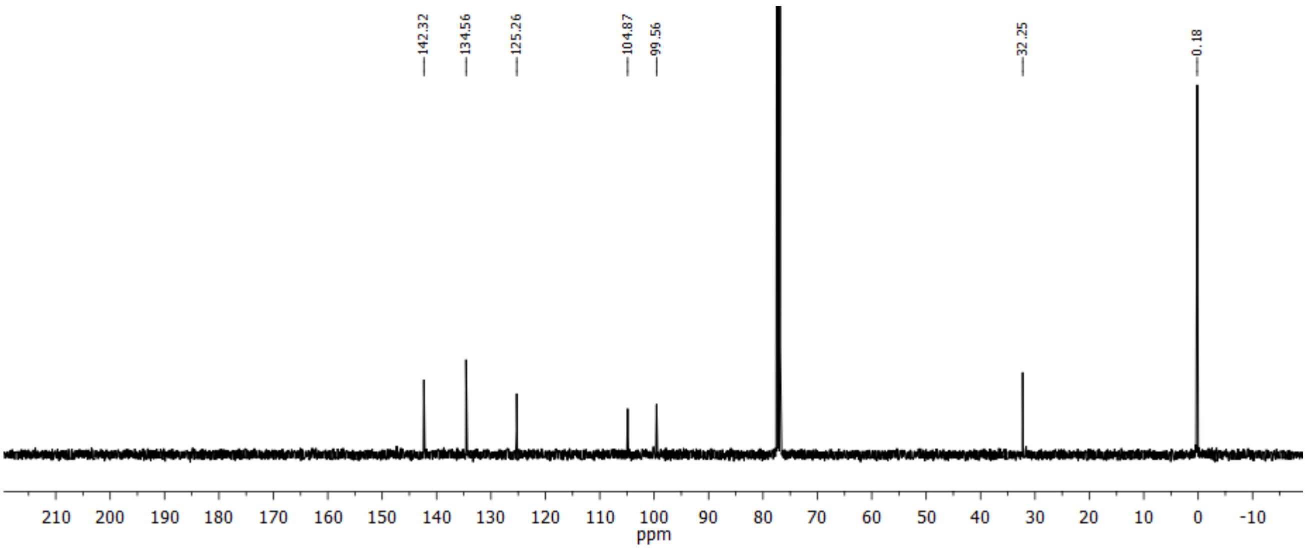


Figure S2. $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) of 4,7,12,15-tetra(trimethylsilylethynyl)[2.2]paracyclophane.

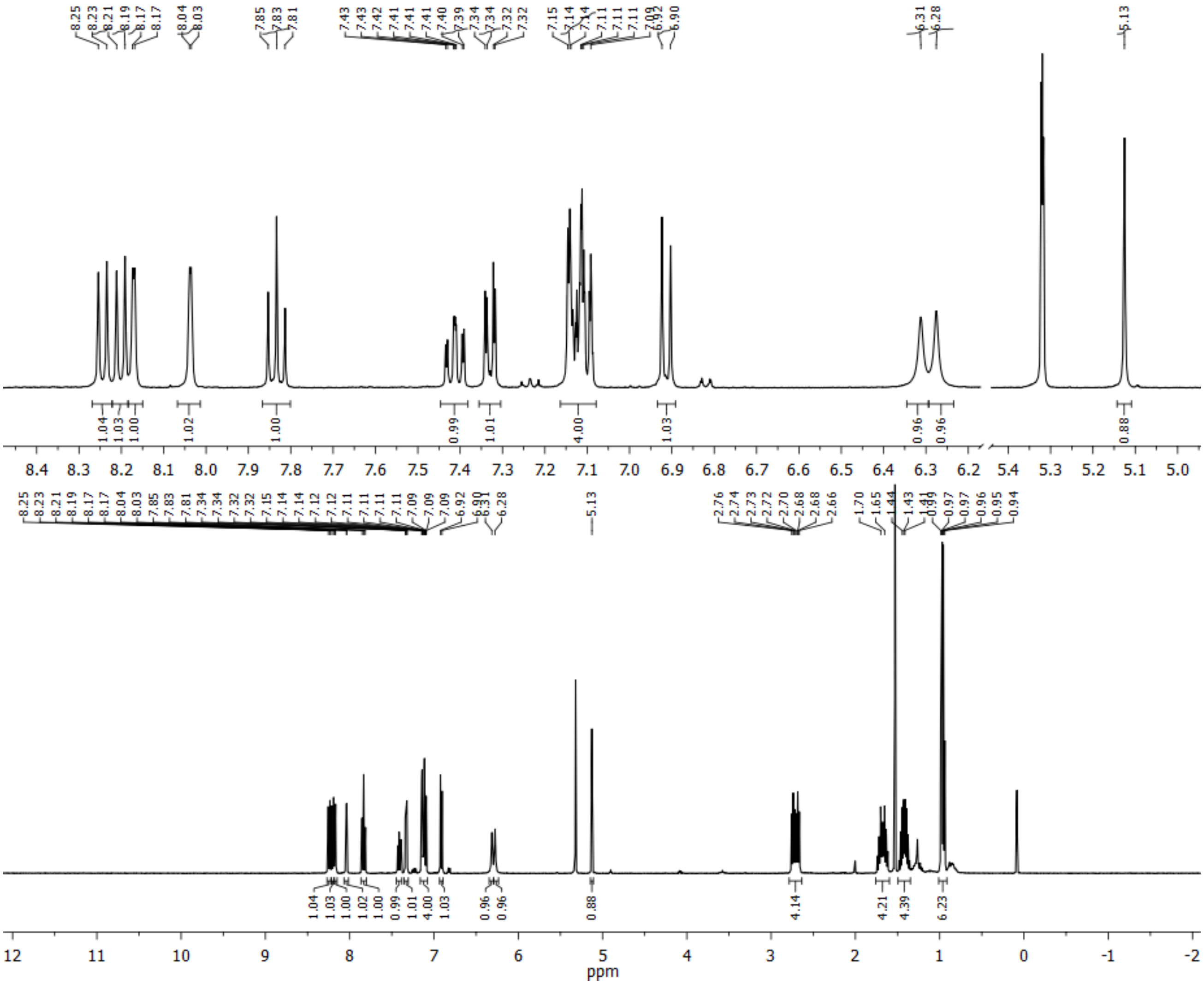


Figure S3. ^{1}H NMR (400 MHz, CD_2Cl_2) of **3*o***.

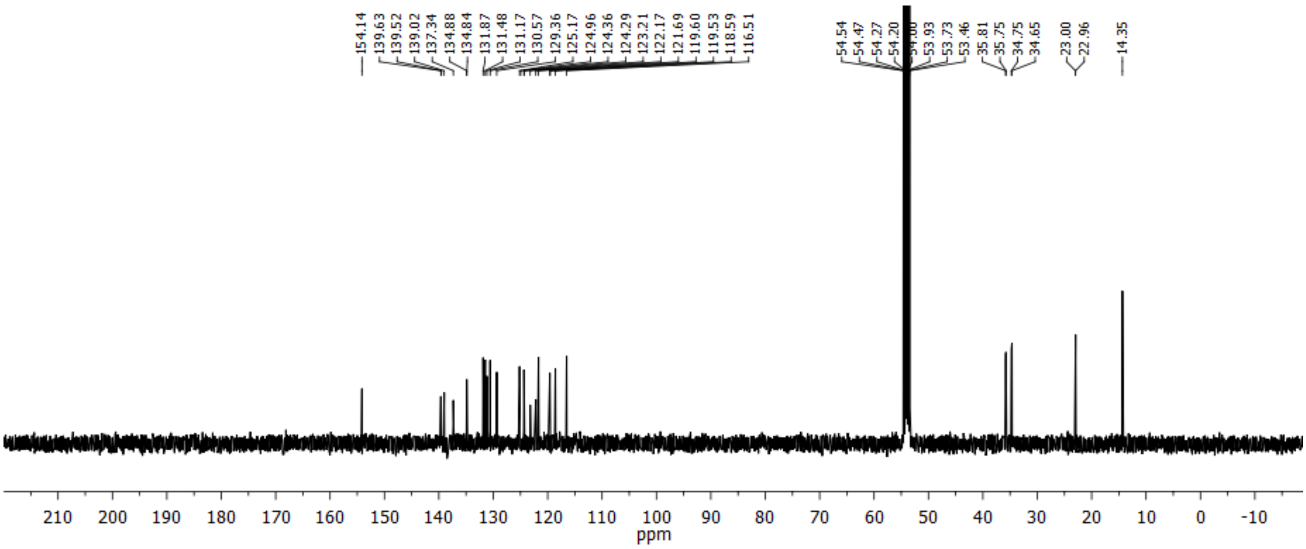


Figure S4. $^{13}C\{^{1}H\}$ NMR (101 MHz, CD_2Cl_2) of **3*o***.

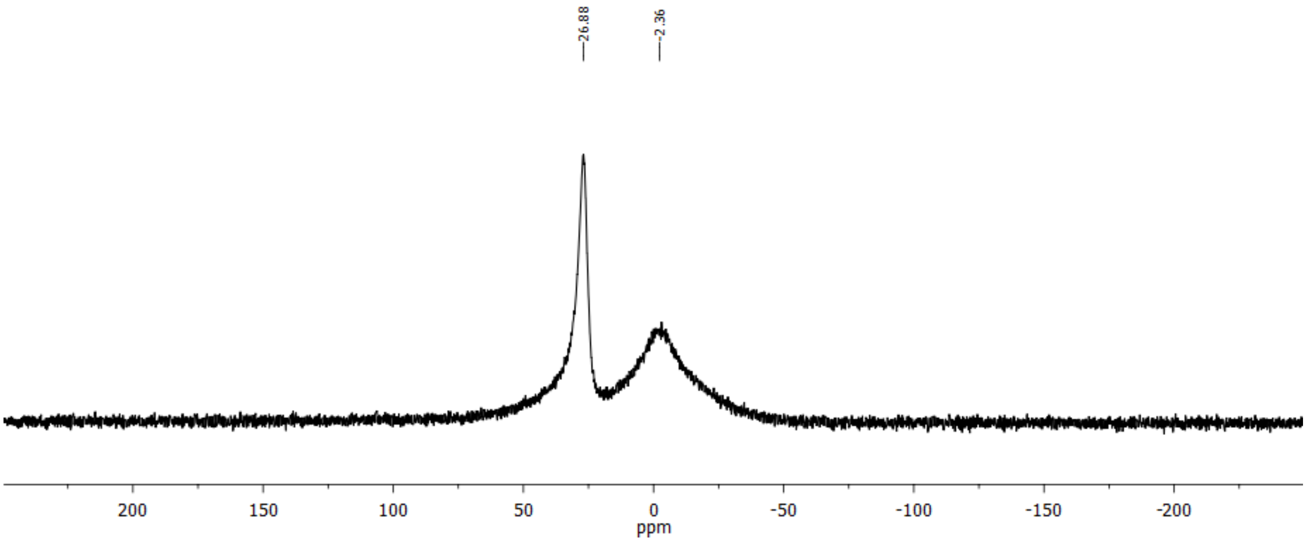


Figure S5. $^{11}B\{1H\}$ NMR (128 MHz, CD_2Cl_2) of **3*o***. Signal at δ -2.36 ppm is related to the NMR tube glass.

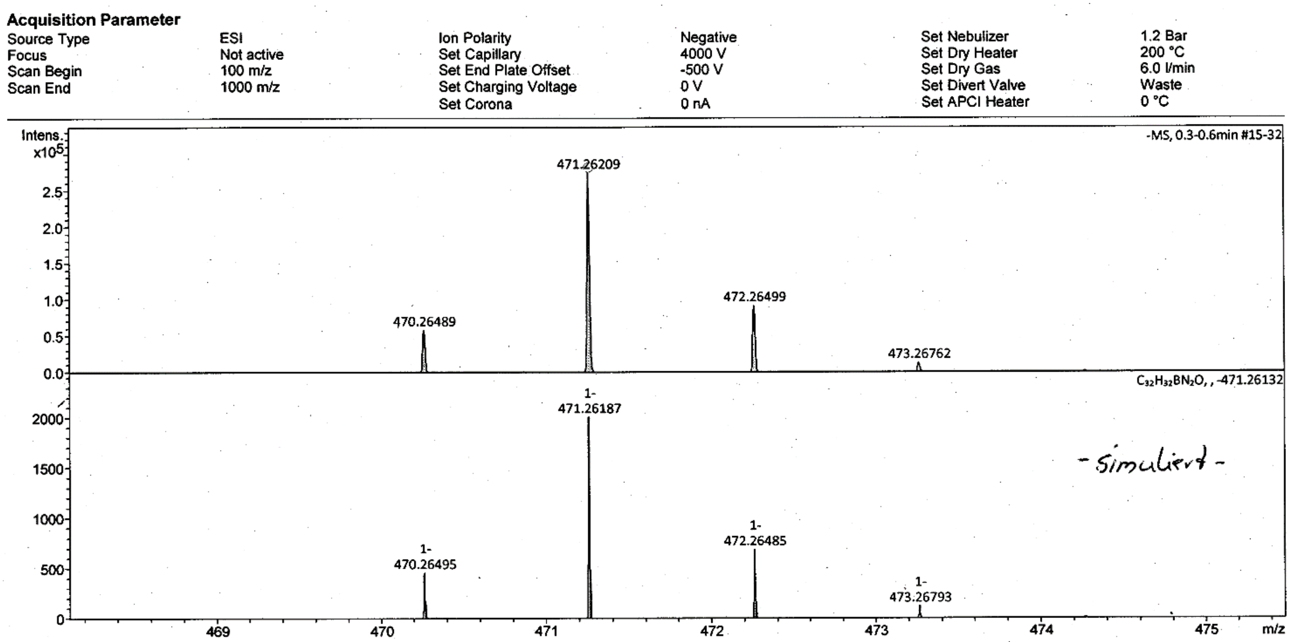


Figure S6. Experimental HR ESI-MS of **3*o*** (top) and theoretical isotopic envelope for $C_{32}H_{32}BN_2O$ $[M-H]^-$ (bottom).

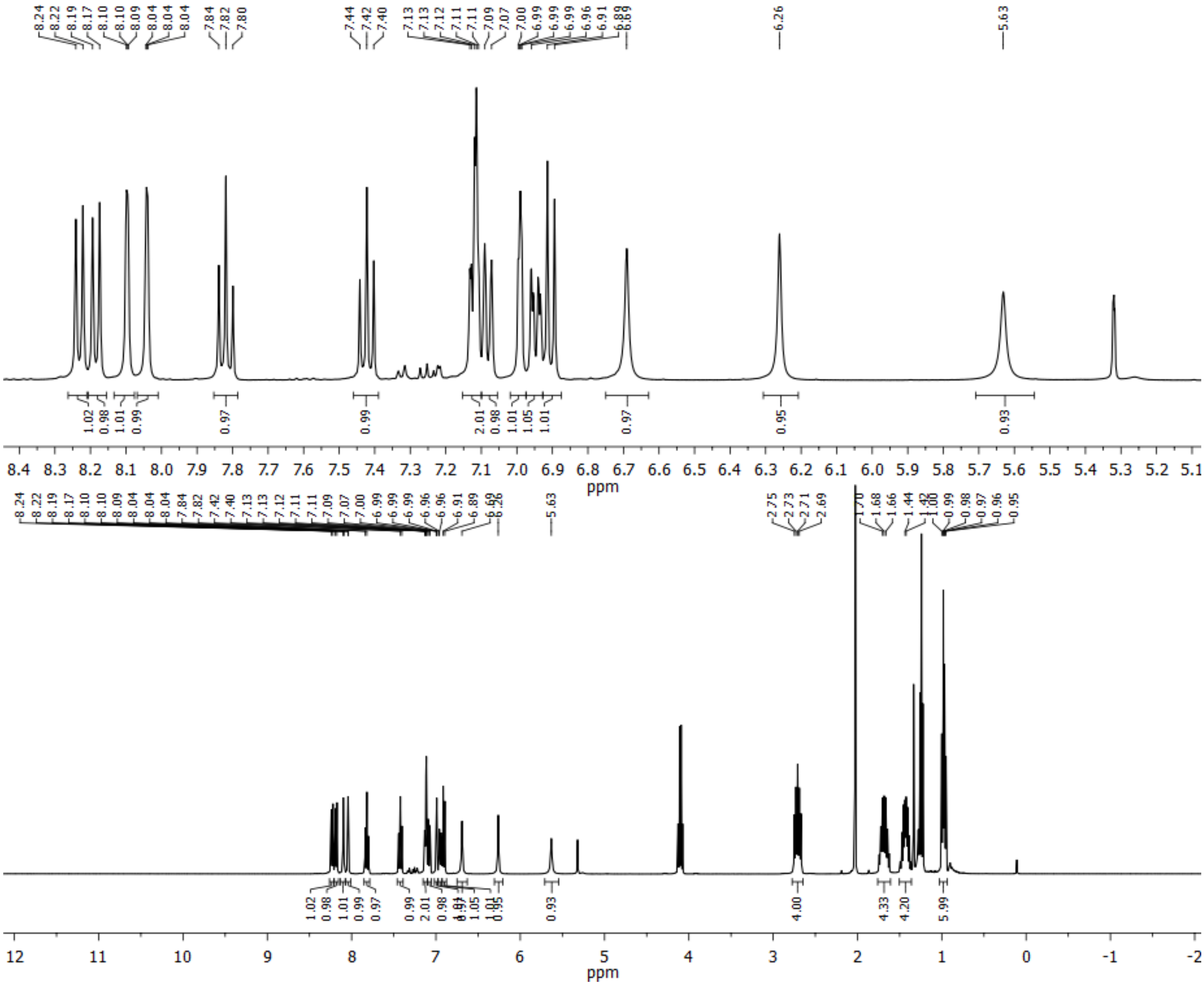


Figure S7. ^{1}H NMR (400 MHz, CD_2Cl_2) of **3*m***.

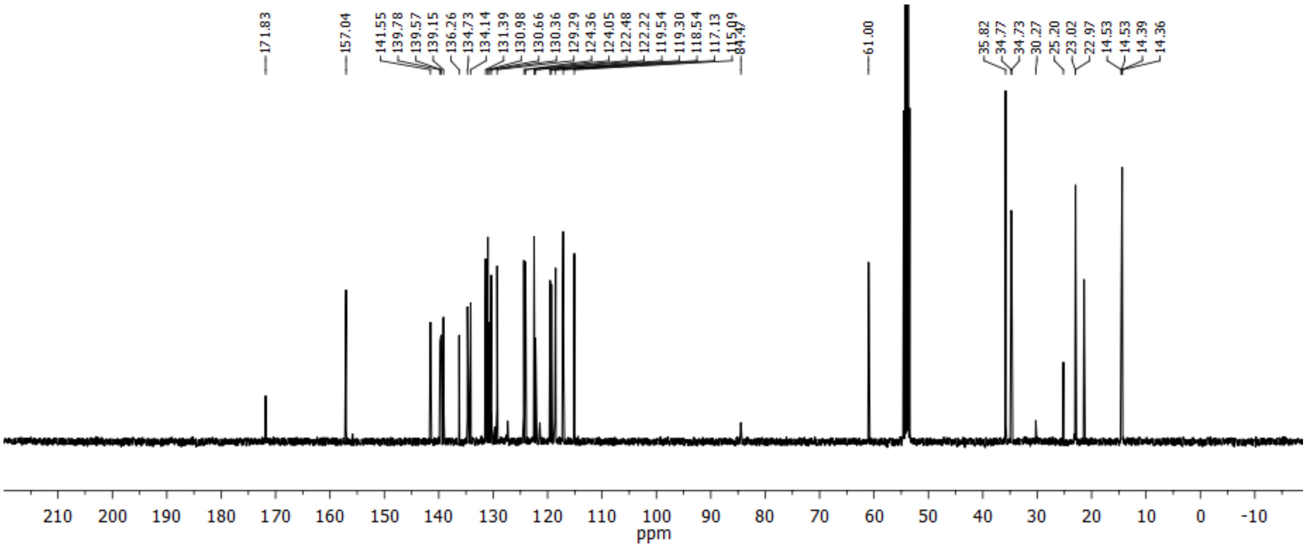


Figure S8. $^{13}C\{^{1}H\}$ NMR (101 MHz, CD_2Cl_2) of **3*m***.

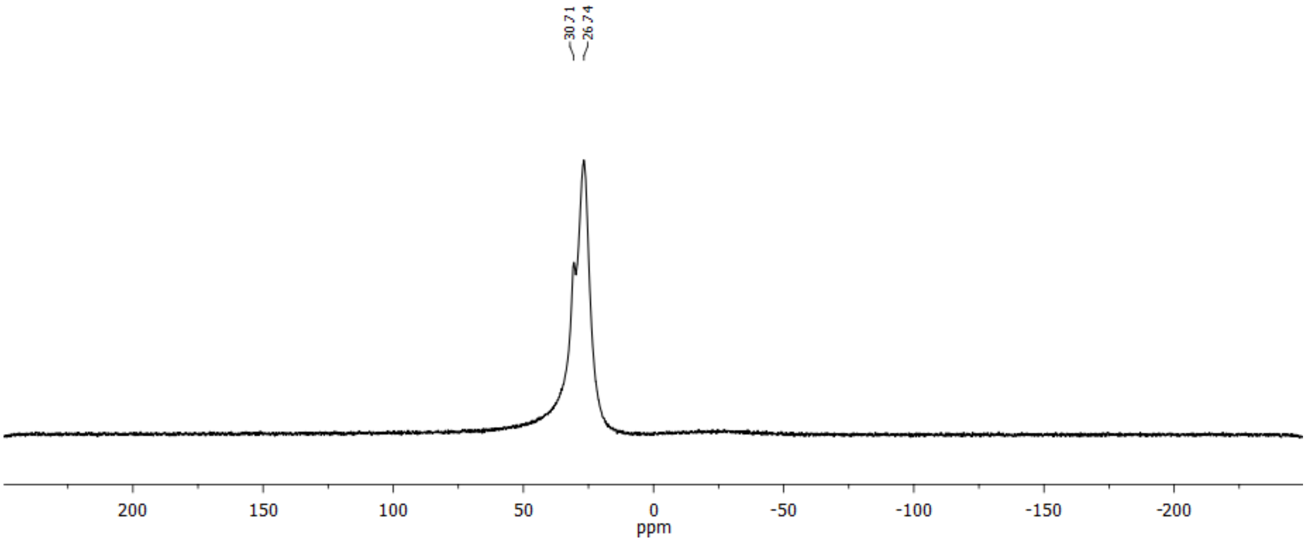


Figure S9. $^{11}B\{1H\}$ NMR (128 MHz, CD_2Cl_2) of **3*m***.

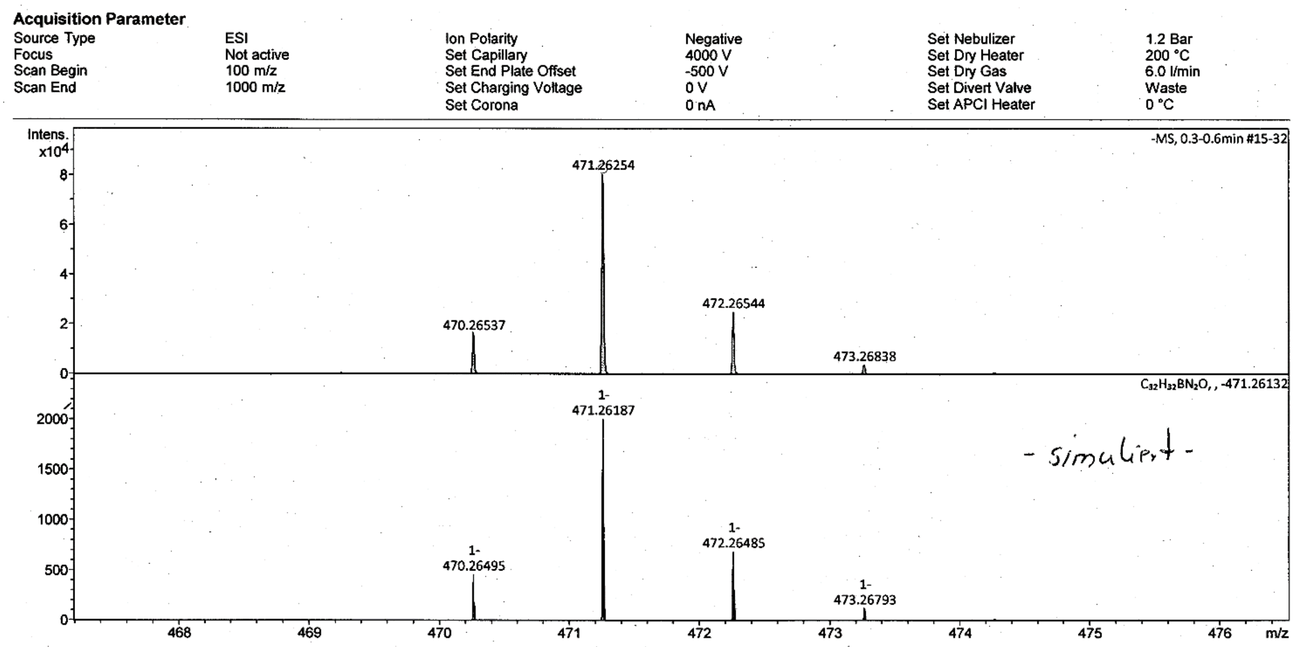


Figure S10. Experimental HR ESI-MS of **3*m*** (top) and theoretical isotopic envelope for $C_{32}H_{32}BN_2O$ $[M\text{-}H]^-$ (bottom).

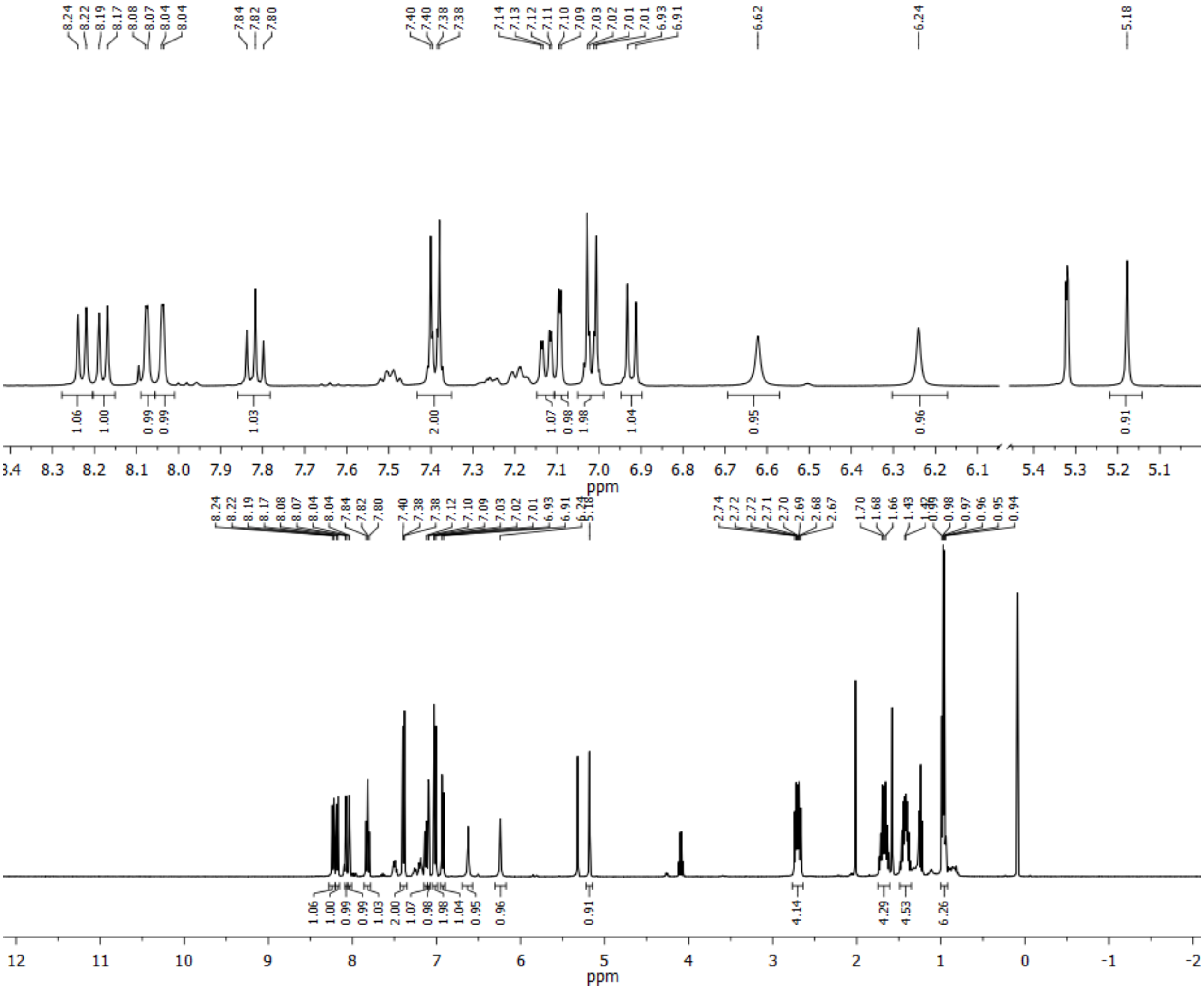


Figure S11. ^{1}H NMR (400 MHz, CD_2Cl_2) of **3*p***.

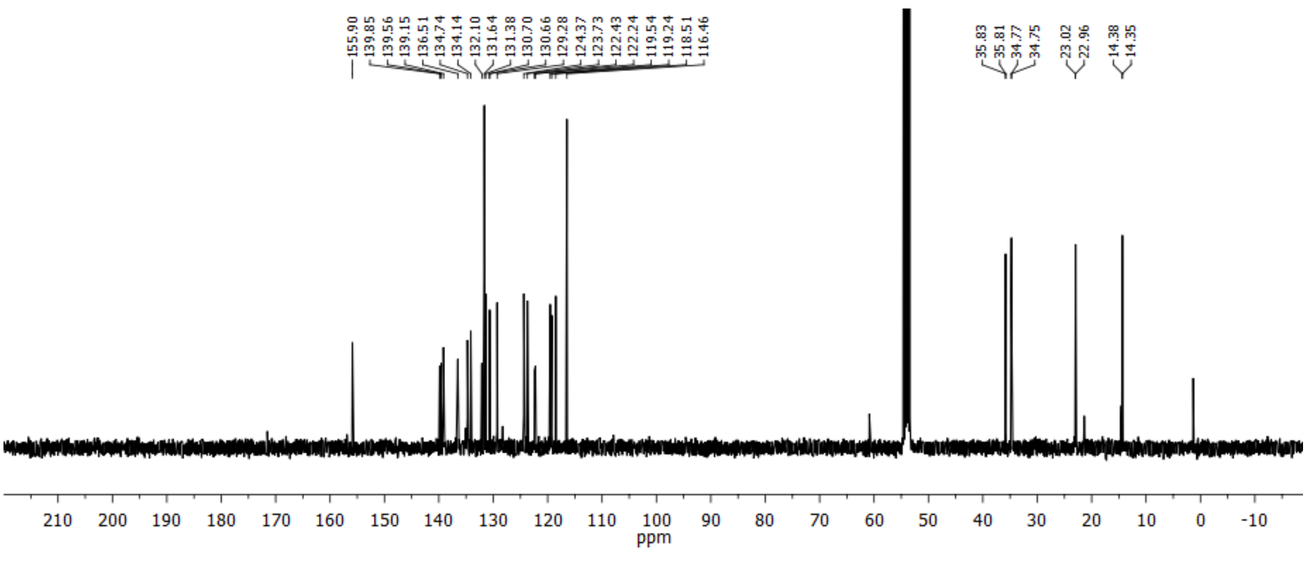


Figure S12. $^{13}C\{^{1}H\}$ NMR (101 MHz, CD_2Cl_2) of **3*p***.

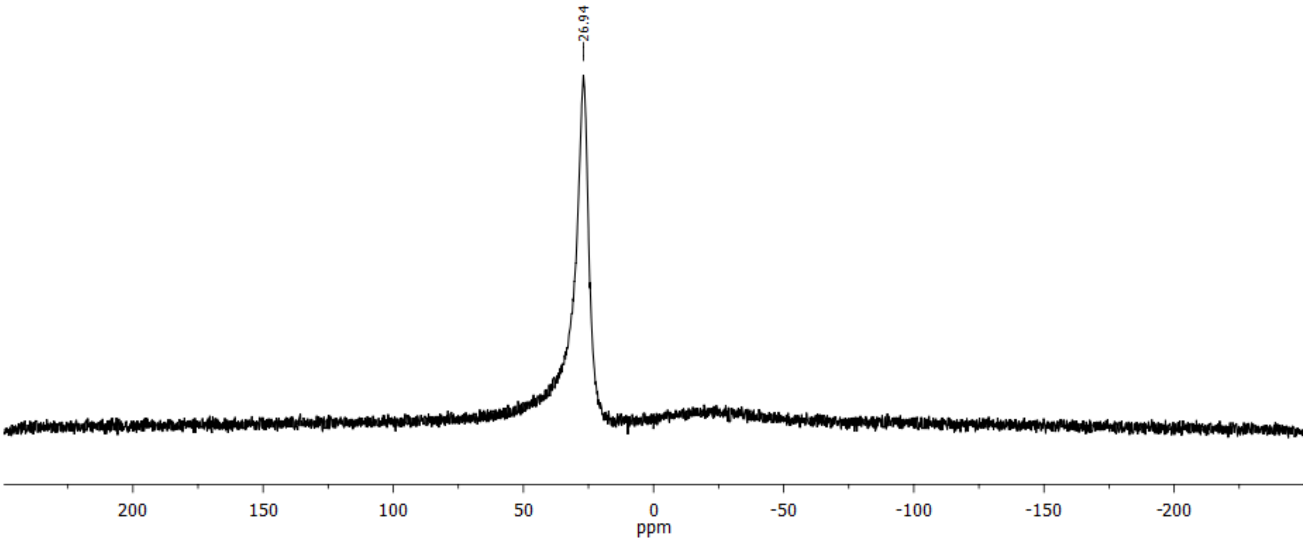


Figure S13. $^{11}B\{1H\}$ NMR (128 MHz, CD_2Cl_2) of **3*p***.

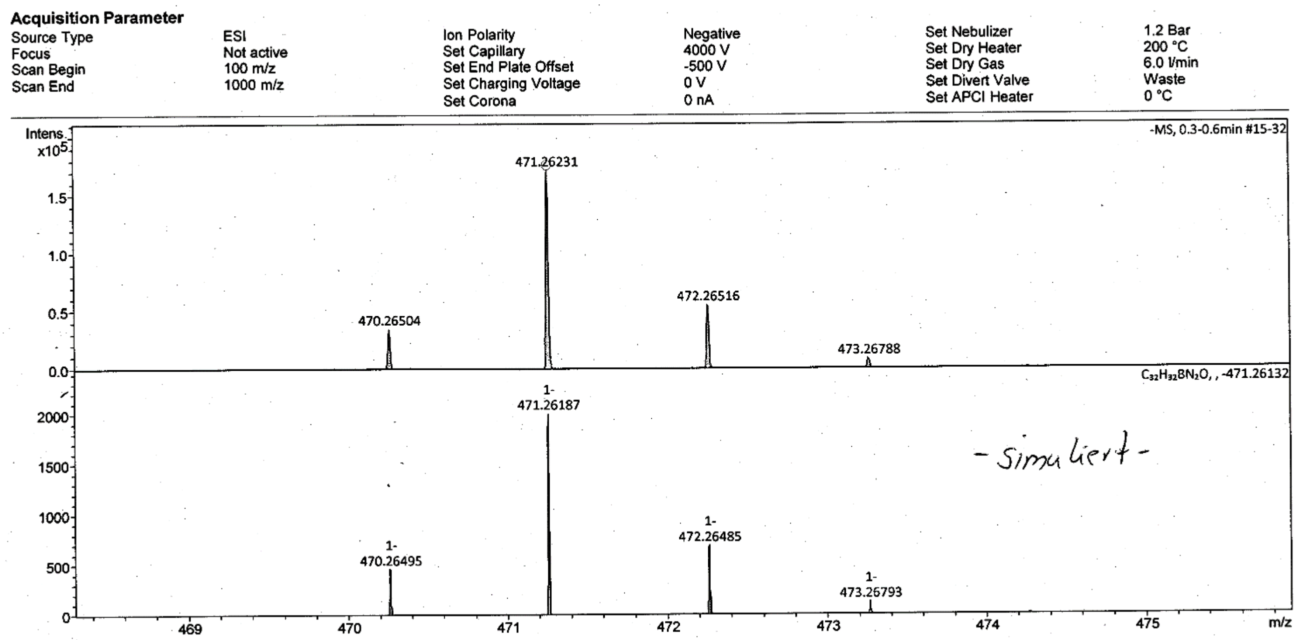


Figure S14. Experimental HR ESI-MS of **3*p*** (top) and theoretical isotopic envelope for $C_{32}H_{32}BN_2O$ $[M-H]^-$ (bottom).

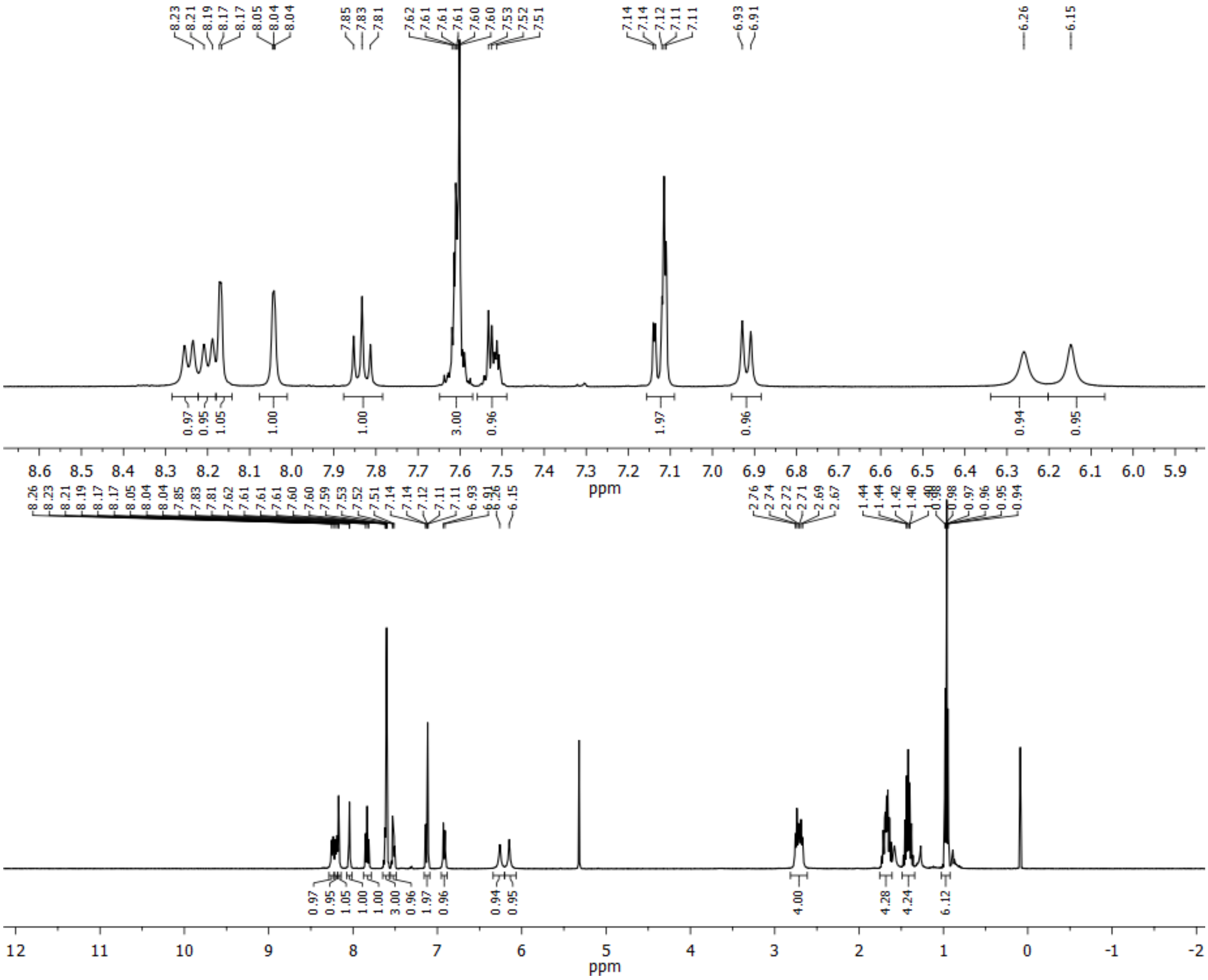


Figure S15. ^{1}H NMR (400 MHz, CD_2Cl_2) of **4*o***.

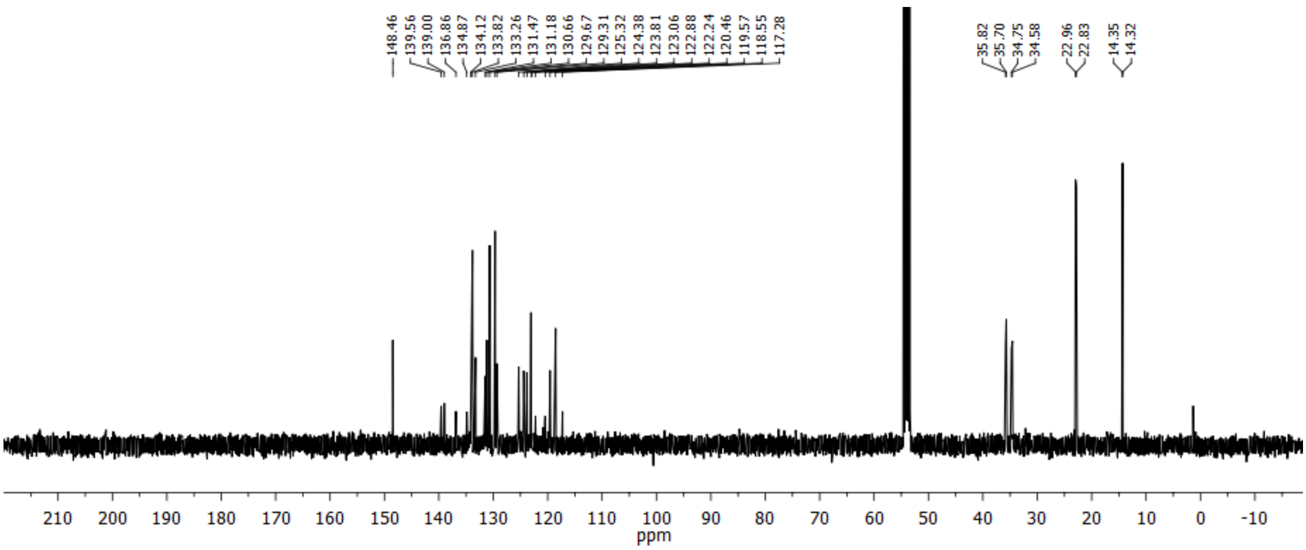


Figure S16. $^{13}C\{^{1}H\}$ NMR (101 MHz, CD_2Cl_2) of **4*o***.

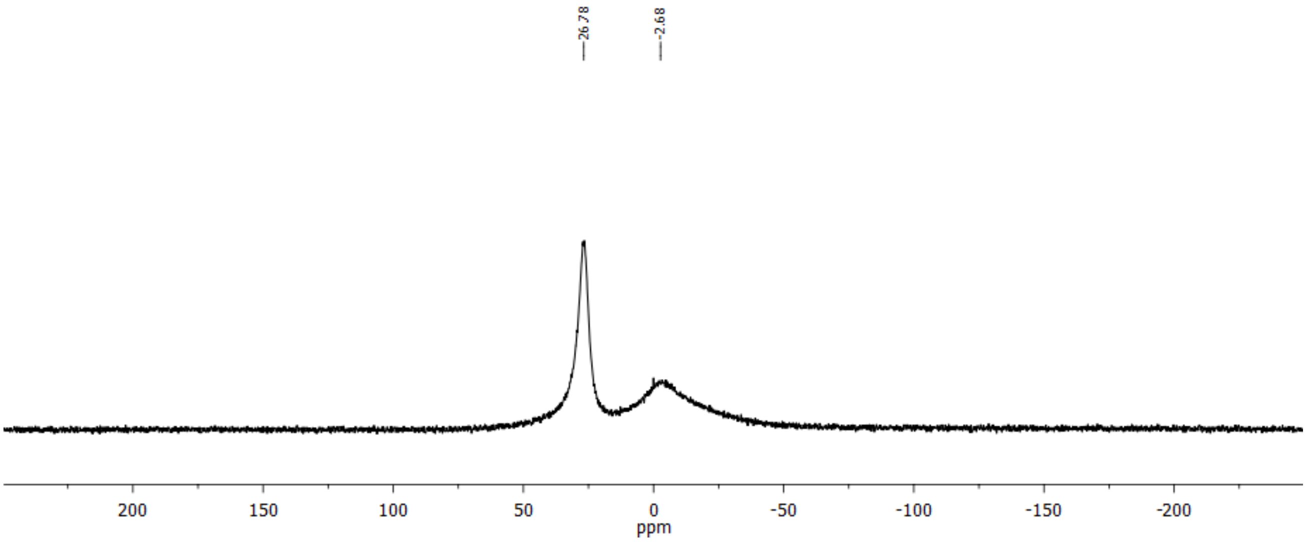


Figure S17. $^{11}B\{1H\}$ NMR (128 MHz, CD_2Cl_2) of **4*o***. Signal at δ -2.68 ppm is related to the NMR tube glass.

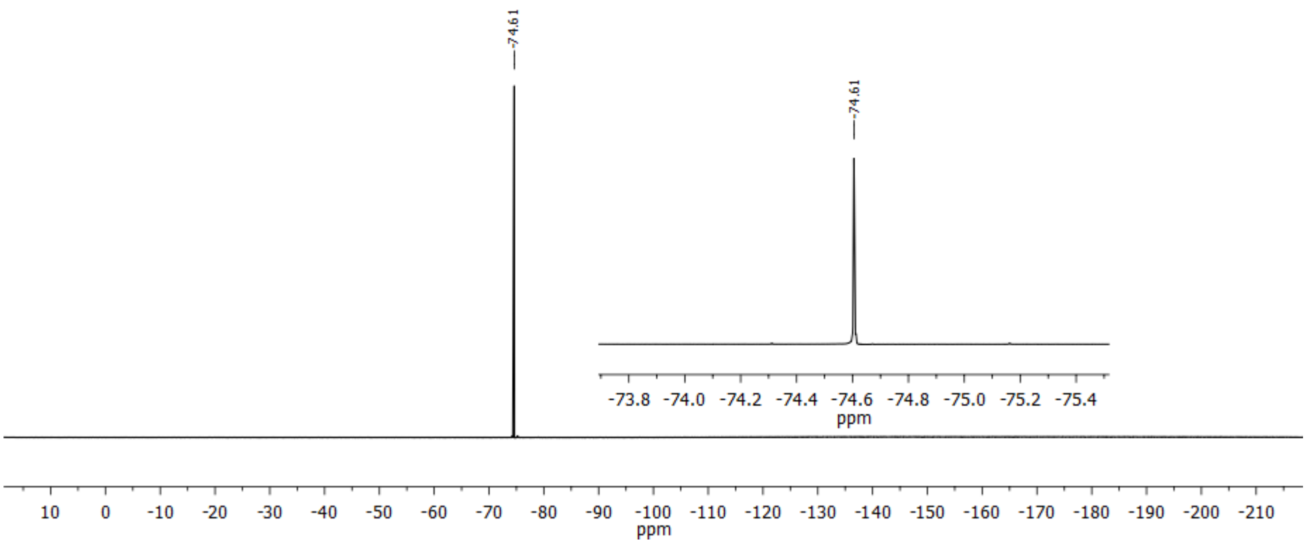


Figure S18. $^{19}F\{1H\}$ NMR (376 MHz, CD_2Cl_2) of **4*o***.

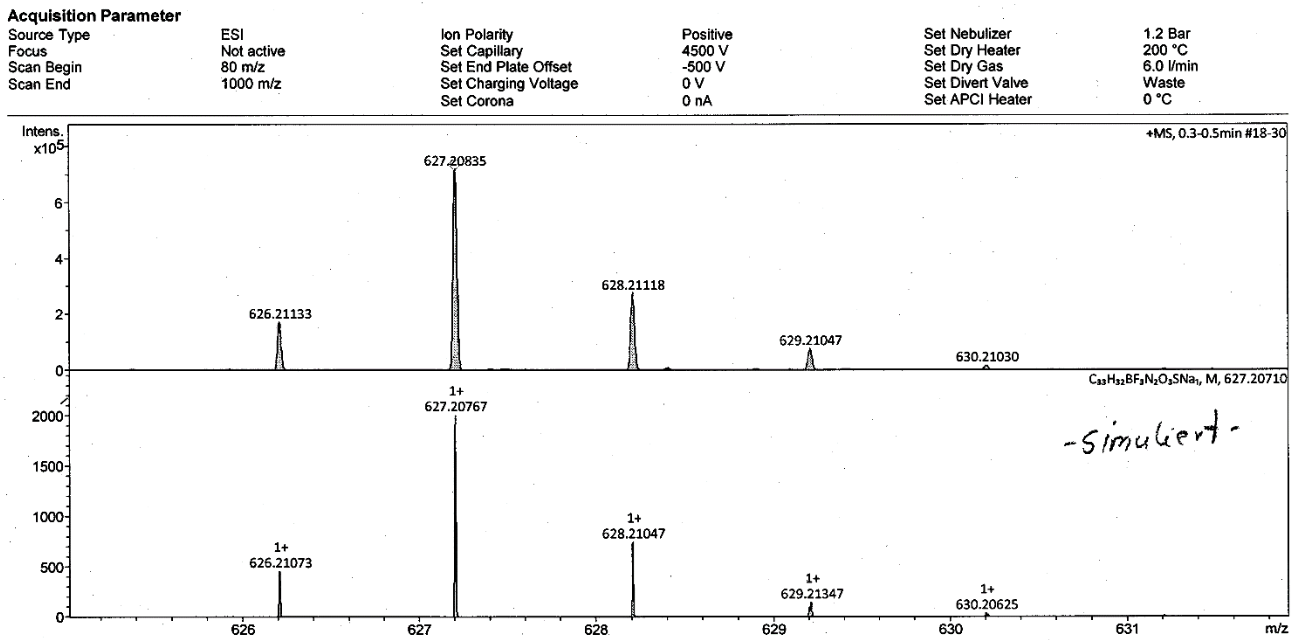


Figure S19. Experimental HR ESI-MS of **4*o*** (top) and theoretical isotopic envelope for $C_{33}H_{32}BF_3N_2O_3SNa$ $[M+Na]^+$ (bottom).

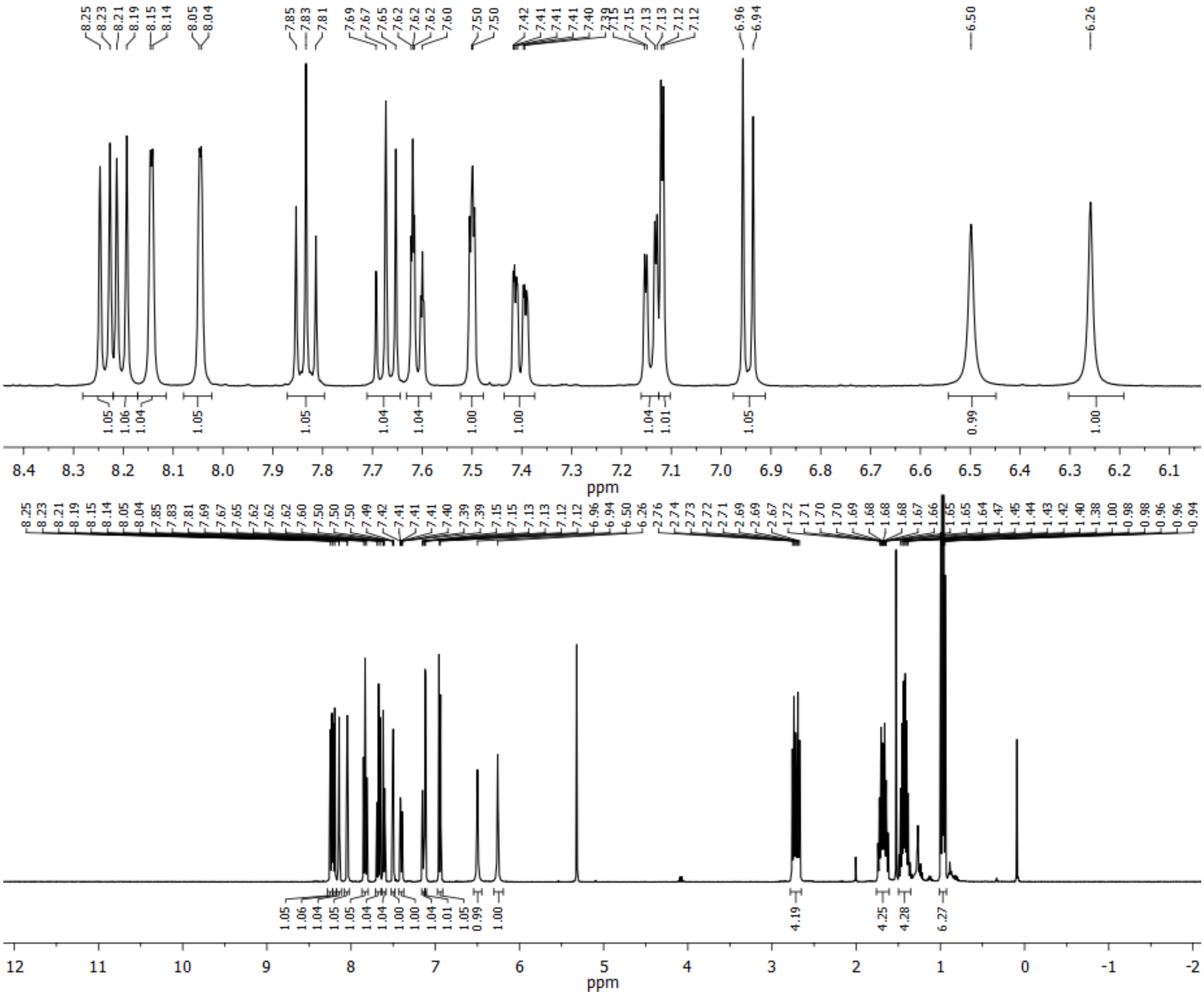


Figure S20. ^1H NMR (400 MHz, CD_2Cl_2) of **4*m***.

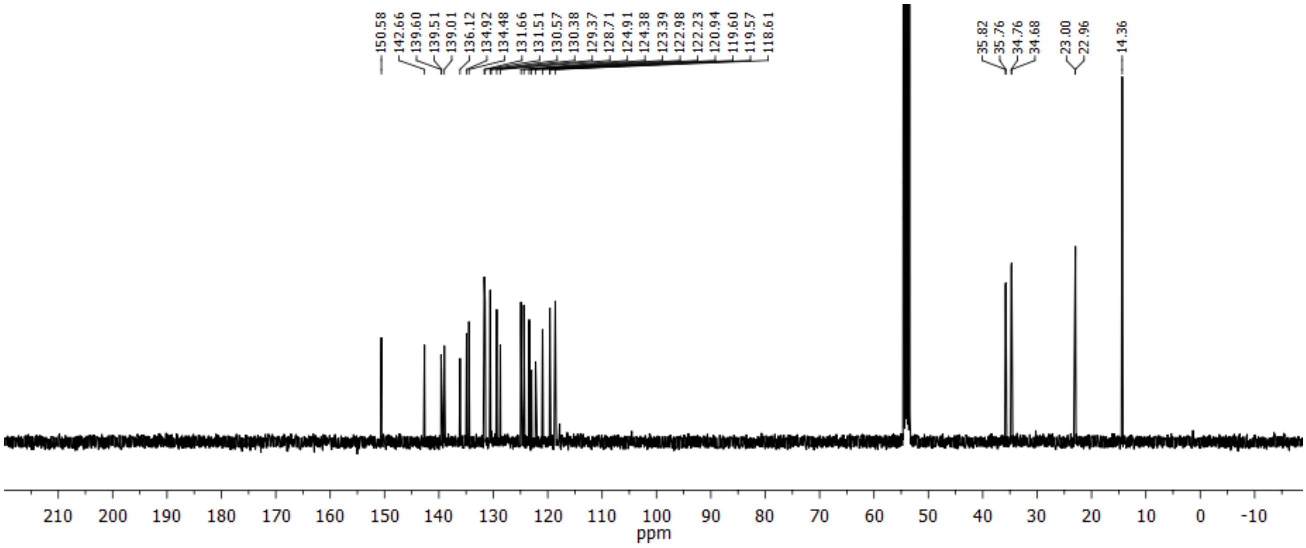


Figure S21. $^{13}C\{^1H\}$ NMR (101 MHz, CD_2Cl_2) of ***4m***.

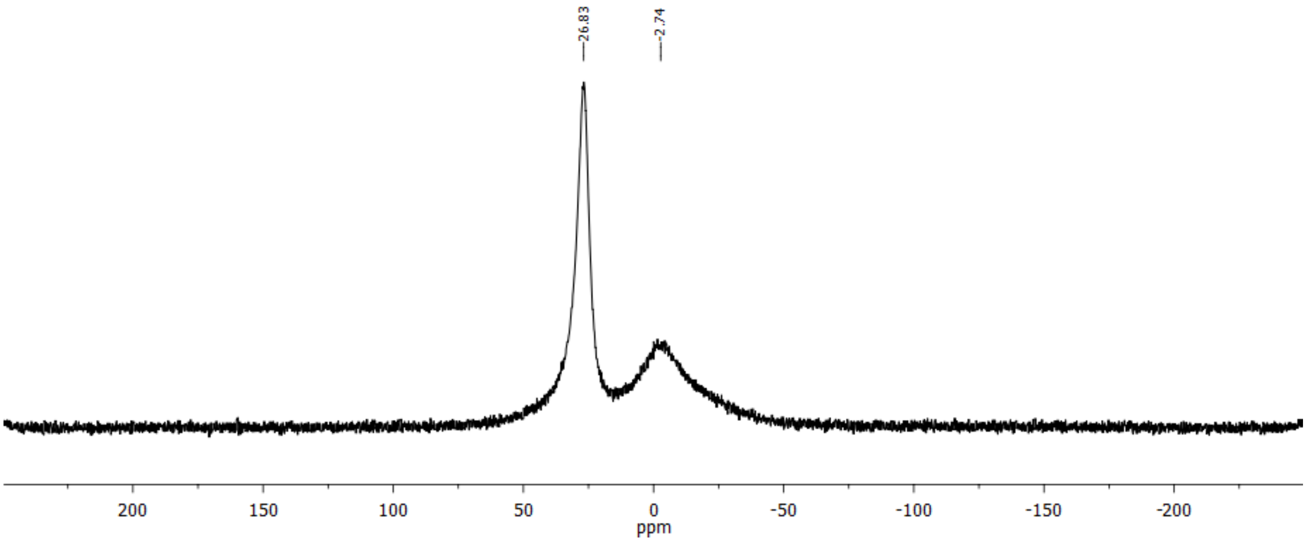


Figure S22. $^{11}B\{1H\}$ NMR (128 MHz, CD_2Cl_2) of ***4m***. Signal at δ -2.74 ppm is related to the NMR tube glass.

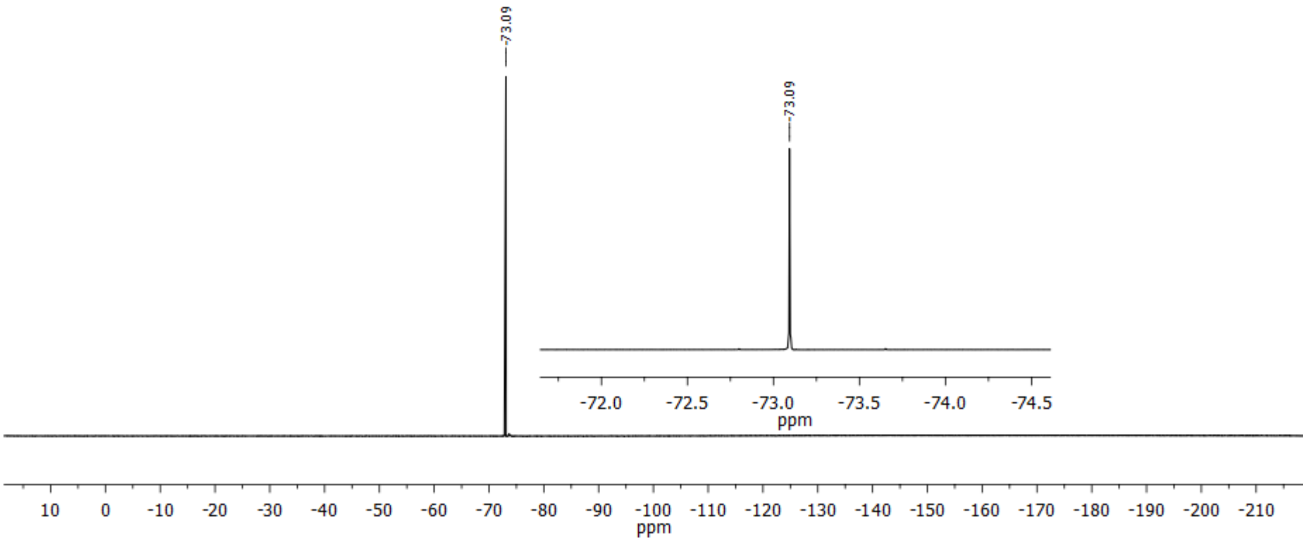


Figure S23. $^{19}F\{1H\}$ NMR (376 MHz, CD_2Cl_2) of ***4m***.

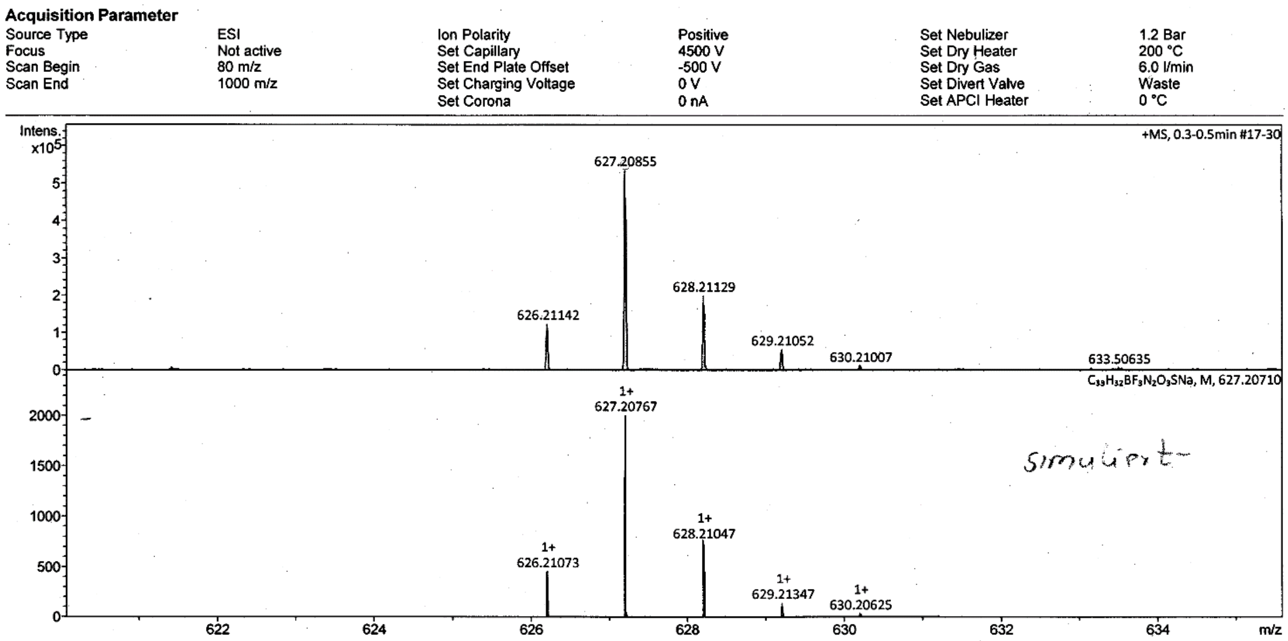


Figure S24. Experimental HR ESI-MS of ***4m*** (top) and theoretical isotopic envelope for $C_{33}H_{32}BF_3N_2O_3SNa$ $[M+Na]^+$ (bottom).

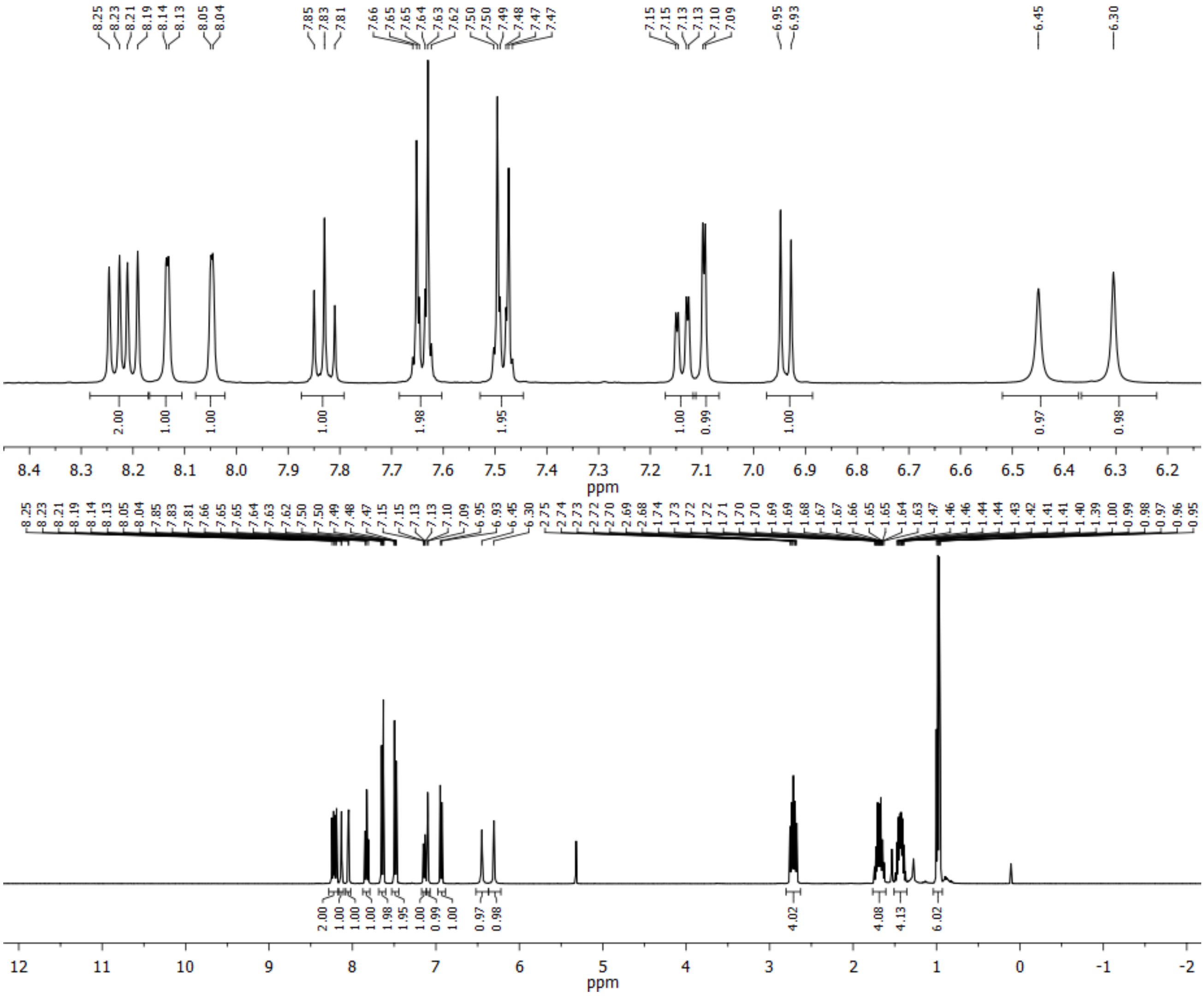


Figure S25. ^{1}H NMR (400 MHz, CD_2Cl_2) of ***4p***.

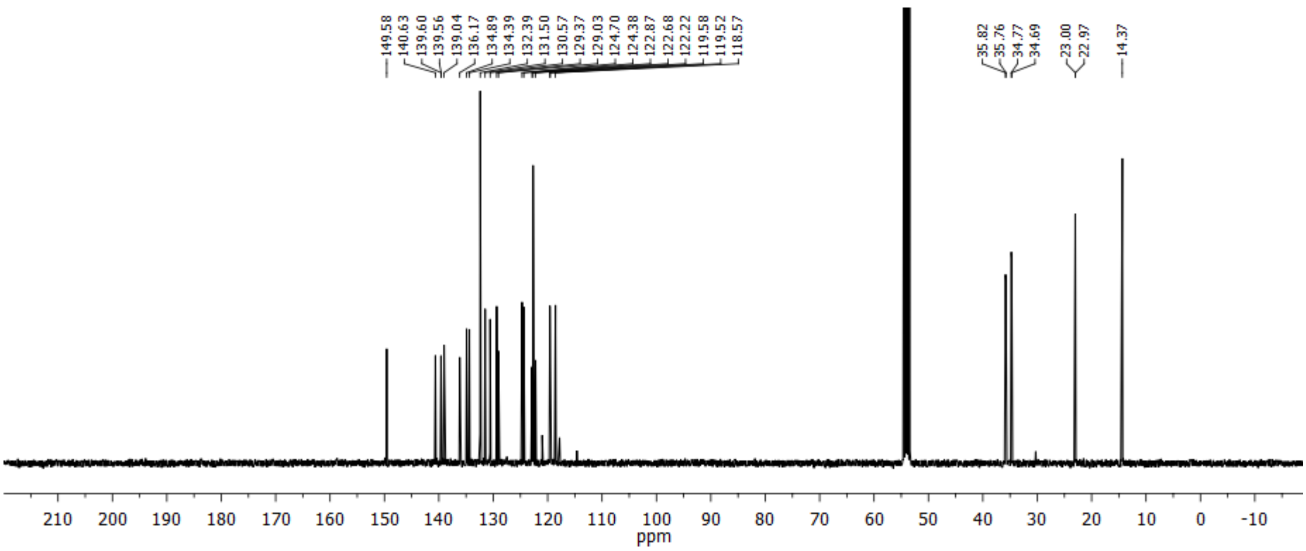


Figure S26. $^{13}C\{^{1}H\}$ NMR (101 MHz, CD_2Cl_2) of ***4p***.

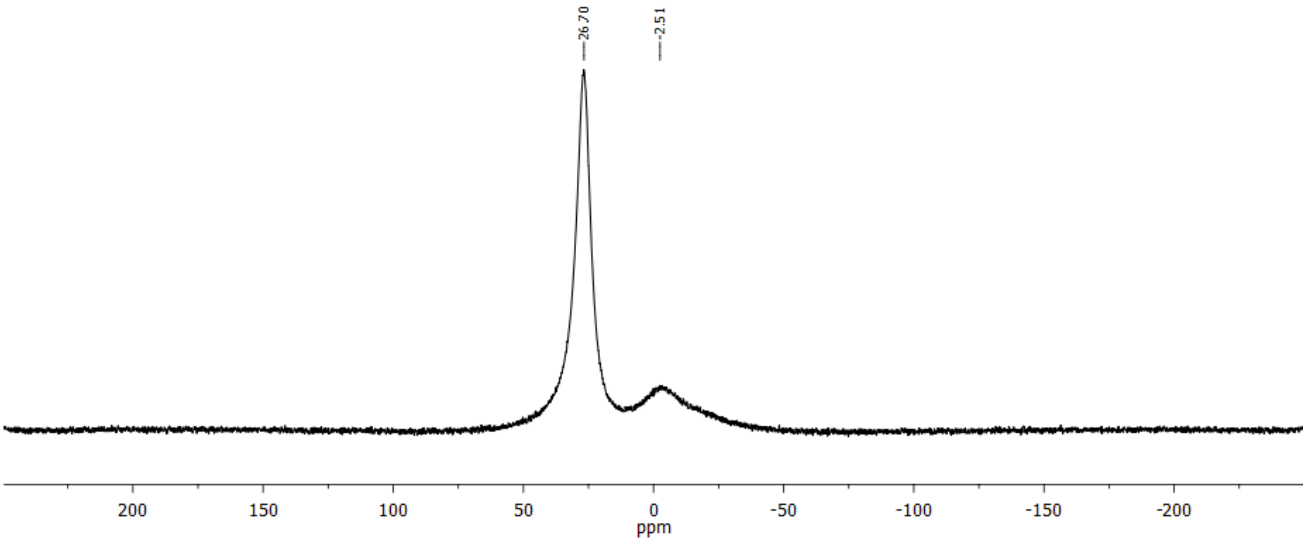


Figure S27. $^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2) of ***4p***. Signal at δ -2.51 ppm is related to the NMR tube glass.

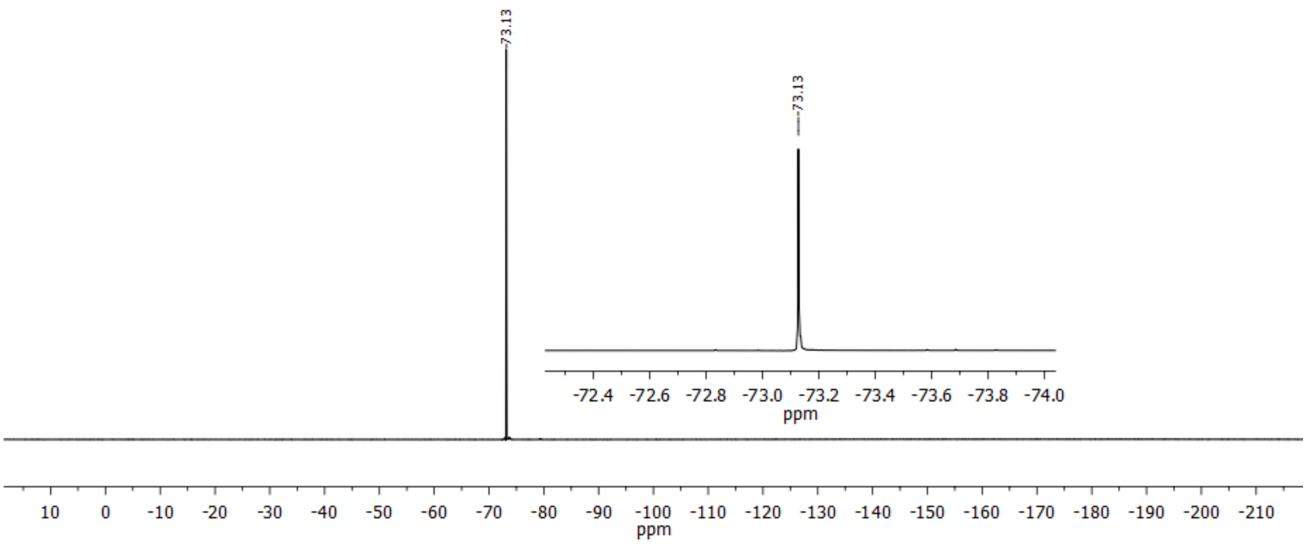


Figure S28. $^{19}F\{^1H\}$ NMR (376 MHz, CD_2Cl_2) of ***4p***.

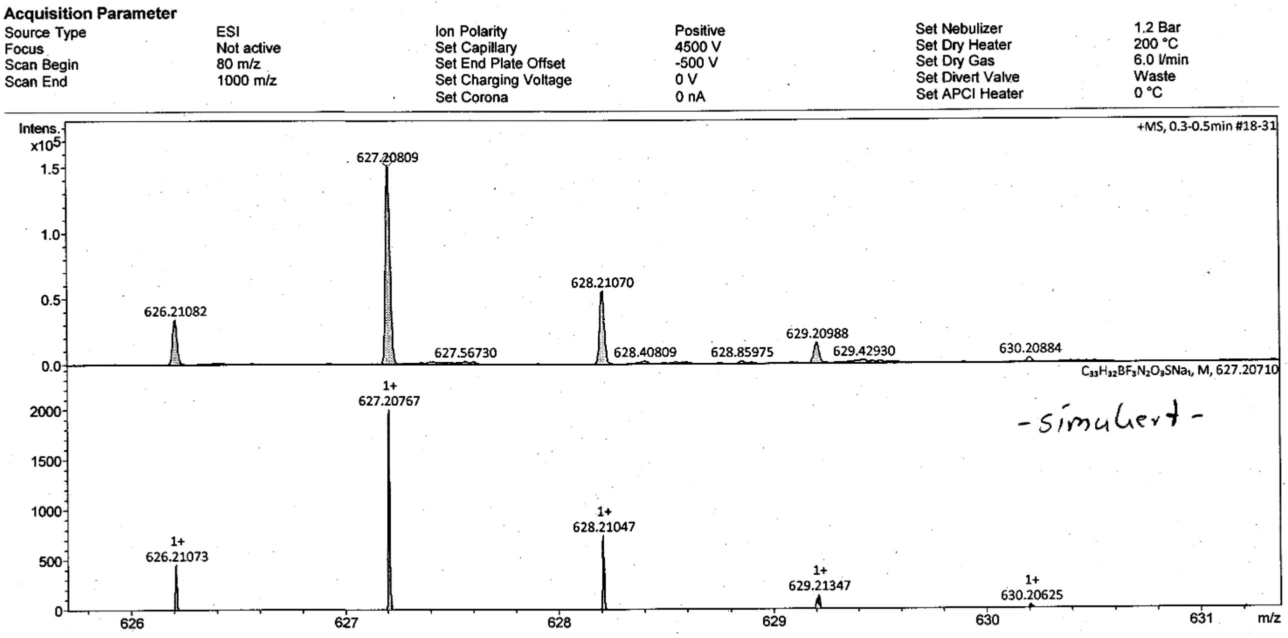


Figure S29. Experimental HR ESI-MS of **4*p*** (top) and theoretical isotopic envelope for $C_{33}H_{32}BF_3N_2O_3SNa$ $[M+Na]^+$ (bottom).

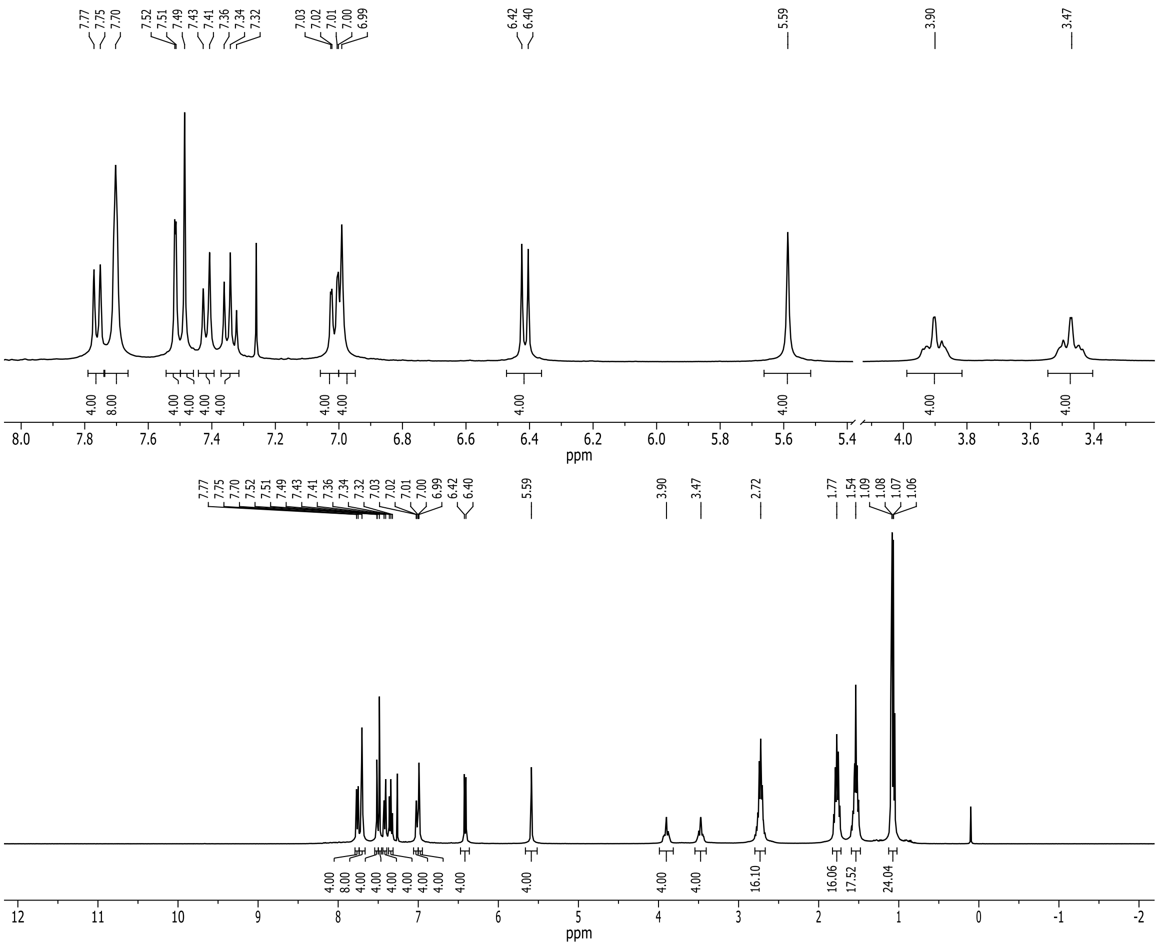


Figure S30. ^1H NMR (400 MHz, $CDCl_3$) of rac-**6**.

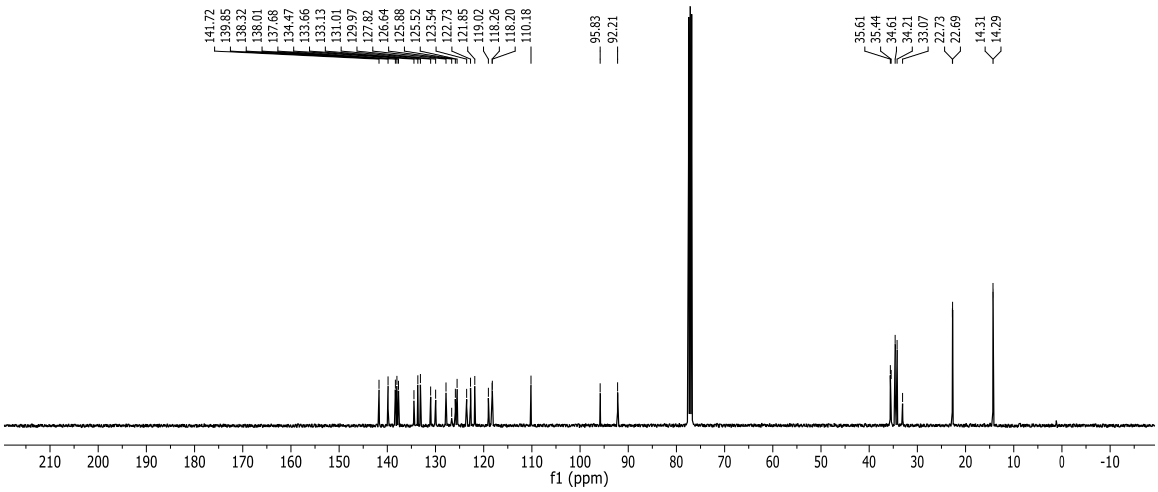


Figure S31. $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) of rac-**6**.

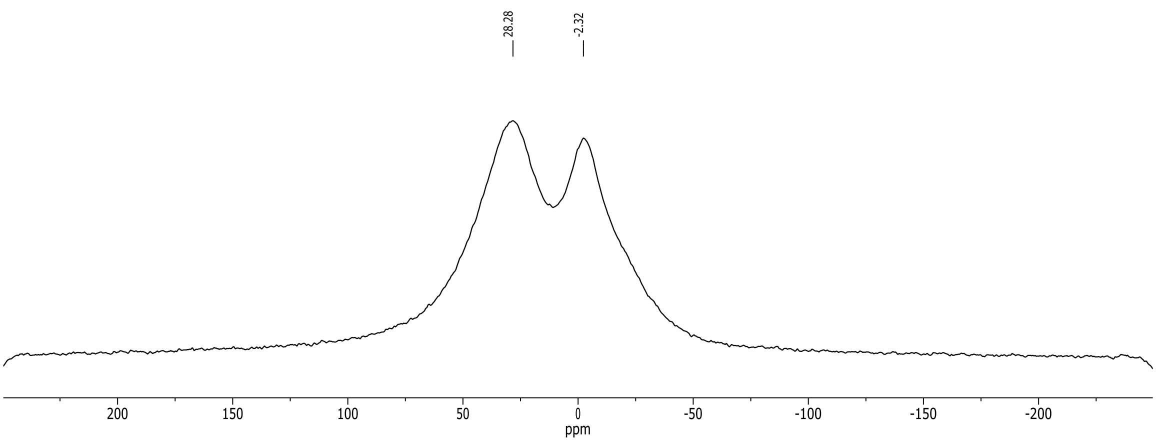


Figure S32. $^{11}B\{1H\}$ NMR (128 MHz, $CDCl_3$) of rac-**6**. Signal at δ -2.32 ppm is related to the NMR tube glass.

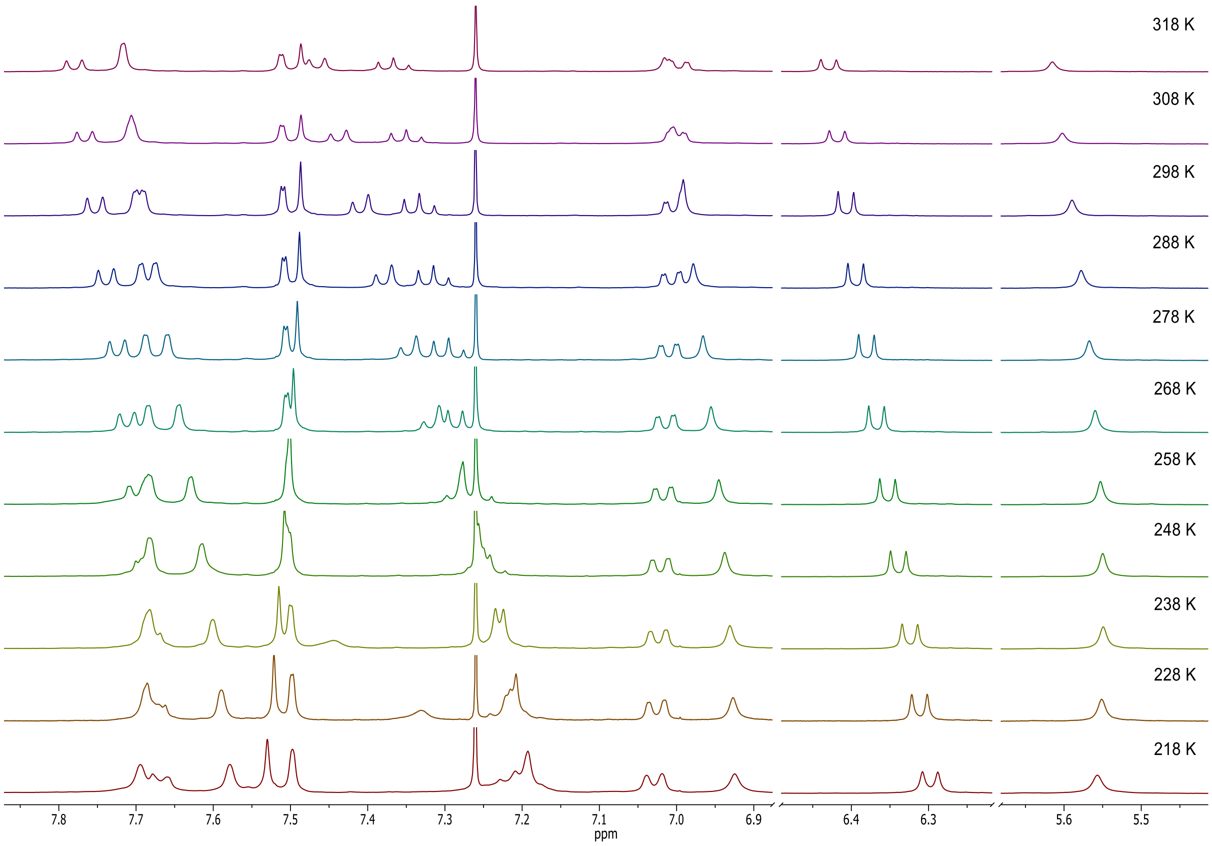


Figure S33. Variable temperature ^{1}H NMR (400 MHz, $CDCl_3$) of rac-6 measured at T = -55 – 45 °C.

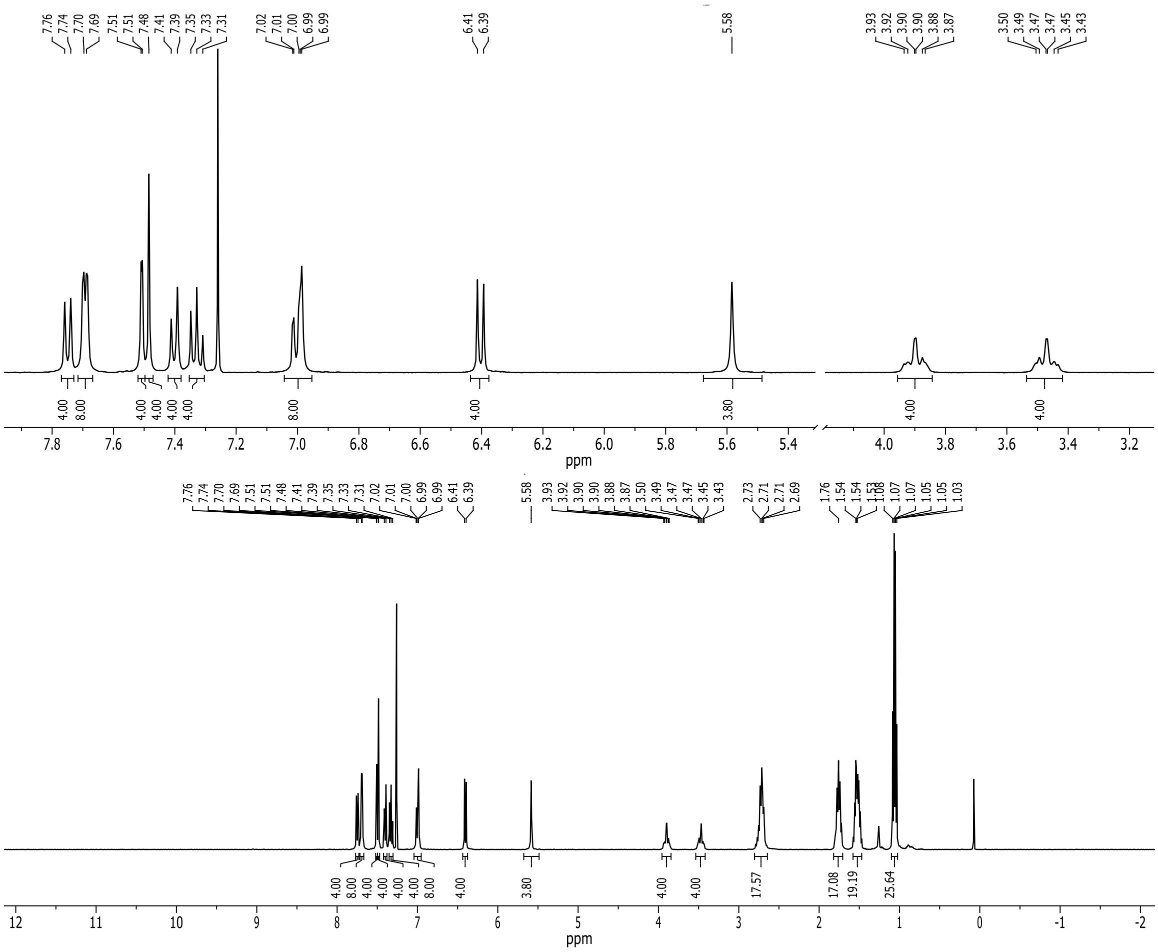


Figure S34. ^{1}H NMR (400 MHz, $CDCl_3$) of (R)-**6**.

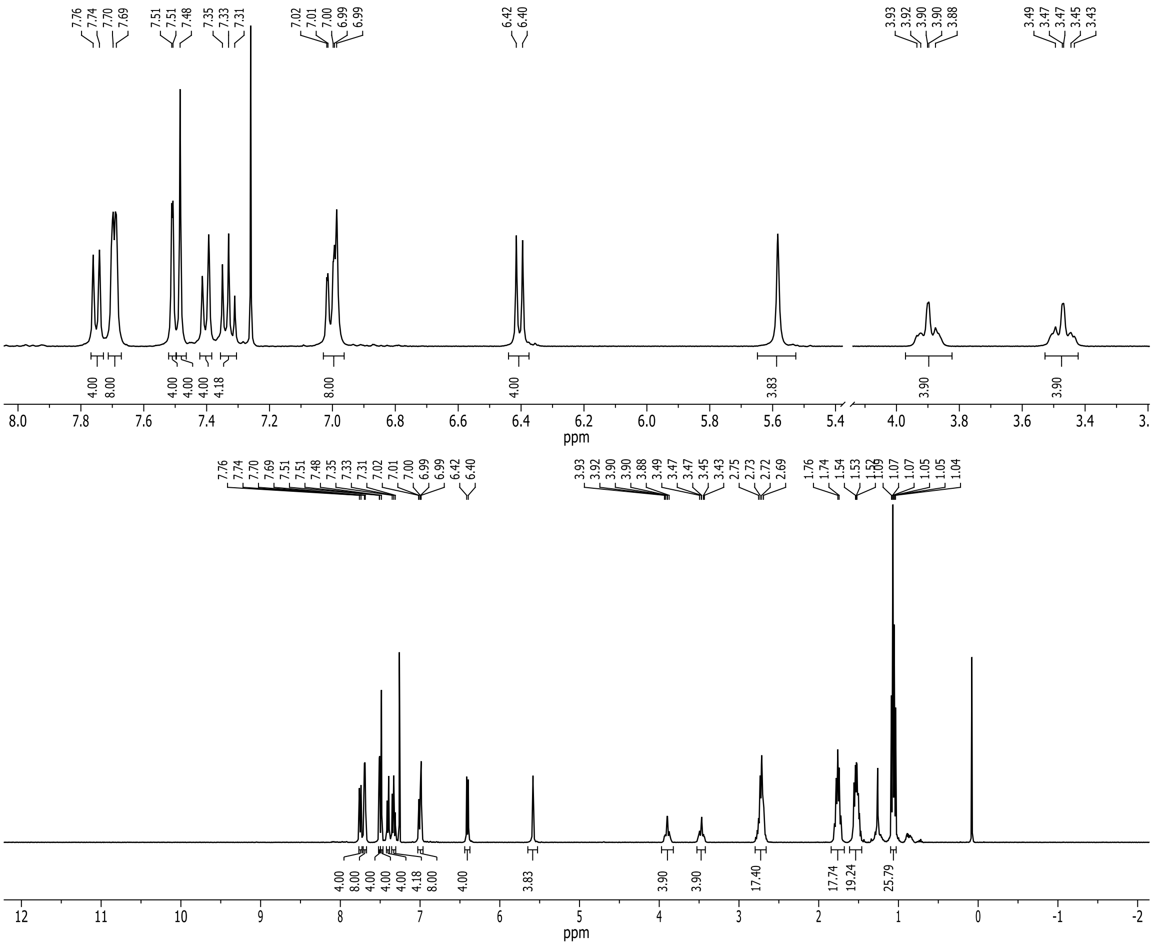


Figure S35. [1]H NMR (400 MHz, $CDCl_3$) of (S)-**6**.

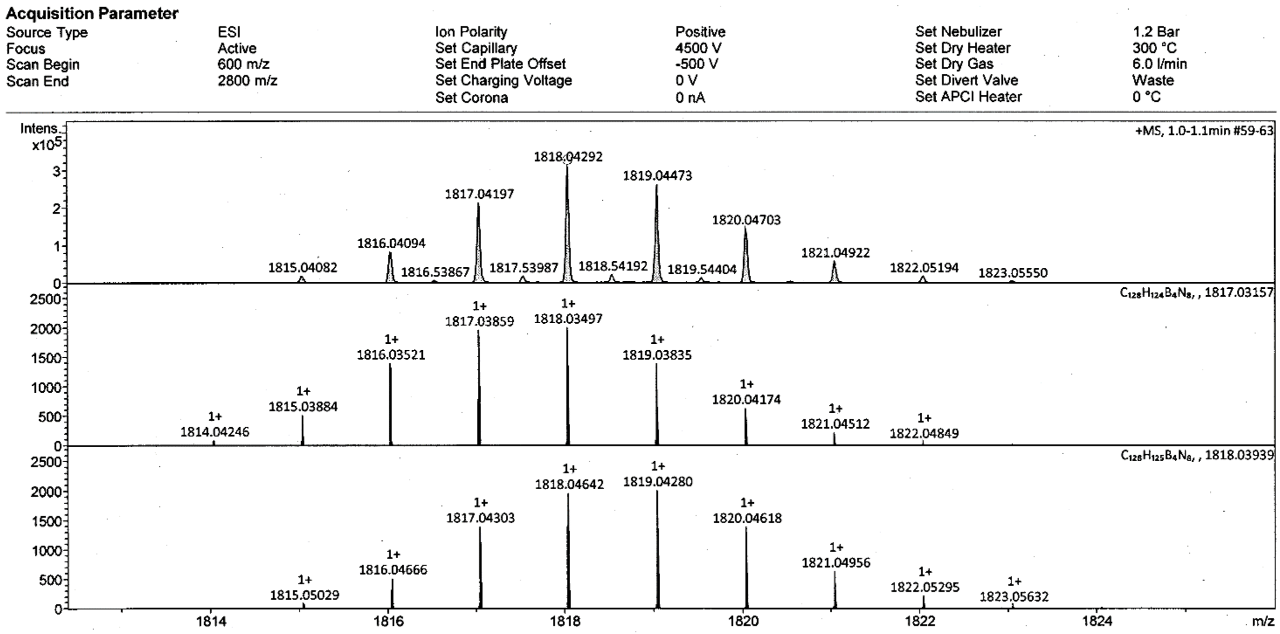


Figure S36. Experimental HR ESI-MS of rac-**6** (top) and theoretical isotopic envelope for $C_{128}H_{124}B_4N_8$ $[M]^+$ and $C_{128}H_{125}B_4N_8$ $[M+H]^+$ (middle and bottom, respectively).

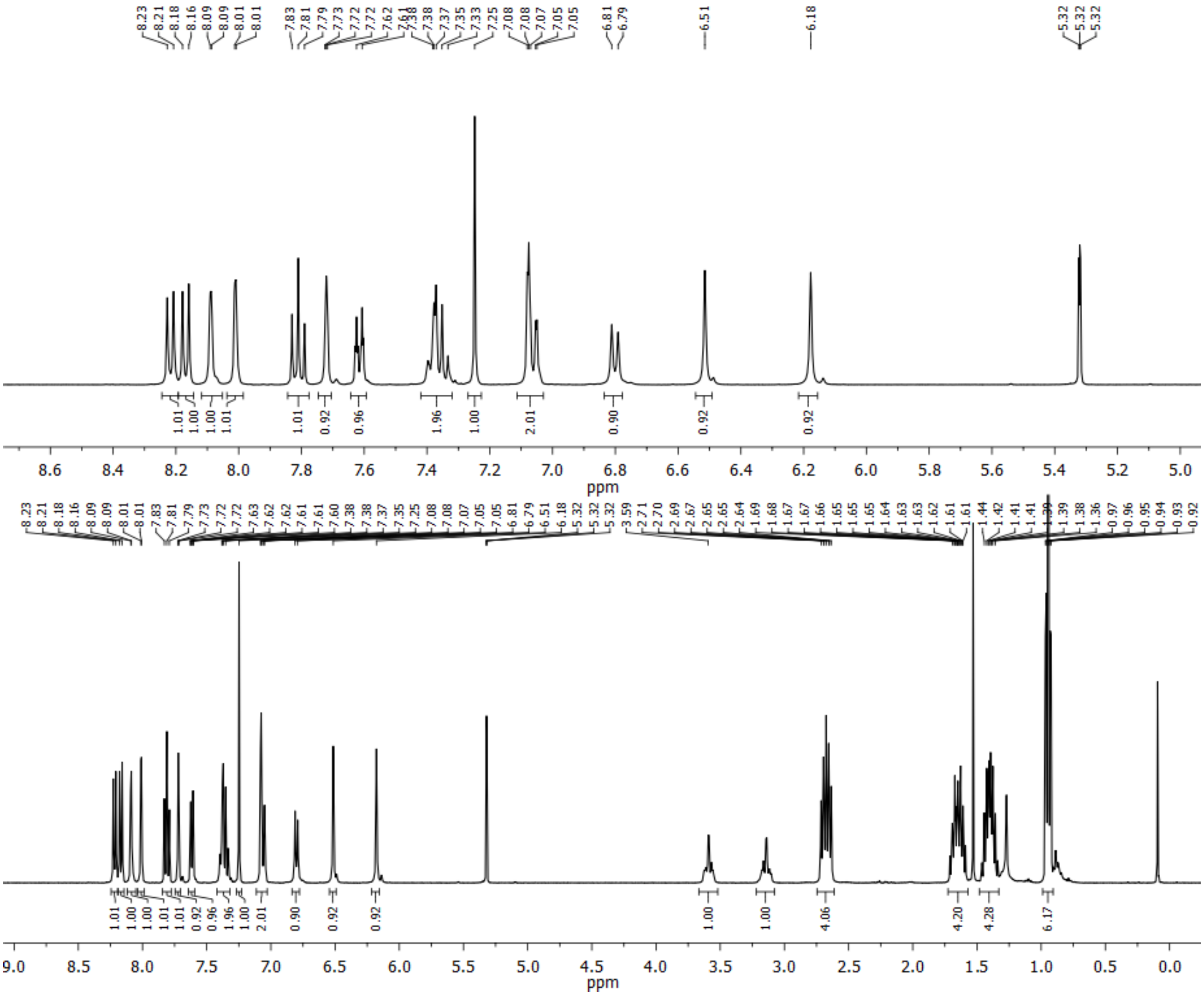


Figure S37. ^{1}H NMR (400 MHz, CD_2Cl_2) of rac-**7*m***.

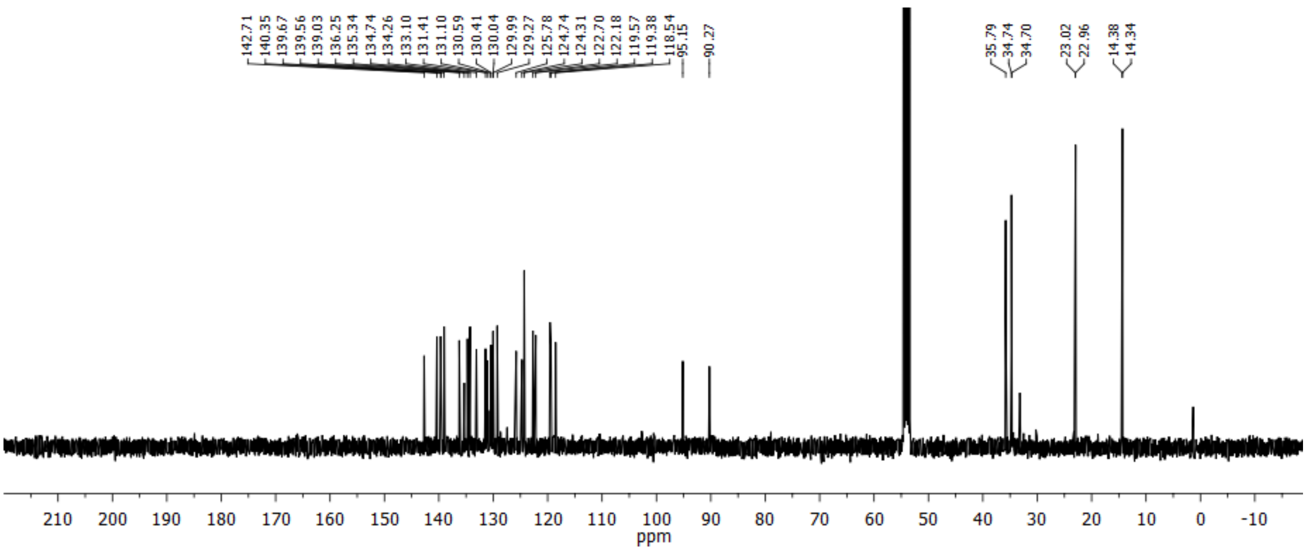


Figure S38. $^{13}C\{^{1}H\}$ NMR (101 MHz, CD_2Cl_2) of rac-**7*m***.

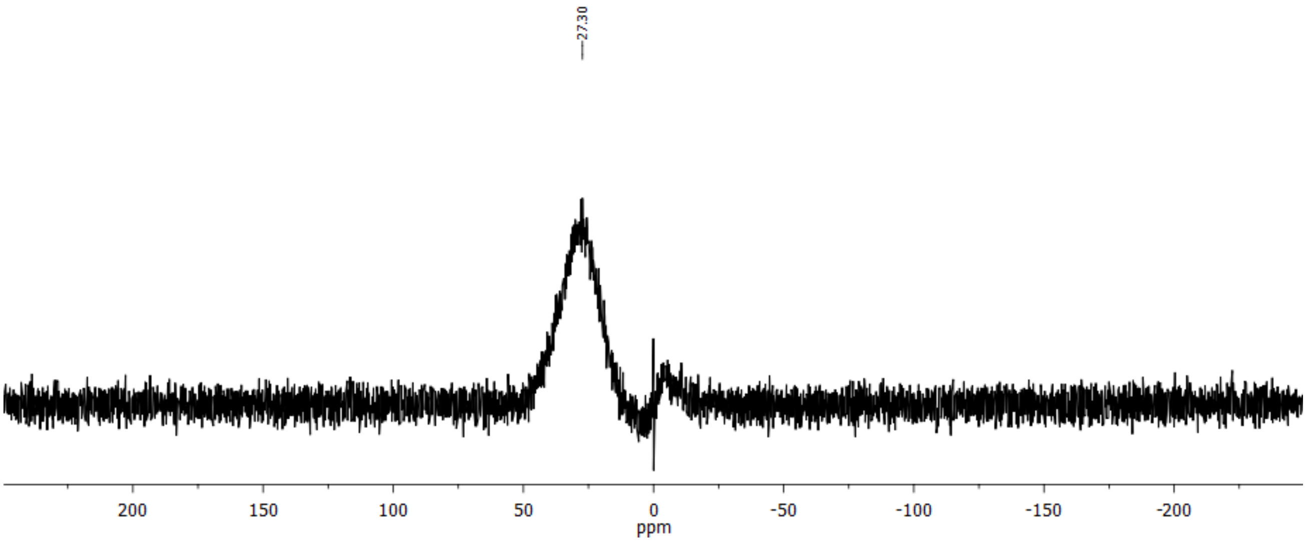


Figure S39. ^{11}B{1H} NMR (128 MHz, $CDCl_3$) of rac-**7*m***.

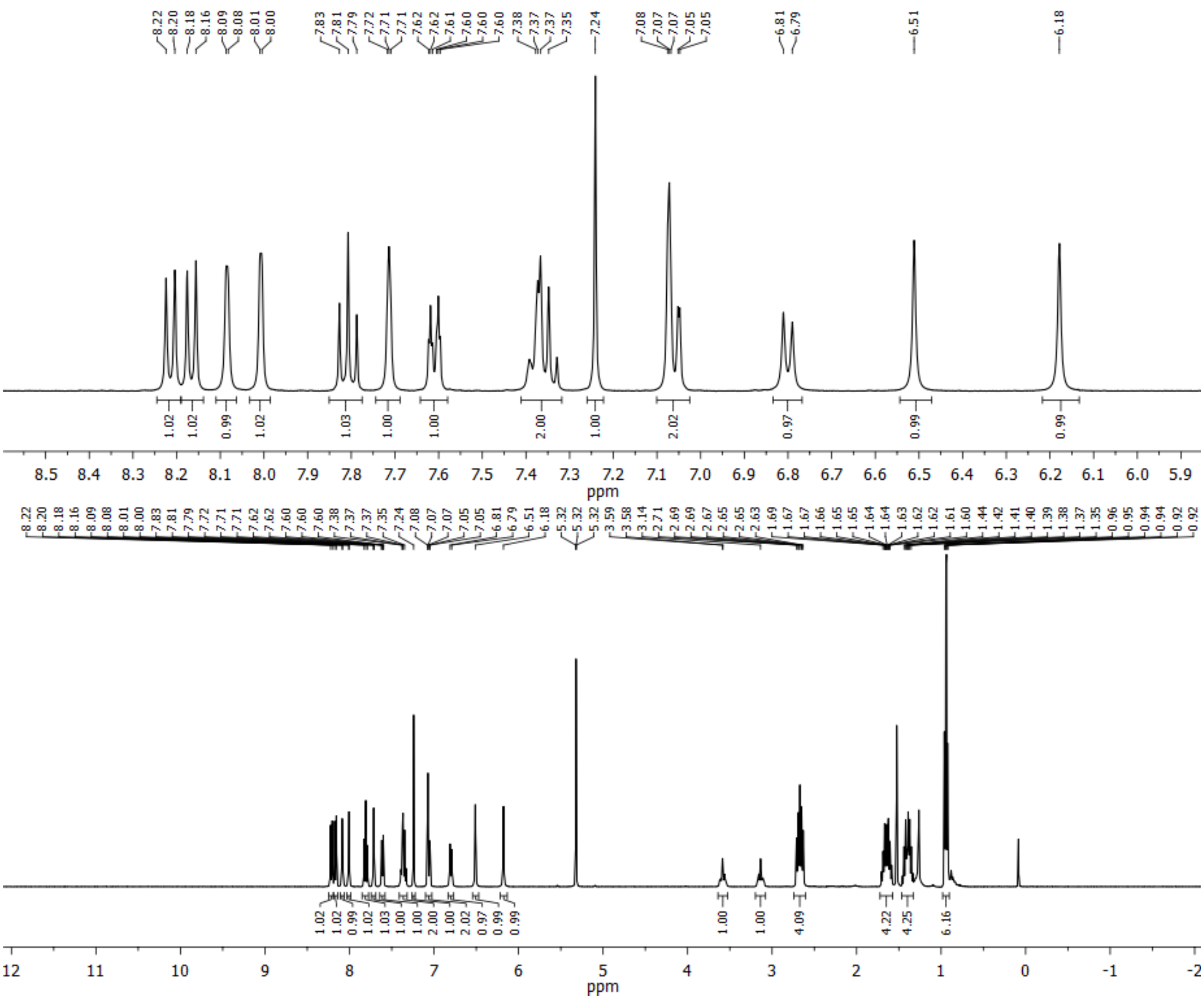


Figure S40. ^{1}H NMR (400 MHz, CD_2Cl_2) of (R)-**7*m***.

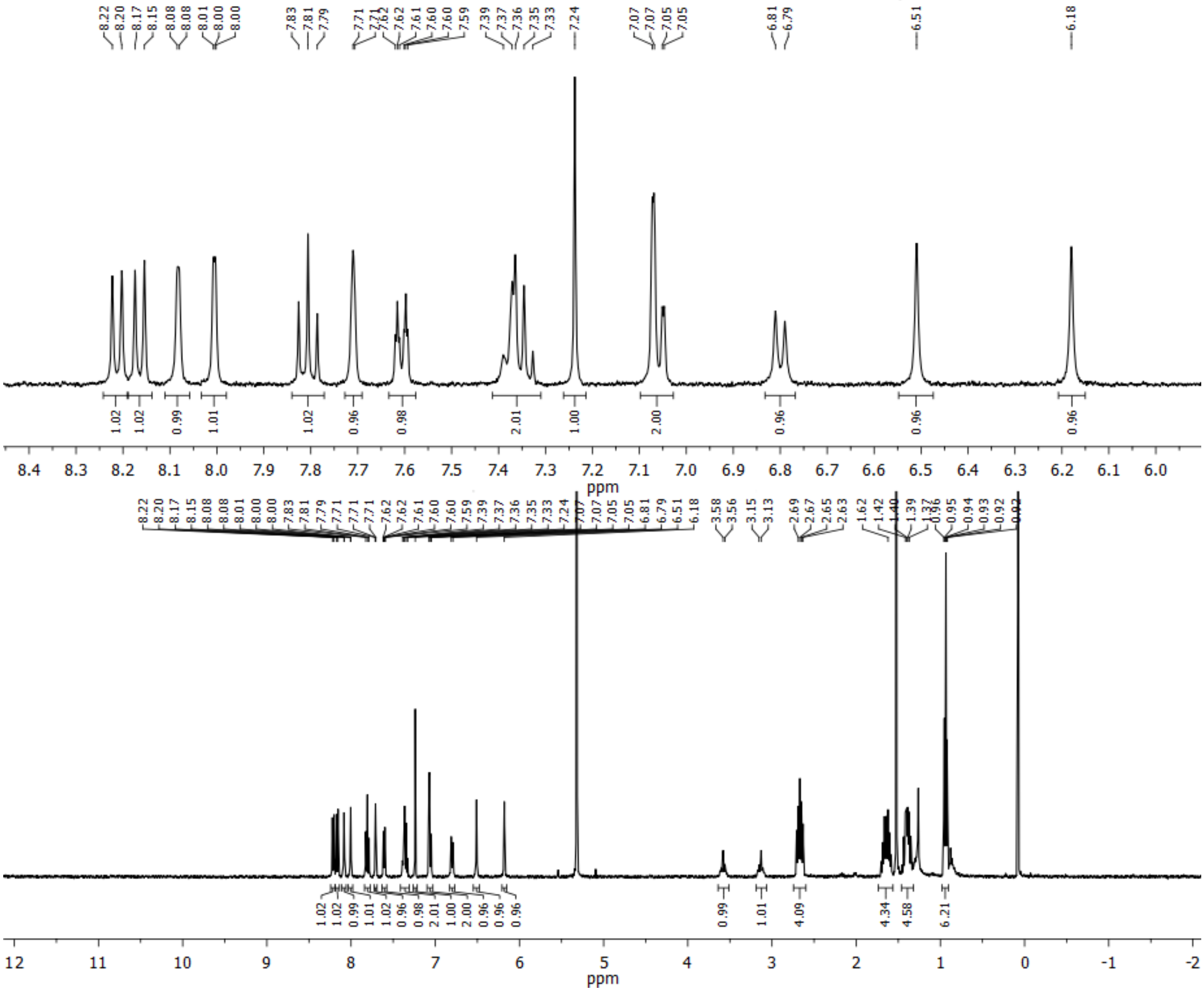


Figure S41. ^{1}H NMR (400 MHz, CD_2Cl_2) of (S)-**7*m***.

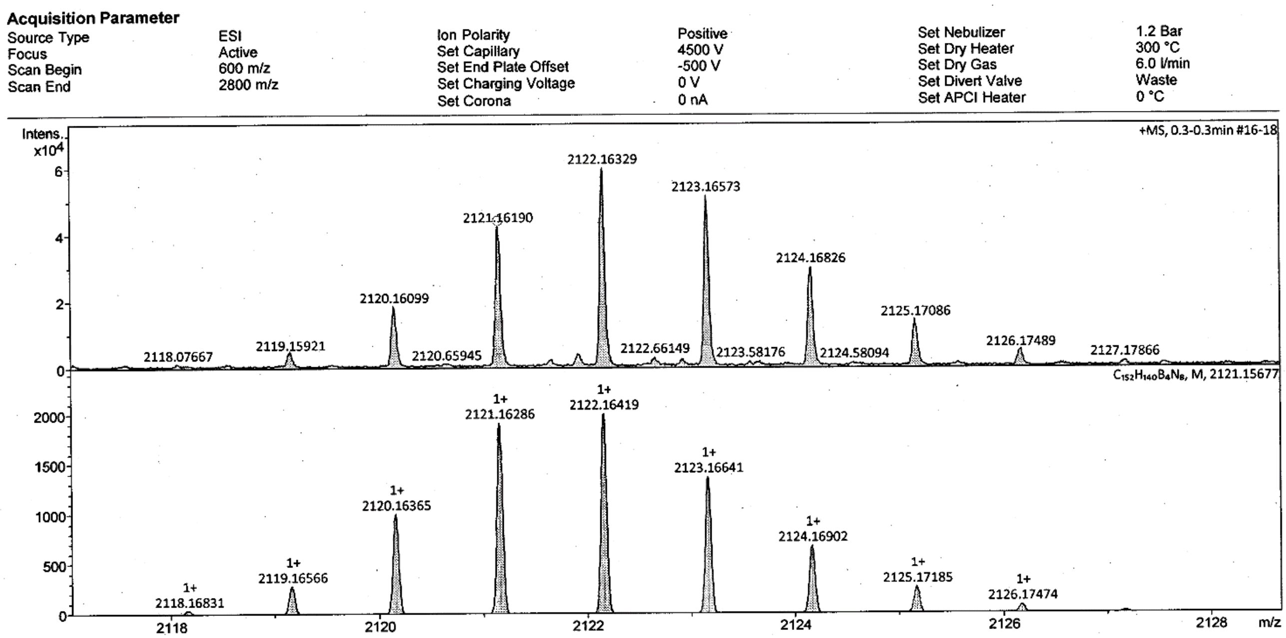


Figure S42. Experimental HR ESI-MS of rac-**7*m*** (top) and theoretical isotopic envelope for $C_{152}H_{140}B_4N_8$ $[M]^+$ (bottom).

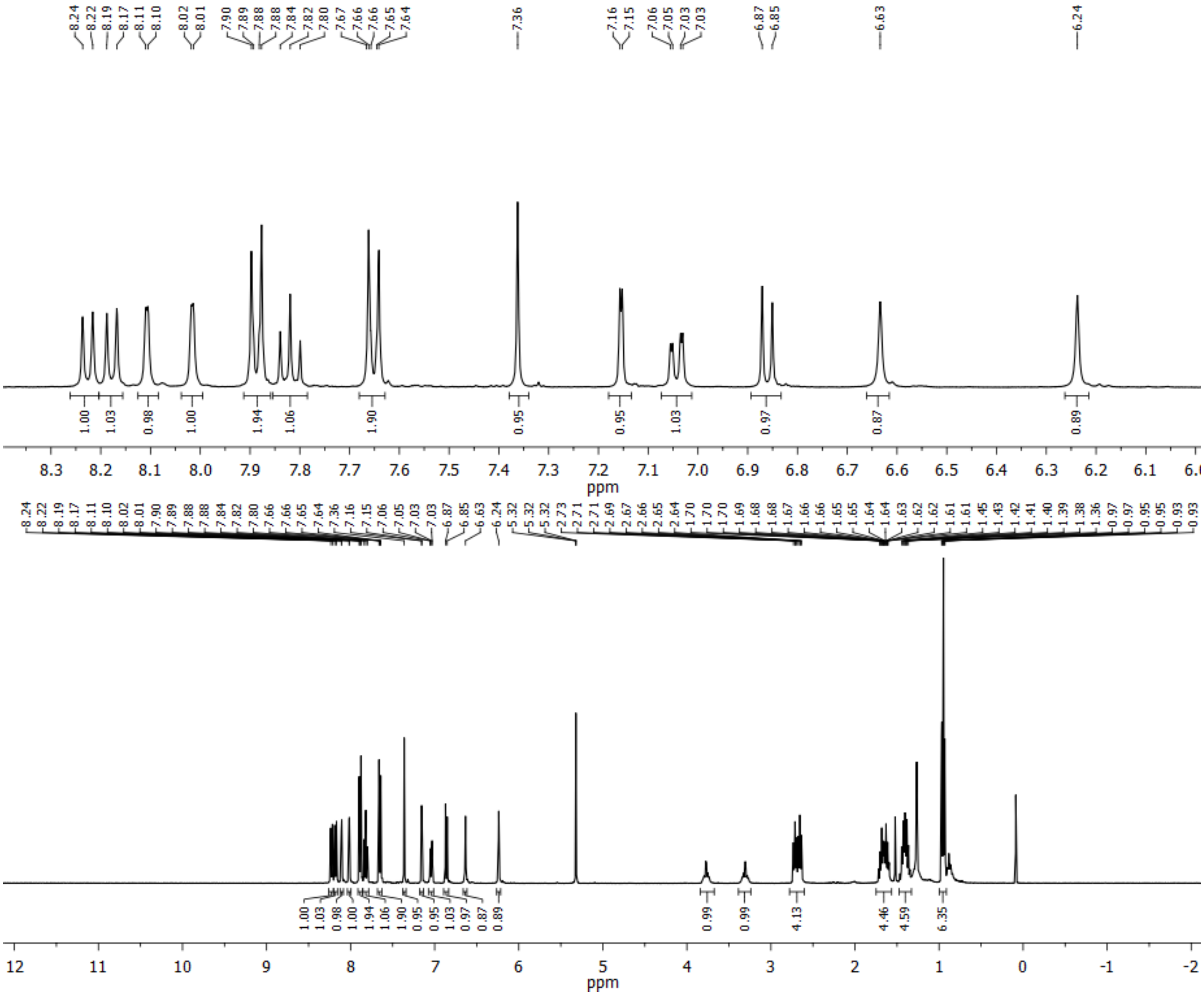


Figure S43. ^{1}H NMR (400 MHz, CD_2Cl_2) of rac-**7*p***.

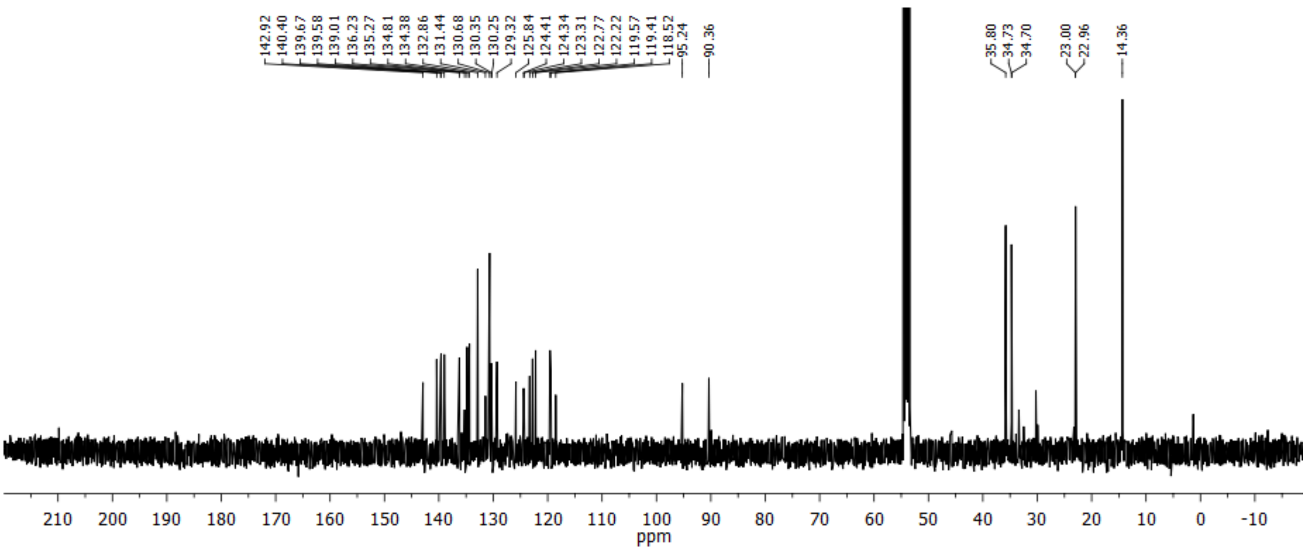


Figure S44. $^{13}C\{^{1}H\}$ NMR (400 MHz, CD_2Cl_2) of rac-**7*p***.

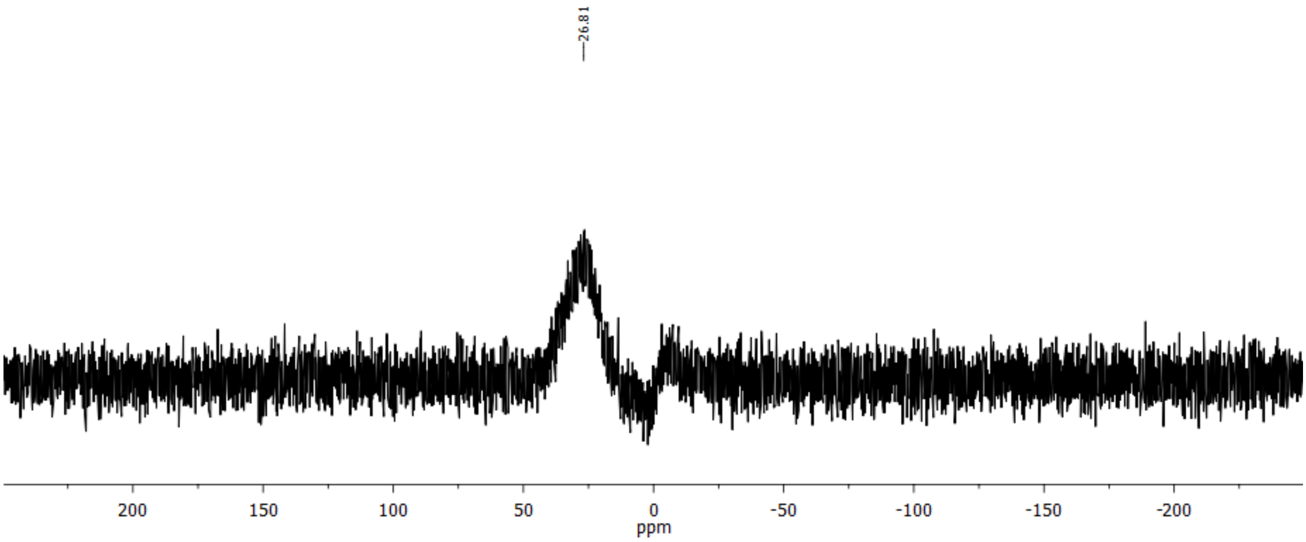


Figure S45. $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$) of rac-**7*p***.

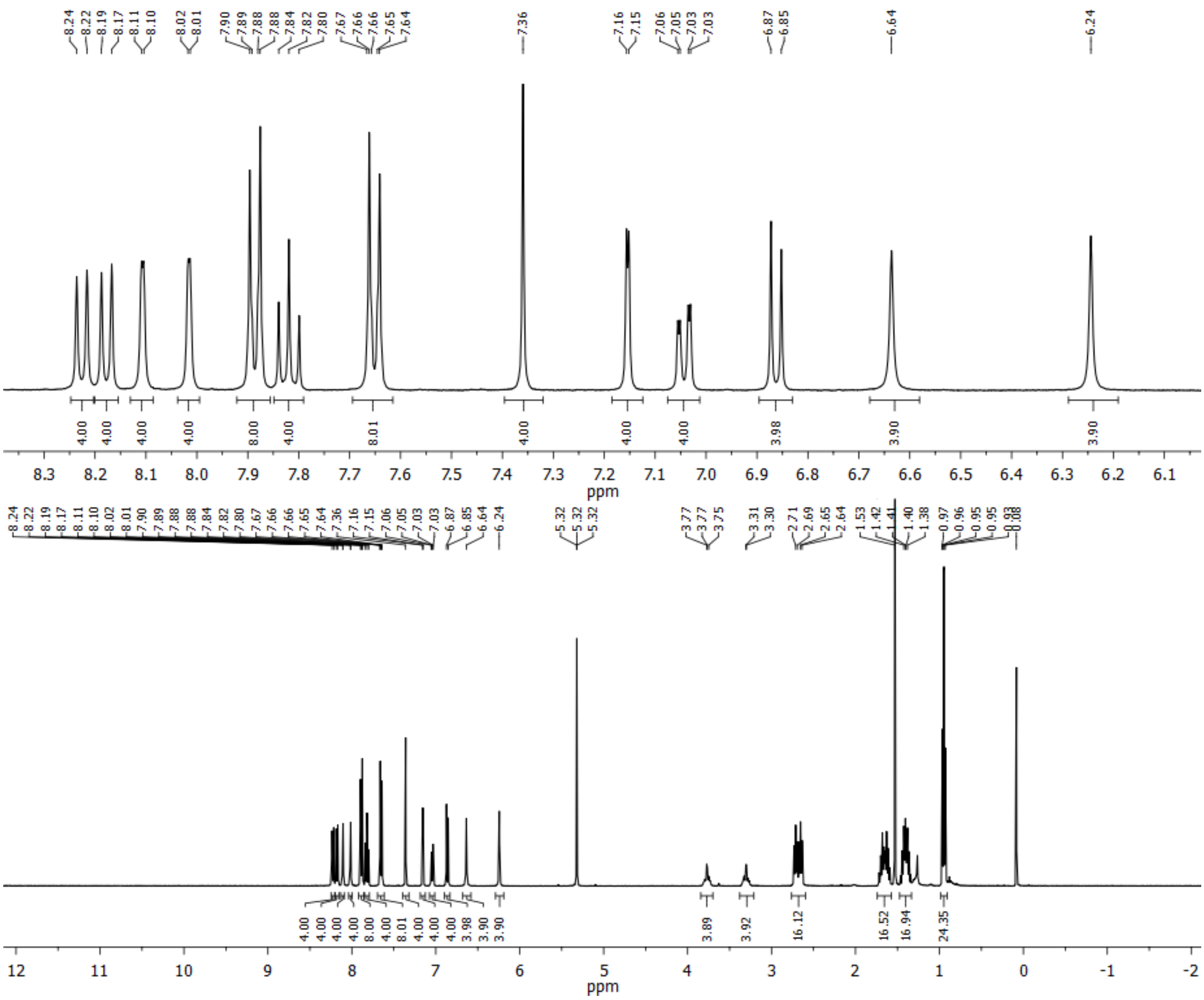


Figure S46. ^1H NMR (400 MHz, CD_2Cl_2) of (R)-**7*p***.

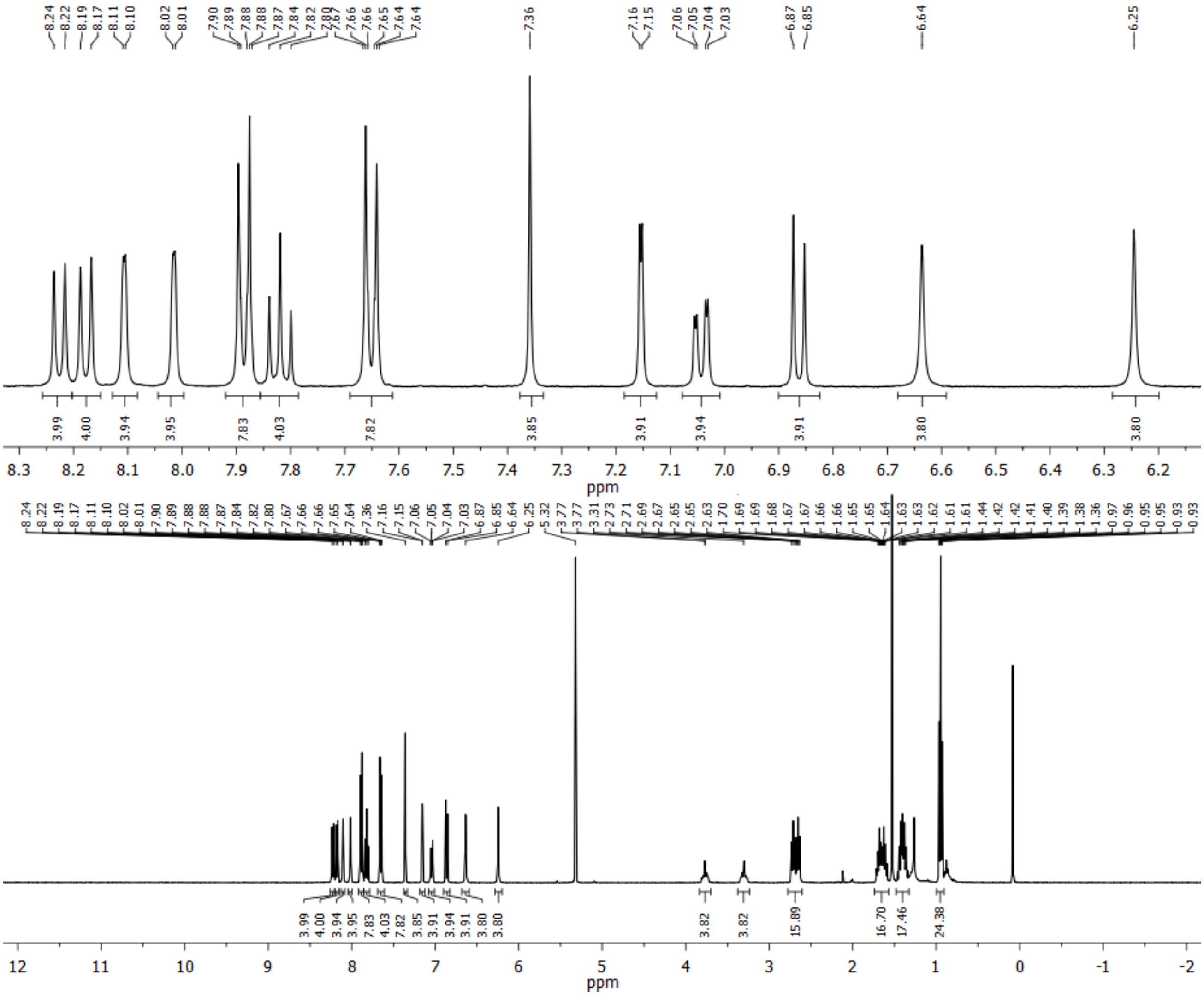


Figure S47. ^{1}H NMR (400 MHz, CD_2Cl_2) of (S)-**7*p***.

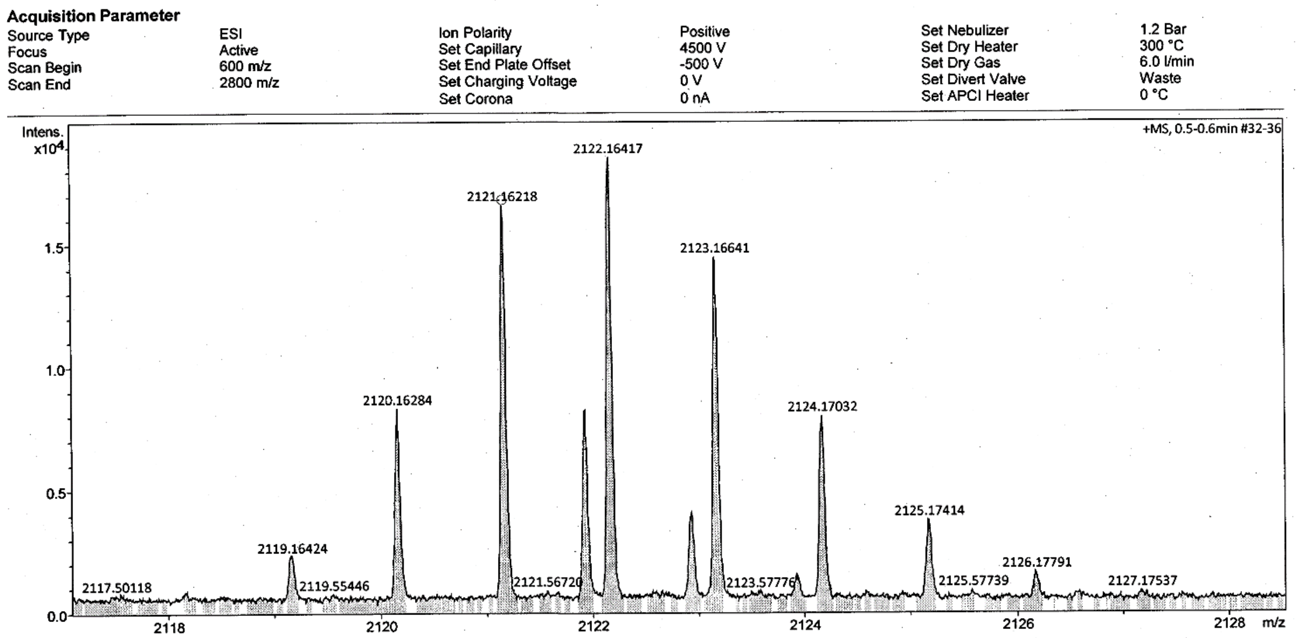


Figure S48. Experimental HR ESI-MS of rac-**7*p*** as $[M]^{+}$.

3. Optical Spectra: UV/Vis, Emission, Excitation, Emission lifetime

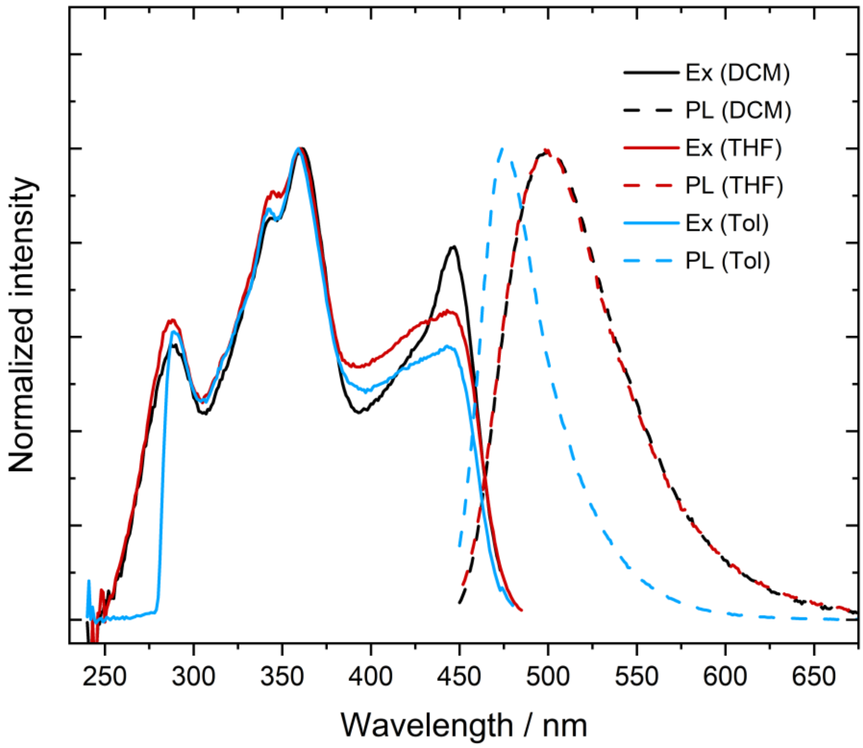


Figure S49. Emission and excitation spectra of rac-**6** in CH_2Cl_2 (λ_{ex} = 445 nm, λ_{em} = 493 nm), THF (λ_{ex} = 492 nm, λ_{em} = 446 nm) and toluene (λ_{ex} = 445 nm, λ_{em} = 476 nm).

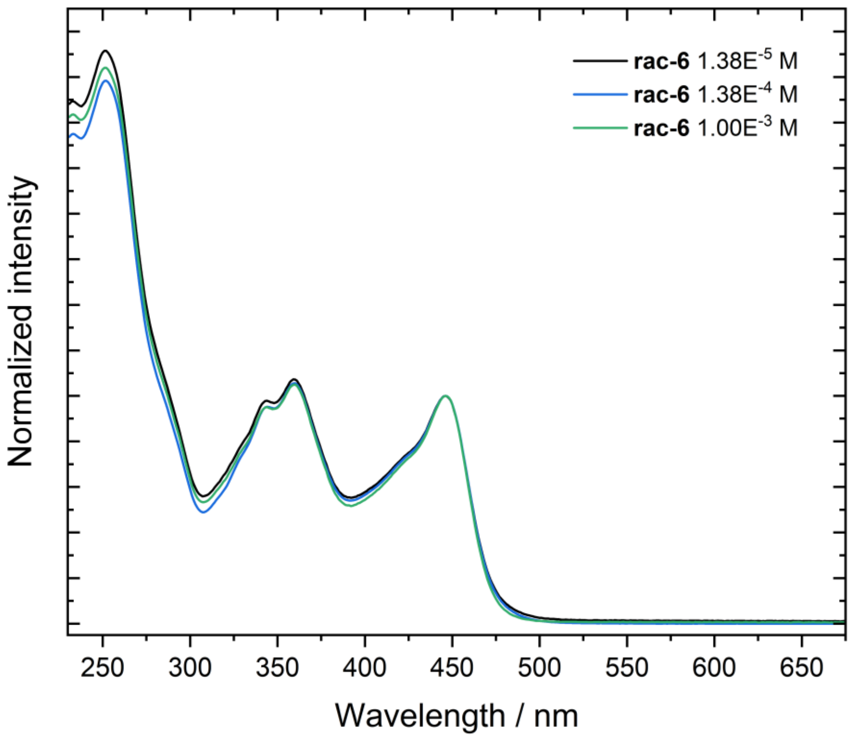


Figure S50. UV/Vis absorption spectra of differently concentrated solutions of rac-**6** in CH_2Cl_2 ($1.38\cdot10^{-5}$ M, $1.38\cdot10^{-4}$ M, and $1.00\cdot10^{-3}$ M).

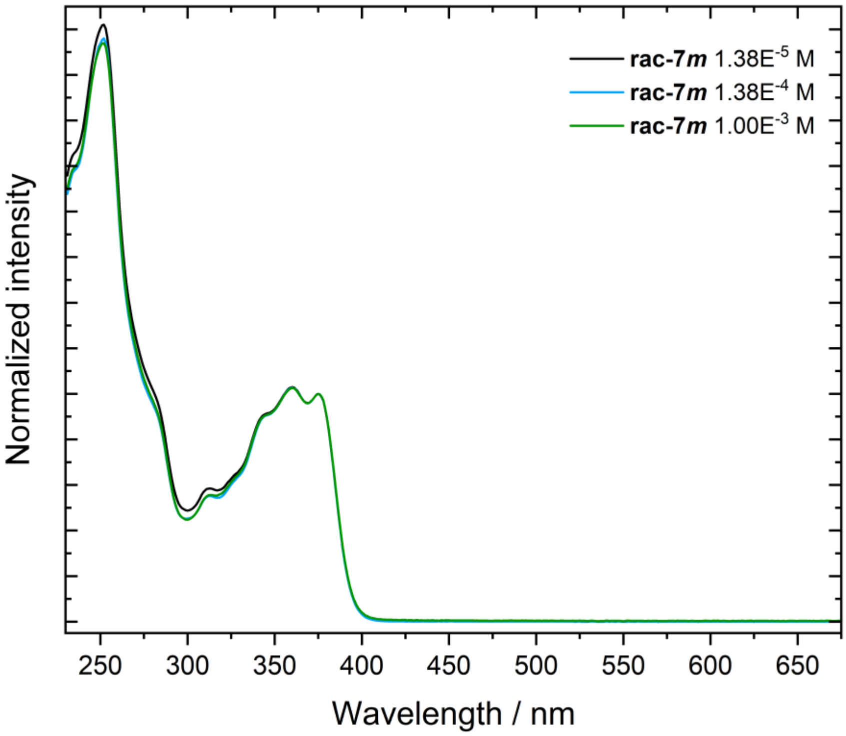


Figure S51. UV/Vis absorption spectra of differently concentrated solutions of rac-**7*m*** in CH_2Cl_2 ($1.38\cdot10^{-5}$ M, $1.38\cdot10^{-4}$ M, and $1.00\cdot10^{-3}$ M).

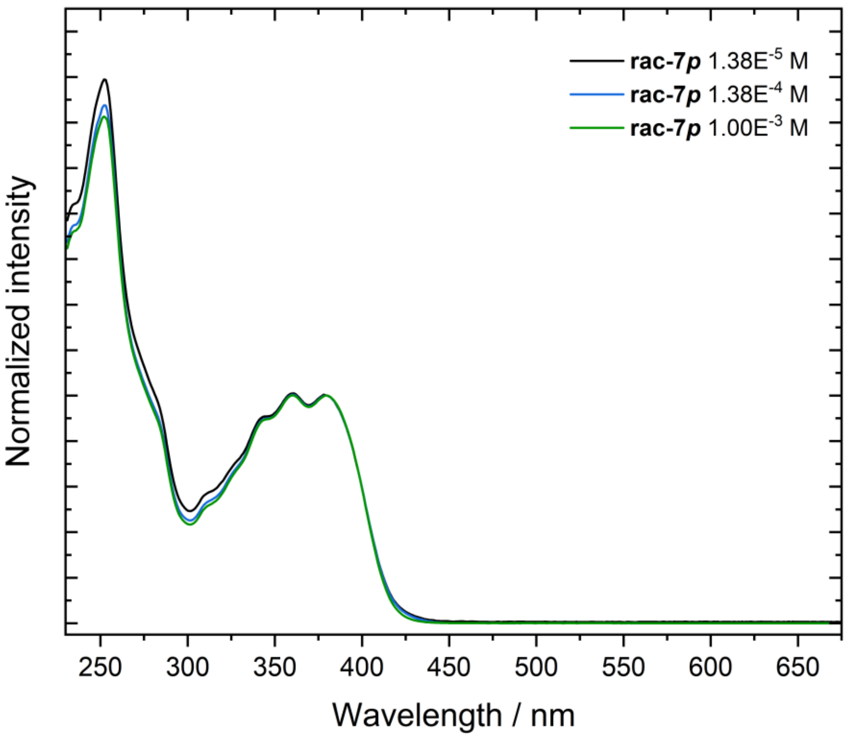


Figure S52. UV/Vis absorption spectra of differently concentrated solutions of rac-**7*p*** in CH_2Cl_2 ($1.38\cdot10^{-5}$ M, $1.38\cdot10^{-4}$ M, and $1.00\cdot10^{-3}$ M).

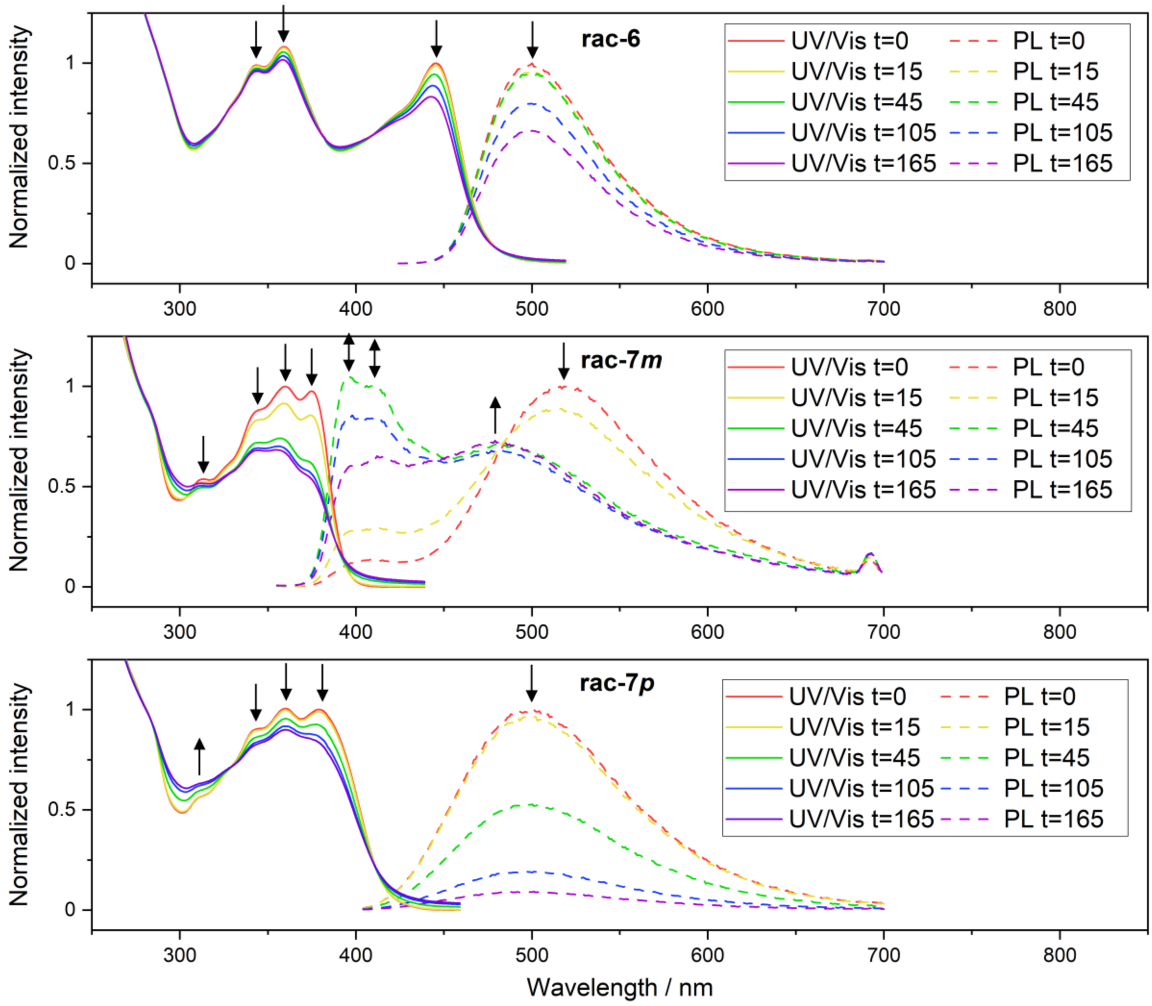


Figure S53. Photodegradation over time of solutions of rac-**6** (top), rac-**7*m*** (middle) and rac-**7*p*** (bottom) in CH_2Cl_2 ($1.00 \cdot 10^{-5}$ M) upon radiation with an UV-Lamp (λ = 366 nm, 2·6 W). Normalization is done by dividing the spectra with the initial maxima at t = 0 min. Times are given in minutes.

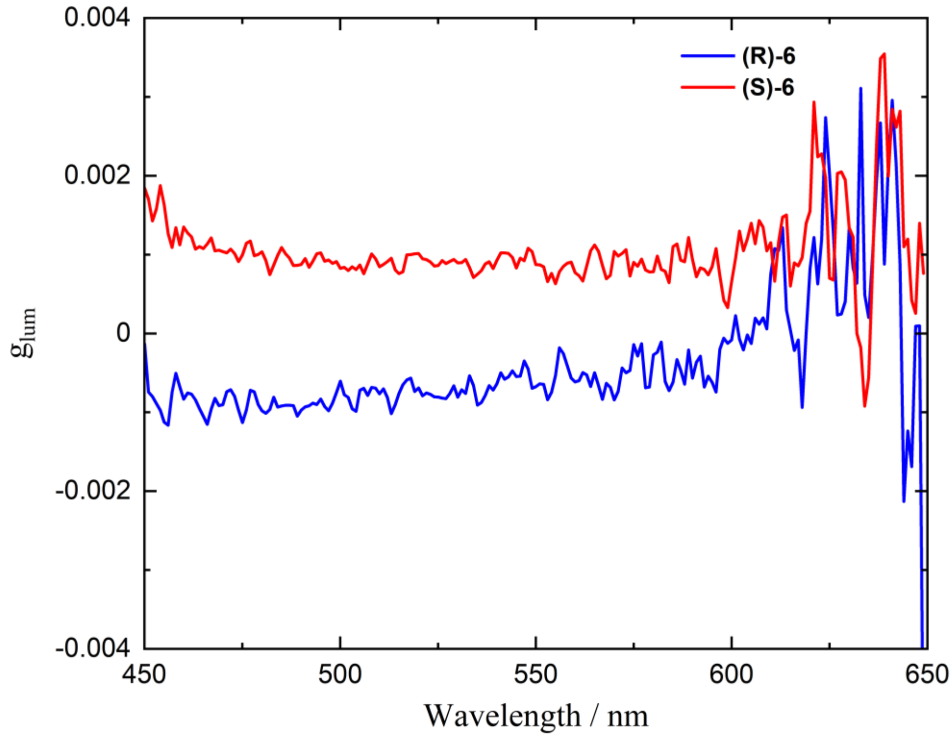


Figure S54. g_{lum} *vs* wavelength plot (λ_{ex} = 365 nm, 2.0·10^{-4} M, CH_2Cl_2, 293 K). Note that on the red edge of the spectrum g_{lum} becomes undefined (and therefore erratic) as total luminescence (I_L+I_R) approaches 0.

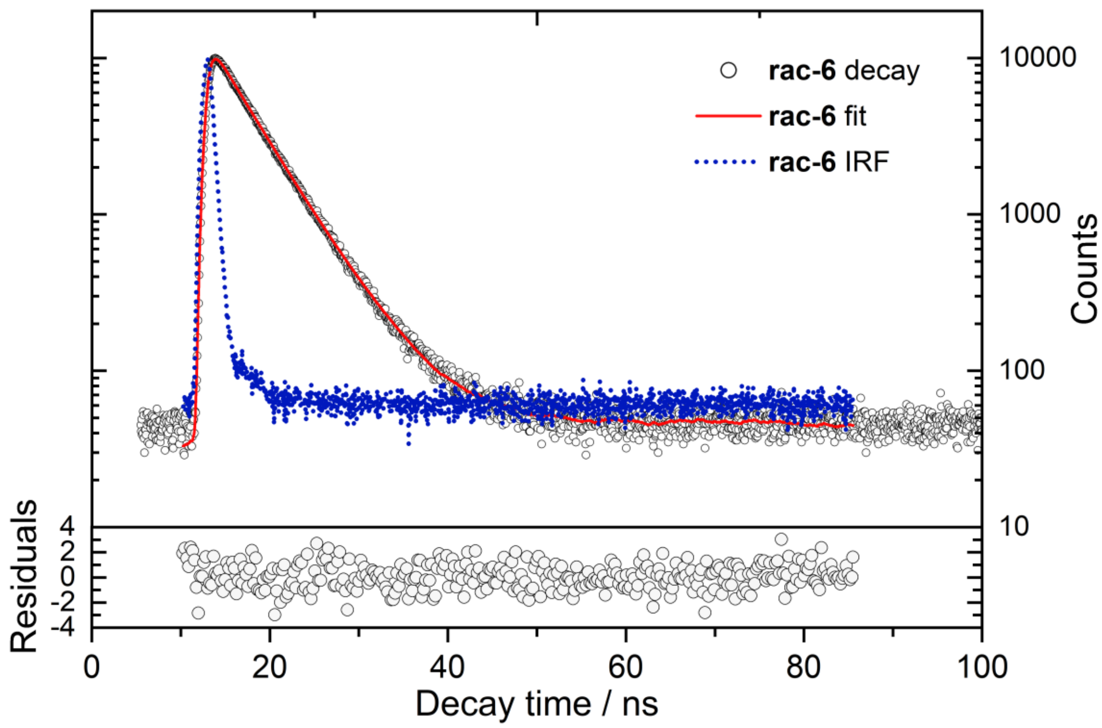


Figure S55. Time-resolved photoluminescence decay curves of rac-**6**. The decay is best fitted to a biexponential equation (χ^2 = 1.07) with 3.34 ns and 5.01 ns (24 % and 76 % relative amplitudes, respectively), taking into account the instruments response function (IRF) by an iterative reconvolution fitting method.

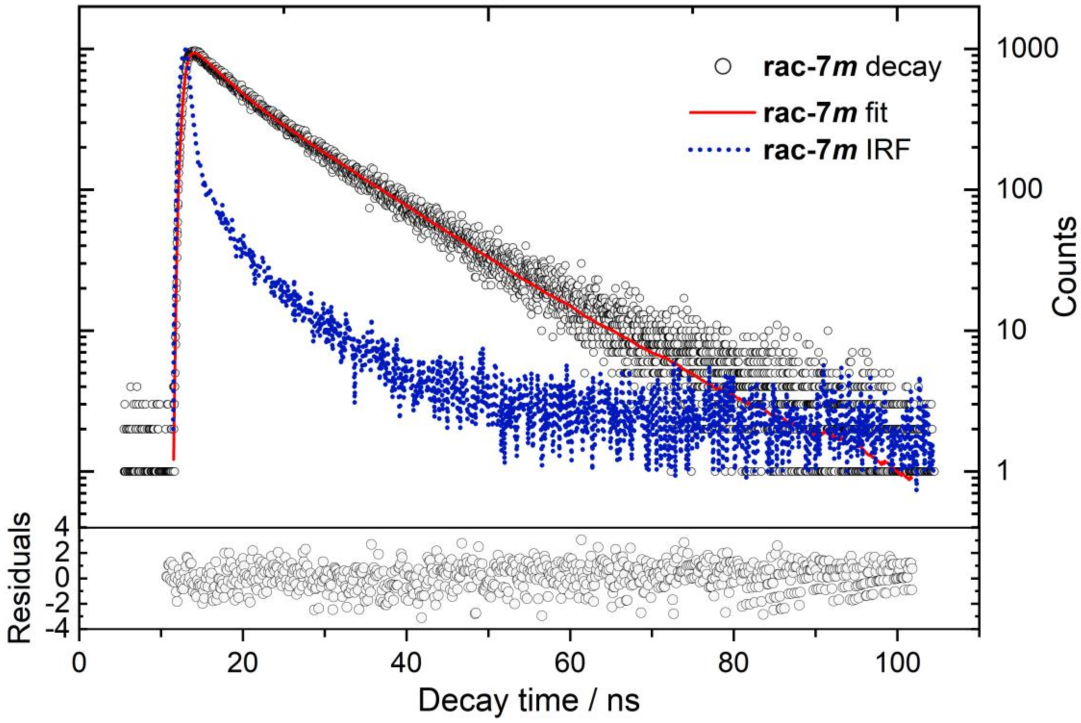


Figure S56. Time-resolved photoluminescence decay curves of rac-**7*m***. The decay is best fitted to a biexponential equation (χ^2 = 1.11) with life times of 3.03 ns and 11.3 ns (36 % and 64 % relative amplitudes, respectively), taking into account the instruments response function (IRF) by an iterative reconvolution fitting method.

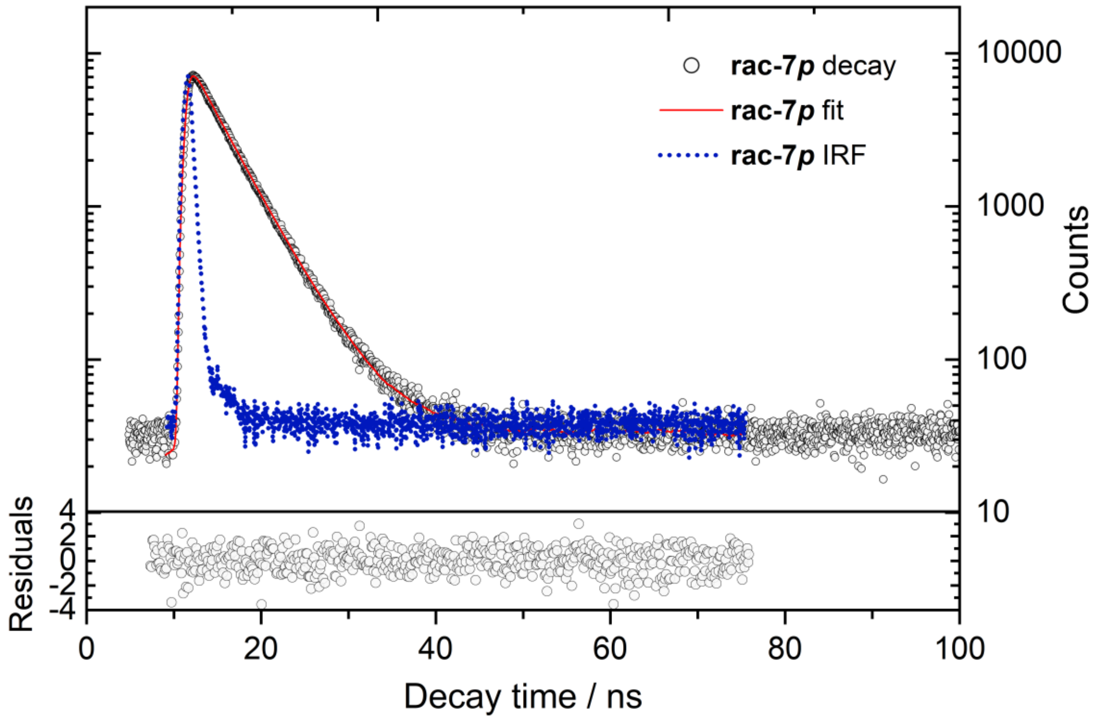


Figure S57. Time-resolved photoluminescence decay curves of rac-**7*p***. The decay is best fitted to a biexponential equation (χ^2 = 1.10) with life times of 2.94 ns and 6.32 ns (29 % and 71 % relative amplitudes, respectively), taking into account the instruments response function (IRF) by an iterative reconvolution fitting method.

4. Electrochemical studies

CH_2Cl_2 stabilized with ethanol (CHEMSOLUTE; HPLC grade) was distilled over P_2O_5 and then over K_2CO_3. CH_3CN (Honeywell Riedel-de Haën; HPLC grade) was distilled successively over P_2O_5, CaH_2 and P_2O_5. The purified solvents were stored under Argon. *Tetrabutylammonium hexafluorophosphate* NBu_4PF_6 (TCI; >98.0%) was recrystallized four times from water/ethanol (3:1) and lyophilized. As the supporting electrolyte, NBu_4PF_6 was dissolved in concentrations of 0.1 M in CH_2Cl_2 and CH_3CN and the electrolytes were degassed by either freeze-pump-thaw or argon bubbling.

Electrochemical measurements were performed in a modified full-glass, gas-tight three-electrode cell as described previously.[7] All experiments were carried out at 17 °C under an argon atmosphere using an ECO-Autolab PGSTAT100 (Metrohm) instrument with GPES-Software 4.9.007. *iR* Drop was compensated by the positive feedback function of the software. A Pt disk electrode tip (Metrohm part no. 6.1204.310; nominal diameter 3 mm; electroactive area A = 0.066 ± 0.003 cm^2) and a GC disk electrode tip (Metrohm part no. 6.1204.300; nominal diameter 3 mm; electroactive area A = 0.065 ± 0.002 cm^2) were used as working electrodes for the positive and negative potential range, respectively. The electrodes were polished using a suspension of α-alumina (Buehler) in deionised water prior to experiments. For the determination of the number of transferred electrons we used a combination of chronoamperometric data and steady-state currents at a microelectrode (Bioanalytical Systems microelectrode tip; nominal radius 50 µm; experimental determined radius r = 44.3 ± 2.2 µm).[8] As counter electrode we used a Pt wire (1 mm diameter). All potentials were determined *vs* Ag/Ag^+ (0.01 M in CH_3CN/0.1 M NBu_4PF_6) by a Haber-Luggin double-reference electrode. The values were rescaled to an external Fc/Fc^+ standard ($E^0(Fc/Fc^+)$ = 207 ± 1 mV *vs* Ag/Ag^+ in CH_2Cl_2).

Scan rates for cyclic voltammograms ranged from 0.02 to 10 V/s. For chronoamperograms we used a step width between 2 and 8 s, while steady-state measurements were conducted at 0.001 to 0.004 V/s. To prove reproducibility all measurements were recorded at different concentrations within one experimental session, and sessions were repeated at least three times. Unless otherwise noted, all current data were background corrected and filtered by the PGSTAT 100's smooth functions Fourier transform (CV) and Savitzky-Golay (CA and microelectrode measurements).

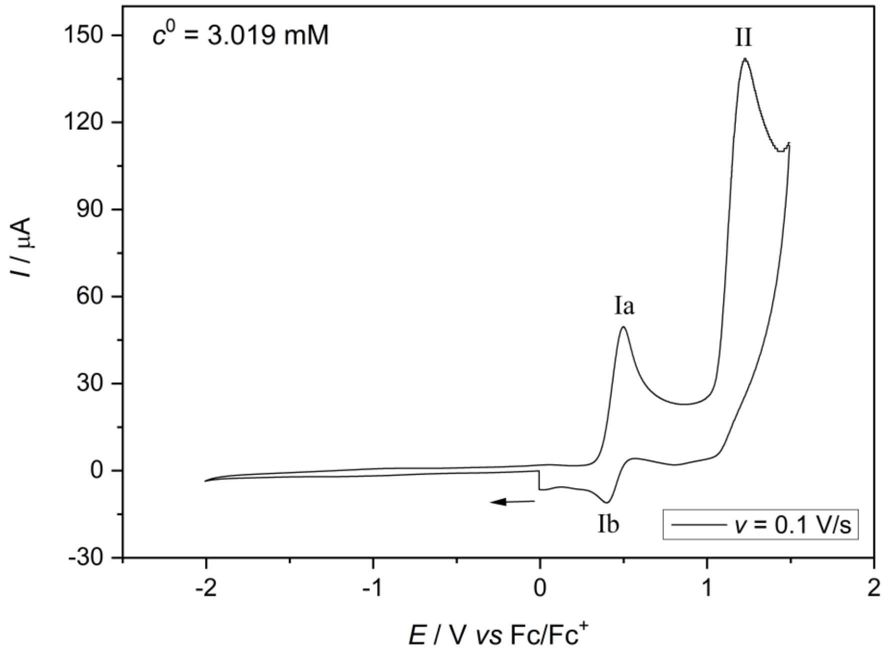


Figure S58. Cyclic voltammogram of NBN-benzotetracene (1) at v = 0.1 V/s in CH_2Cl_2/0.1 M NBu_4PF_6 (not background corrected).

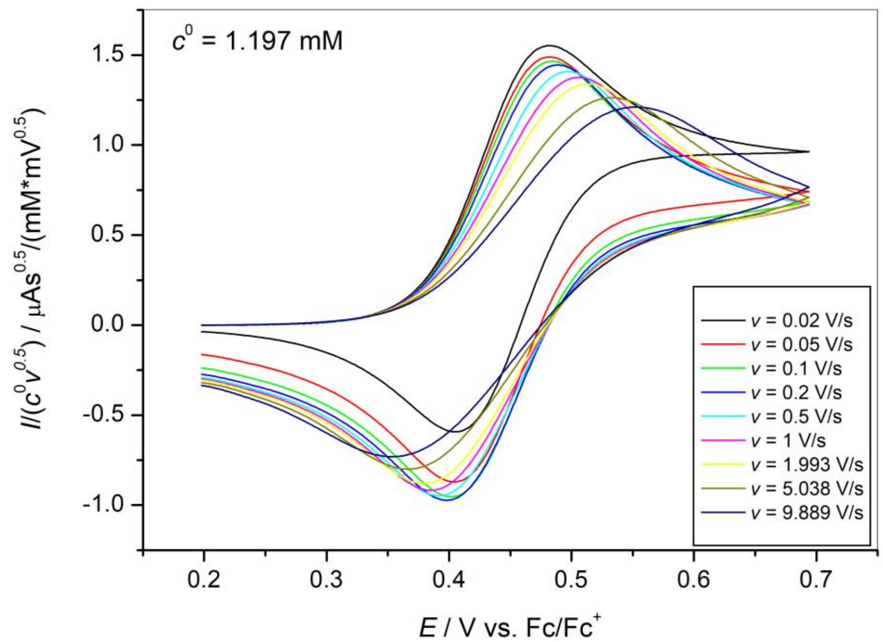


Figure S59. Normalized cyclic voltammogram of the first oxidation I of 1 at various scan rates v in CH_2Cl_2/0.1 M NBu_4PF_6.

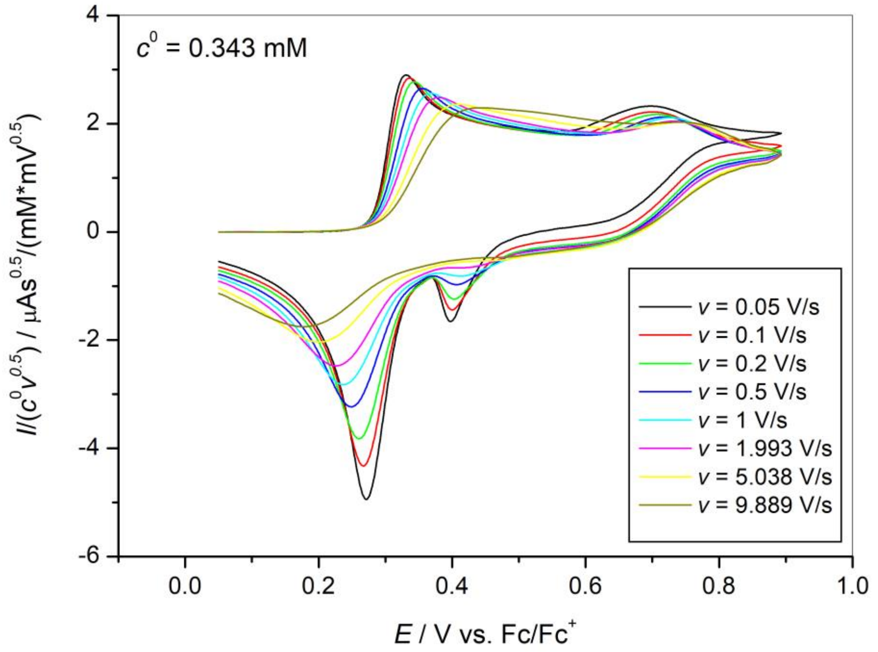


Figure S60. Normalized cyclic voltammograms of the first and second oxidations of rac-6 at various scan rates v in CH_2Cl_2/0.1 M NBu_4PF_6.

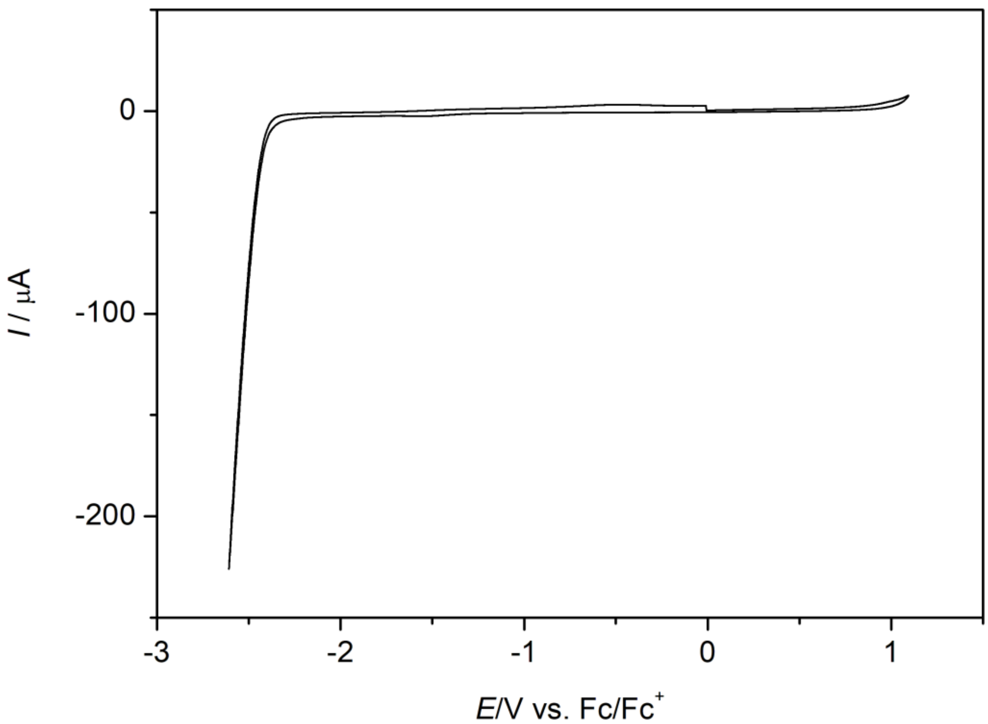


Fig. **S61**: Cyclic voltammogram of rac-**5** at v = 0.2 V/s in CH_2Cl_2/0.1 M NBu_4PF_6 (concentration c^0 = 0.901 mM, GC electrode).

5. Computational studies

Conformer Analysis and Frontier Molecular Orbitals

The structures were optimized using the TPSS[9] meta functional in conjunction and the resolution of the identity approximation (Figure S62). The study of Grimme et al. suggests that the description of the intermolecular interaction of the [2.2]PCP framework requires large Gaussian type basis sets.[10] For this reason, the geometry optimizations were performed using the def2-QZVP basis set along with the recommended fitting bases required for the RI approximation.[11,12] In addition, dispersion interactions between the NBN-moieties were dealt with using Grimme's D3 scheme along with Becke-Johnson damping.[13,14] The TPSS and computations were performed with the Turbomole program.[15]

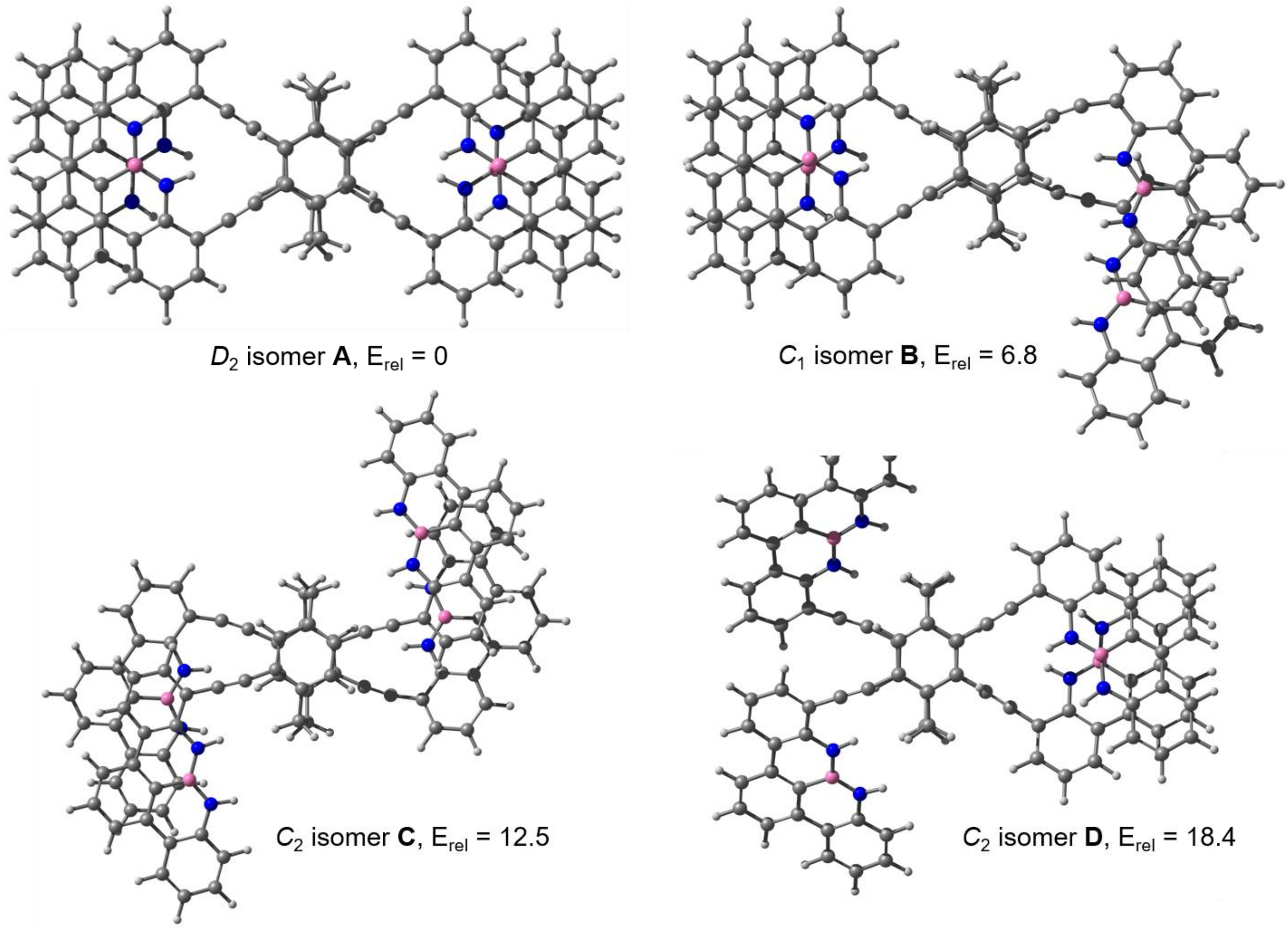


Figure S62. Computed structures of four isomers of the target compound (R)-**6'**. Relative energies computed at the RI-TPSS-D3(BJ)/def2-QZVP level of theory are given in kcal mol^{-1}.

Based on the most favorable D_2 isomer of **6'**, the compounds with one ("monomer") and two NBN-tetracene units were computed at the RI-TPSS-D3(BJ)/def2-QZVP level of theory. The latter have their NBN-tetracene units either attached to two different PCP arene rings allowing face-to-face interaction ("dimer through space") or to the same PCP arene ring allowing conjugation through its π system ("dimer through bond"). The frontier molecular orbital energies and energy gaps were computed (see Figure S63) in subsequent single point computations using the B3LYP[16,17] hybrid density functional in conjunction with the def2-QZVP basis set with the Gaussian 16 program.[18]

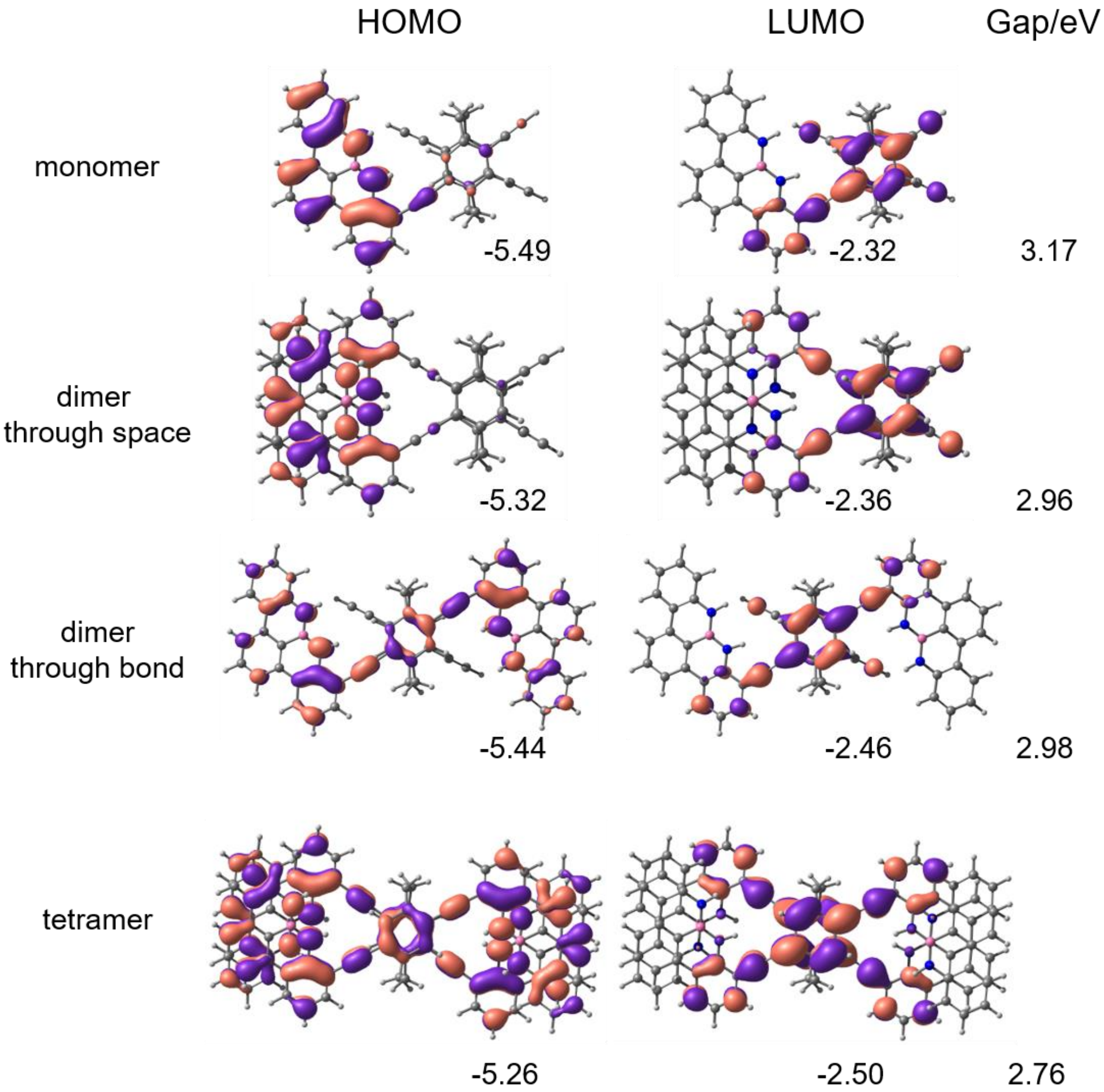


Figure S63. Frontier molecular orbitals, their energies (in eV) and energy gap (in eV) as computed at the B3LYP/def2-QZVP//RI-TPSS-D3(BJ)/def2-QZVP level of theory.

Comparison of the molecular orbitals and their energies for "monomer", "dimers" and "tetramer" shows that the π orbitals of the PCP mix into the HOMO of the NBN-tetracene unit once through bond conjugation is possible between these units. The LUMO is located primarily on the PCP core for the entire series. Due to through-bond conjugation, the HOMO energy is hardly changed while the LUMO energy is lowered. The through space interaction in the dimer raises the energy of the HOMO and hardly effects the energy of the LUMO. A combination of through space and through bond interactions in the tetramer results in a higher HOMO and lower LUMO energy, and thus the smallest HOMO-LUMO energy gap of 2.76 eV that is in good agreement with the optical gap.

Optical spectra (Absorption and ECD)

The energy of the lowest excited states and associated oscillator strengths were computed at the optimized geometry (RI-TPSS-D3(BJ)/def2-QZVP) using the algebraic diagrammatic construction through second order ADC(2)[19] and time-dependent density functional theory (TD-DFT)[20] along with the def2-TZVP basis set.[21] The CAM-B3LYP,[22] ωB97XD,[23] and M06-2X[24] functionals were chosen. To speed-up the ADC(2) computations, the resolution of the identity approximation[25] along with the recommended fitting basis set was employed.[21] The ADC(2) computations were performed with the Turbomole program,[15] while the TD-DFT computations were run with Gaussian 16.[18] Using the M06-2X functional, the 100 lowest energy excited states were computed for plotting of the absorption and ECD spectra below (Figures S64 and S65).

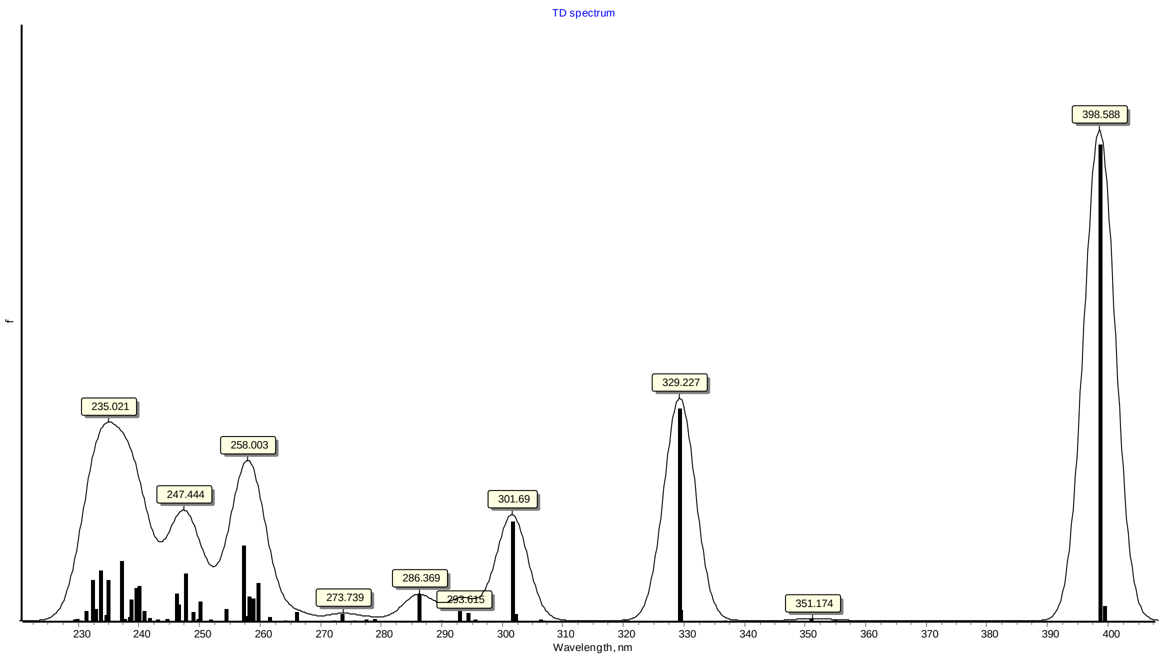


Figure S64. Absorption spectrum of (R)-6' including the first 100 excited states computed at the M062X/def2-TZVP level of theory.

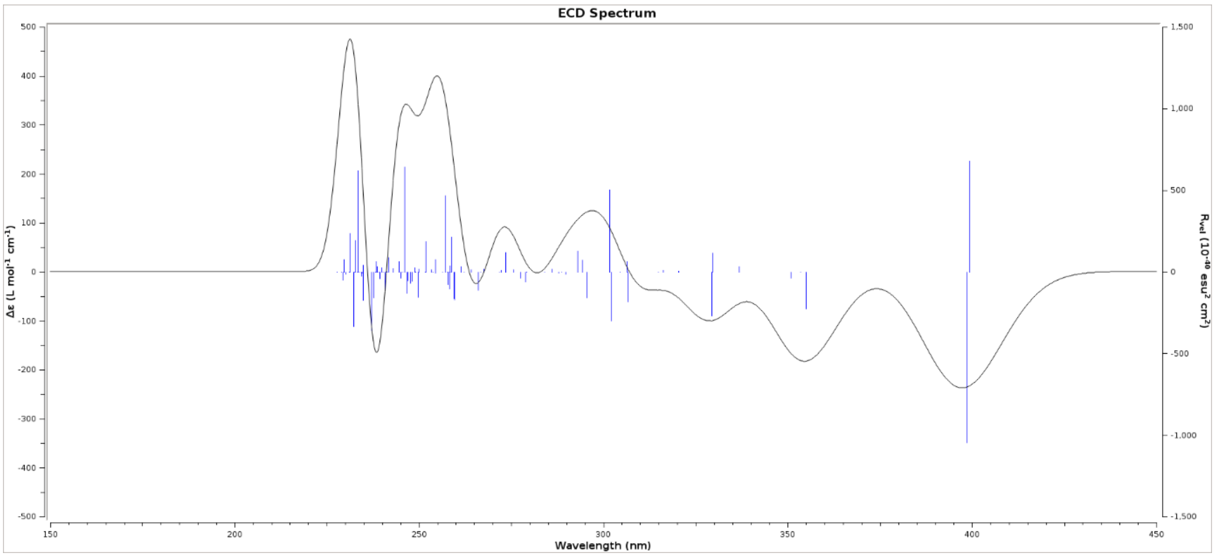


Figure S65. ECD spectrum of (R)-6' including the first 100 excited states computed at the M062X/def2-TZVP level of theory.

Dissymmetry Factor $g_{lum,calcd.}$

For detailed information on the procedure to calculate the g_{lum} value of compounds we refer to Kubo et al.[26] The geometries of the S_1 states were optimized by analytic gradients[27,28] using TD-DFT along with the def2-SV(P)[29] basis set. For (R)-6', Ph-PCP, Naph-PCP, and Anth-PCP' the meta-hybrid GGA M06-2X[24] functional was used, while (R)-6' was also studied with the Coulomb-attenuating method corrected CAM-B3LYP[22] (with and without using Grimme's D3 scheme along with Becke-Johnson damping)[13,14] and ωB97XD[23] functionals. These computations were run with the *Gaussian* 16 package.[18]

The dissymmetry factor $g_{lum,calcd.}$ was calculated as follows: $g = 4R/(D+G)$. R is the rotatory strength defined by the inner product of transition electric and magnetic dipole moments (it can be either calculated via $R = |\mu_e|\cdot|\mu_m|\cdot\cos\theta$ or taken from the R(length) column in the tables below), and D and G are the electric and magnetic dipole strengths defined by the square of transition electric and magnetic dipole moments, respectively ($D = |\mu_e|^2$; $G = |\mu_m|^2$). E_{ex} is the excitation energy calculated by TD-DFT method.

Table S1. Cartesian coordinates (Å) and transition moments of optimized structure of (R)-**6'** in the lowest-energy excited state (S_1) calculated at the M06-2X/def2-SV(P) level of theory.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.074347	1.417330	-1.420925
2	6	0	1.222457	0.643868	-1.554322
3	6	0	1.171649	-0.764474	-1.548419
4	6	0	-0.074328	-1.417247	-1.420907

5	6	0	-1.222430	-0.643784	-1.554440
6	6	0	-1.171626	0.764562	-1.548569
7	1	0	2.200554	1.129410	-1.496399
8	1	0	-2.200532	-1.129330	-1.496605
9	6	0	0.172610	2.802585	-0.827102
10	1	0	-0.507247	3.506757	-1.332982
11	1	0	1.201135	3.172755	-0.962207
12	6	0	-0.178394	2.805951	0.721253
13	1	0	-1.203954	3.184566	0.853978
14	1	0	0.507654	3.506788	1.224981
15	6	0	0.094070	-1.424504	1.321034
16	6	0	1.227468	-0.661785	1.459787
17	6	0	1.181617	0.770154	1.457721
18	6	0	-0.094288	1.424432	1.321030
19	6	0	-1.227702	0.661708	1.459652
20	6	0	-1.181857	-0.770240	1.457599
21	1	0	2.207071	-1.140674	1.375972
22	1	0	-2.207292	1.140595	1.375711
23	6	0	0.178266	-2.805987	0.721198
24	6	0	-0.172628	-2.802551	-0.827184
25	1	0	0.507288	-3.506695	-1.333026
26	1	0	-1.201131	-3.172732	-0.962410
27	1	0	-0.507775	-3.506877	1.224863
28	1	0	1.203843	-3.184564	0.853964
29	6	0	-2.391041	1.502881	-1.450971
30	6	0	-3.426455	2.136190	-1.339640
31	6	0	2.391058	-1.502790	-1.450727
32	6	0	3.426454	-2.136120	-1.339348
33	6	0	-2.368110	-1.498531	1.378054
34	6	0	-3.417182	-2.141960	1.268141
35	6	0	2.367893	1.498425	1.378274
36	6	0	3.416990	2.141791	1.268240
37	6	0	-7.021200	4.313590	-1.098679
38	6	0	-5.807107	4.981604	-0.980478
39	6	0	-4.619407	4.261390	-1.055477
40	6	0	-4.646786	2.873988	-1.236076
41	1	0	-7.941435	4.895503	-1.038572
42	1	0	-5.787992	6.063891	-0.839857
43	1	0	-3.651462	4.761658	-0.982842
44	6	0	-7.102788	2.924519	-1.282426
45	6	0	-5.889866	2.188287	-1.335049
46	7	0	-5.893998	0.816046	-1.476842
47	6	0	-8.406711	2.235525	-1.403208
48	1	0	-4.971265	0.389371	-1.511496
49	5	0	-7.105953	0.060571	-1.561179
50	6	0	-8.429261	0.829194	-1.538334
51	6	0	-9.642854	0.112266	-1.634605
52	7	0	-7.161062	-1.358487	-1.652870
53	1	0	-6.332350	-1.945596	-1.627931
54	6	0	-9.600165	-1.360541	-1.755294
55	6	0	-8.360777	-2.049633	-1.756462
56	6	0	-8.338669	-3.451826	-1.854903
57	6	0	-9.513910	-4.180187	-1.947157
58	6	0	-10.744523	-3.515475	-1.951860

59	6	0	-10.771082	-2.131465	-1.859890
60	1	0	-7.370735	-3.961388	-1.849784
61	1	0	-9.471652	-5.269722	-2.023200
62	1	0	-11.677998	-4.076423	-2.031572
63	1	0	-11.739942	-1.630151	-1.865452
64	6	0	7.021098	-4.313698	-1.098500
65	6	0	4.646756	-2.873973	-1.235851
66	6	0	4.619306	-4.261364	-1.055197
67	6	0	5.806970	-4.981641	-0.980228
68	1	0	7.941299	-4.895666	-1.038421
69	1	0	3.651336	-4.761574	-0.982480
70	1	0	5.787800	-6.063922	-0.839566
71	6	0	5.889868	-2.188349	-1.334925
72	6	0	7.102754	-2.924639	-1.282309
73	6	0	8.406711	-2.235720	-1.403177
74	5	0	7.106057	-0.060703	-1.561115
75	6	0	8.429329	-0.829387	-1.538271
76	6	0	9.642955	-0.112526	-1.634622
77	6	0	8.360987	2.049437	-1.756425
78	6	0	9.600342	1.360286	-1.755272
79	6	0	10.771299	2.131159	-1.859764
80	6	0	10.744809	3.515174	-1.951692
81	6	0	9.514227	4.179942	-1.947014
82	6	0	8.338947	3.451632	-1.854819
83	1	0	11.740141	1.629810	-1.865227
84	1	0	11.678316	4.076081	-2.031310
85	1	0	9.472021	5.269481	-2.023030
86	1	0	7.371035	3.961239	-1.849710
87	6	0	4.611688	2.872542	1.184861
88	6	0	4.598166	4.272468	0.994711
89	6	0	5.786911	4.979355	0.947240
90	6	0	7.008355	4.312884	1.095097
91	1	0	5.775328	6.061557	0.802041
92	1	0	7.926781	4.898455	1.051326
93	1	0	3.634790	4.776193	0.895843
94	6	0	7.088116	2.926671	1.285676
95	6	0	5.872297	2.188248	1.312169
96	7	0	5.870975	0.827384	1.454353
97	6	0	8.385216	2.235670	1.436586
98	1	0	4.946779	0.399587	1.455104
99	6	0	8.403471	0.829165	1.573873
100	5	0	7.083124	0.063446	1.564365
101	7	0	7.125987	-1.353140	1.658365
102	6	0	9.612592	0.109337	1.696280
103	1	0	6.296717	-1.937653	1.600068
104	6	0	8.320244	-2.047871	1.788816
105	6	0	9.561871	-1.361886	1.816138
106	6	0	10.727589	-2.137580	1.946995
107	6	0	10.692819	-3.520856	2.038071
108	6	0	9.459746	-4.182076	2.005186
109	6	0	8.290005	-3.450382	1.886516
110	1	0	11.697891	-1.639904	1.973894
111	1	0	11.622023	-4.085628	2.138033
112	1	0	9.412713	-5.271470	2.079483

113	1	0	7.320574	-3.956216	1.857779
114	6	0	-7.008687	-4.312876	1.095764
115	6	0	-4.611922	-2.872672	1.185104
116	6	0	-4.598496	-4.272644	0.995254
117	6	0	-5.787289	-4.979468	0.948038
118	1	0	-7.927153	-4.898400	1.052188
119	1	0	-3.635154	-4.776449	0.896444
120	1	0	-5.775783	-6.061710	0.803134
121	6	0	-5.872477	-2.188281	1.312324
122	6	0	-7.088349	-2.926609	1.285964
123	6	0	-8.385394	-2.235457	1.436642
124	7	0	-5.871030	-0.827401	1.454320
125	1	0	-4.946797	-0.399685	1.454988
126	5	0	-7.083110	-0.063350	1.564350
127	6	0	-8.403521	-0.828949	1.573915
128	6	0	-9.612579	-0.108999	1.696229
129	7	0	-7.125844	1.353243	1.658256
130	1	0	-6.296528	1.937681	1.599867
131	6	0	-9.561716	1.362212	1.816152
132	6	0	-8.320028	2.048085	1.788778
133	6	0	-8.289658	3.450595	1.886447
134	6	0	-9.459325	4.182392	2.005208
135	6	0	-10.692453	3.521280	2.038200
136	6	0	-10.727353	2.138008	1.947113
137	1	0	-7.320187	3.956346	1.857617
138	1	0	-9.412188	5.271782	2.079494
139	1	0	-11.621598	4.086132	2.138260
140	1	0	-11.697698	1.640416	1.974088
141	7	0	5.894065	-0.816118	-1.476787
142	1	0	4.971349	-0.389401	-1.511431
143	7	0	7.161238	1.358348	-1.652840
144	1	0	6.332552	1.945496	-1.627980
145	6	0	9.626806	-2.923823	-1.370973
146	6	0	10.844922	-0.834278	-1.592883
147	6	0	10.824290	-2.220082	-1.465459
148	1	0	11.809251	-0.328555	-1.654448
149	1	0	11.768904	-2.768941	-1.429457
150	1	0	9.667259	-4.007851	-1.261891
151	6	0	10.817357	0.828757	1.679229
152	6	0	9.607655	2.920997	1.429635
153	6	0	10.801539	2.214471	1.550061
154	1	0	11.779164	0.321040	1.760542
155	1	0	9.652197	4.004756	1.319457
156	1	0	11.747668	2.761497	1.532483
157	6	0	-9.607909	-2.920647	1.429441
158	6	0	-10.817418	-0.828289	1.678978
159	6	0	-10.801732	-2.213996	1.549708
160	1	0	-11.779183	-0.320472	1.760166
161	1	0	-11.747921	-2.760911	1.531907
162	1	0	-9.652557	-4.004388	1.319126
163	6	0	-10.844860	0.833949	-1.592739
164	6	0	-9.626844	2.923557	-1.370877
165	6	0	-10.824294	2.219751	-1.465296
166	1	0	-11.809168	0.328171	-1.654182

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    167          1          0      -11.768939    2.768552   -1.429172
    168          1          0       -9.667349    4.007578   -1.261756
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 Ground to excited state transition electric dipole moments (Au):
     state          X           Y           Z        Dip. S.      Osc.
       1        -4.2732     -0.8060      0.0000     18.9095      1.3296
 Ground to excited state transition velocity dipole moments (Au):
     state          X           Y           Z        Dip. S.      Osc.
       1         0.4669      0.0877     -0.0000      0.2257      1.4265
 Ground to excited state transition magnetic dipole moments (Au):
     state          X           Y           Z
       1        -0.5607      1.8253      0.0002
 Ground to excited state transition velocity quadrupole moments (Au):
     state          XX          YY          ZZ          XY          XZ         YZ
       1       -0.0001     -0.0000     -0.0000      0.0000      1.1636     0.2869

  <0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>
  Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
     state          XX          YY          ZZ    R(velocity)   E-M Angle
       1       194.4675   -428.6337   -448.4745   -227.5469       96.44

 1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]
  Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
     state          XX          YY          ZZ     R(length)
       1     -1694.4593   1040.4063     -0.0000   -218.0177

 1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)
     state          X           Y           Z        Dip. S.   Osc.(frdel)
       1        -1.9952     -0.0707     -0.0000      2.0659      1.3772

 ----------------------------------------------------------------------
 Excitation energies and oscillator strengths:
 ----------------------------------------------------------------------
 Excited State 1:   Singlet-A   2.8701 eV  431.99 nm  f=1.3296  <S**2>=0.000
      352 -> 357        0.16199
      354 -> 357        0.27846
      356 -> 357       -0.56820
      356 -> 358        0.16364
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```

Summary of chiroptical properties of (R)-6' (M06-2X/def2-SV(P))

state	$\lvert\mu_e\rvert$ /10^{-20} esu-cm	$\lvert\mu_m\rvert$ /10^{-20} erg/Gauss	$\cos\theta$ (E-M Angle)	$g_{lum,calcd.}$ (4R/(D+G))	E_{ex} /nm
1	1106	1.771	-0.111	-0.000713	432

Table S2. Cartesian coordinates (Å) and transition moments of optimized structure of (R)-**6'** in the lowest-energy excited state (S_1) calculated at the CAM-B3LYP/def2-SV(P) level of theory.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.056229	-1.415110	-1.544511
2	6	0	-1.210224	-0.652065	-1.681979
3	6	0	-1.181840	0.754644	-1.693312
4	6	0	0.056210	1.415200	-1.544406
5	6	0	1.210212	0.652165	-1.681884
6	6	0	1.181828	-0.754546	-1.693320
7	1	0	-2.181539	-1.149720	-1.635925
8	1	0	2.181524	1.149817	-1.635756
9	6	0	-0.145861	-2.801927	-0.953504
10	1	0	0.562592	-3.491588	-1.437864
11	1	0	-1.158188	-3.197568	-1.126959
12	6	0	0.149349	-2.805463	0.607616
13	1	0	1.158169	-3.211376	0.776560
14	1	0	-0.565258	-3.491265	1.090227
15	6	0	-0.078000	1.423948	1.209804
16	6	0	-1.215743	0.672214	1.347804
17	6	0	-1.191734	-0.760273	1.380108
18	6	0	0.077976	-1.424065	1.209696
19	6	0	1.215725	-0.672338	1.347706
20	6	0	1.191718	0.760146	1.380115
21	1	0	-2.189675	1.159790	1.260495
22	1	0	2.189653	-1.159910	1.260323
23	6	0	-0.149391	2.805389	0.607826
24	6	0	0.145819	2.801975	-0.953294
25	1	0	-0.562633	3.491672	-1.437606
26	1	0	1.158146	3.197632	-1.126711
27	1	0	0.565214	3.491159	1.090485
28	1	0	-1.158212	3.211285	0.776808
29	6	0	2.413115	-1.478337	-1.675999
30	6	0	3.462621	-2.091429	-1.662812
31	6	0	-2.413125	1.478440	-1.676011
32	6	0	-3.462618	2.091553	-1.662810
33	6	0	2.384770	1.473928	1.416647
34	6	0	3.448155	2.098758	1.444698
35	6	0	-2.384779	-1.474065	1.416644
36	6	0	-3.448162	-2.098903	1.444661
37	6	0	7.116573	-4.180576	-1.682138
38	6	0	5.922995	-4.888961	-1.629875
39	6	0	4.717006	-4.199726	-1.622545
40	6	0	4.702604	-2.802253	-1.658488
41	1	0	8.051104	-4.741545	-1.690912
42	1	0	5.934522	-5.980869	-1.602621
43	1	0	3.766162	-4.735909	-1.594377
44	6	0	7.159314	-2.780061	-1.723544
45	6	0	5.926373	-2.080742	-1.700976
46	7	0	5.895227	-0.700516	-1.719459
47	6	0	8.441188	-2.041441	-1.792702

48	1	0	4.961566	-0.301051	-1.709619
49	5	0	7.078387	0.093522	-1.766829
50	6	0	8.420223	-0.629941	-1.820917
51	6	0	9.608846	0.130034	-1.887613
52	7	0	7.086496	1.512628	-1.761902
53	1	0	6.239228	2.066124	-1.696493
54	6	0	9.518953	1.606282	-1.906251
55	6	0	8.260789	2.251869	-1.834741
56	6	0	8.191470	3.653762	-1.838056
57	6	0	9.337432	4.426037	-1.917798
58	6	0	10.586187	3.805666	-1.994673
59	6	0	10.659907	2.421700	-1.986913
60	1	0	7.209421	4.131227	-1.773147
61	1	0	9.258241	5.516540	-1.922002
62	1	0	11.499435	4.401812	-2.061407
63	1	0	11.644173	1.955746	-2.046619
64	6	0	-7.116578	4.180687	-1.682020
65	6	0	-4.702607	2.802368	-1.658459
66	6	0	-4.717010	4.199841	-1.622472
67	6	0	-5.923000	4.889075	-1.629762
68	1	0	-8.051112	4.741651	-1.690749
69	1	0	-3.766166	4.736024	-1.594300
70	1	0	-5.934529	5.980982	-1.602478
71	6	0	-5.926373	2.080857	-1.700964
72	6	0	-7.159315	2.780173	-1.723475
73	6	0	-8.441189	2.041552	-1.792616
74	5	0	-7.078380	-0.093409	-1.766858
75	6	0	-8.420221	0.630052	-1.820863
76	6	0	-9.608844	-0.129925	-1.887529
77	6	0	-8.260778	-2.251757	-1.834801
78	6	0	-9.518947	-1.606172	-1.906218
79	6	0	-10.659903	-2.421591	-1.986845
80	6	0	-10.586178	-3.805556	-1.994670
81	6	0	-9.337416	-4.425926	-1.917899
82	6	0	-8.191453	-3.653650	-1.838186
83	1	0	-11.644175	-1.955639	-2.046469
84	1	0	-11.499428	-4.401703	-2.061373
85	1	0	-9.258221	-5.516429	-1.922158
86	1	0	-7.209399	-4.131115	-1.773359
87	6	0	-4.658235	-2.802510	1.511176
88	6	0	-4.686708	-4.213434	1.462443
89	6	0	-5.888843	-4.888934	1.551685
90	6	0	-7.084316	-4.180414	1.695450
91	1	0	-5.908306	-5.980823	1.516516
92	1	0	-8.014039	-4.744757	1.763672
93	1	0	-3.743299	-4.753302	1.361399
94	6	0	-7.124867	-2.782131	1.750073
95	6	0	-5.894915	-2.081275	1.644657
96	7	0	-5.859552	-0.711612	1.665655
97	6	0	-8.395282	-2.041341	1.910482
98	1	0	-4.928293	-0.312766	1.580722
99	6	0	-8.370921	-0.629461	1.936202
100	5	0	-7.038676	0.090758	1.788387
101	7	0	-7.037705	1.507270	1.779432

102	6	0	-9.550120	0.133632	2.082017
103	1	0	-6.195823	2.056976	1.645164
104	6	0	-8.202033	2.250589	1.927112
105	6	0	-9.454344	1.608622	2.087862
106	6	0	-10.584761	2.428741	2.241505
107	6	0	-10.505645	3.812050	2.236017
108	6	0	-9.262942	4.428420	2.070433
109	6	0	-8.127576	3.652437	1.917518
110	1	0	-11.564178	1.966686	2.370410
111	1	0	-11.410271	4.411957	2.360933
112	1	0	-9.181049	5.518648	2.062569
113	1	0	-7.150827	4.125941	1.782508
114	6	0	7.084280	4.180305	1.695603
115	6	0	4.658219	2.802381	1.511244
116	6	0	4.686676	4.213306	1.462568
117	6	0	5.888802	4.888816	1.551853
118	1	0	8.013994	4.744657	1.763873
119	1	0	3.743261	4.753167	1.361536
120	1	0	5.908253	5.980706	1.516726
121	6	0	5.894907	2.081153	1.644700
122	6	0	7.124849	2.782019	1.750162
123	6	0	8.395272	2.041239	1.910557
124	7	0	5.859564	0.711487	1.665640
125	1	0	4.928314	0.312631	1.580658
126	5	0	7.038692	-0.090871	1.788374
127	6	0	8.370925	0.629359	1.936257
128	6	0	9.550129	-0.133724	2.082071
129	7	0	7.037744	-1.507383	1.779347
130	1	0	6.195875	-2.057093	1.645007
131	6	0	9.454368	-1.608715	2.087891
132	6	0	8.202073	-2.250692	1.927054
133	6	0	8.127637	-3.652541	1.917403
134	6	0	9.263004	-4.428514	2.070366
135	6	0	10.505687	-3.812133	2.236061
136	6	0	10.584784	-2.428823	2.241596
137	1	0	7.150904	-4.126054	1.782308
138	1	0	9.181127	-5.518742	2.062458
139	1	0	11.410311	-4.412032	2.361030
140	1	0	11.564184	-1.966759	2.370597
141	7	0	-5.895221	0.700631	-1.719513
142	1	0	-4.961559	0.301170	-1.709709
143	7	0	-7.086484	-1.512515	-1.761986
144	1	0	-6.239212	-2.066011	-1.696637
145	6	0	-9.681942	2.688115	-1.830973
146	6	0	-10.829980	0.554501	-1.926427
147	6	0	-10.854408	1.943885	-1.897474
148	1	0	-11.776620	0.015547	-1.974984
149	1	0	-11.816169	2.463569	-1.924654
150	1	0	-9.755661	3.775411	-1.805639
151	6	0	-10.767317	-0.548419	2.207148
152	6	0	-9.631940	-2.685088	2.036049
153	6	0	-10.795508	-1.937933	2.183013
154	1	0	-11.707492	-0.007699	2.319746
155	1	0	-9.708978	-3.772279	2.017099

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   156          1          0      -11.753943   -2.455750    2.278040
   157          6          0        9.631924    2.684996    2.036131
   158          6          0       10.767319    0.548336    2.207215
   159          6          0       10.795499    1.937851    2.183091
   160          1          0       11.707499    0.007623    2.319809
   161          1          0       11.753928    2.455675    2.278127
   162          1          0        9.708953    3.772187    2.017176
   163          6          0       10.829978   -0.554394   -1.926581
   164          6          0        9.681939   -2.688007   -1.831111
   165          6          0       10.854404   -1.943778   -1.897651
   166          1          0       11.776617   -0.015442   -1.975180
   167          1          0       11.816163   -2.463465   -1.924889
   168          1          0        9.755657   -3.775302   -1.805789
 ---------------------------------------------------------------------

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 Ground to excited state transition electric dipole moments (Au):
     state          X           Y           Z        Dip. S.      Osc.
       1        -4.3348     -0.8721     -0.0000     19.5509      1.3805
       2        -3.5611      0.5691      0.0000     13.0056      1.0453
  Ground to excited state transition velocity dipole moments (Au):
     state          X           Y           Z        Dip. S.      Osc.
       1         0.4559      0.0912      0.0000      0.2162      1.3606
       2         0.4273     -0.0678     -0.0000      0.1872      1.0349
  Ground to excited state transition magnetic dipole moments (Au):
     state          X           Y           Z
       1        -0.3536      1.7957      0.0002
       2        -0.5716     -2.0673     -0.0001

  Ground to excited state transition velocity quadrupole moments (Au):
     state          XX          YY          ZZ          XY          XZ          YZ
       1      -0.0000     -0.0000      0.0000     -0.0001      1.6181      0.4193
       2       0.0001     -0.0000      0.0000      0.0000     -1.5522      0.3825

  <0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>
  Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
     state          XX          YY          ZZ     R(velocity)    E-M Angle
       1        54.0859    100.0064   -136.4035      5.8963        89.82
       2       102.3753   -236.9902   -476.2458   -203.6202        96.44

 1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]
  Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
     state          XX          YY          ZZ     R(length)
       1     -1083.7985   1107.4356      0.0000      7.8791
       2     -1439.3986    831.9950      0.0000   -202.4679

 1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)
     state          X           Y           Z        Dip. S.   Osc.(frdel)
       1        -1.9762     -0.0796     -0.0000      2.0558      1.3705
       2        -1.5216     -0.0386     -0.0000      1.5601      1.0401
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---------------------------------------------------------------------
Excitation energies and oscillator strengths:
---------------------------------------------------------------------
Excited State 1:      Singlet-A   2.8822 eV 430.17 nm f=1.3805 <S**2>=0.000
     352 -> 357        0.18038
     354 -> 357        0.21224
     356 -> 357        0.58504
     356 -> 358       -0.16226

Excited State 2:      Singlet-A   3.2804 eV 377.95 nm f=1.0453 <S**2>=0.000
     351 -> 357        0.30778
     351 -> 358        0.19165
     352 -> 357        0.13598
     352 -> 358        0.12107
     354 -> 357       -0.32466
     354 -> 358       -0.21335
     356 -> 357        0.22140
     356 -> 358        0.27781
```

Summary of chiroptical properties of (R)-6' (CAM-B3LYP/def2-SV(P))

state	$\lvert\mu_e\rvert$ /10^{-20} esu-cm	$\lvert\mu_m\rvert$ /10^{-20} erg/Gauss	cosθ (E-M Angle)	$g_{lum,calcd.}$ (4R/(D+G))	E_{ex} /nm
1	1125	1.697	0.004	0.000025	430
2	917	1.989	-0.111	-0.000963	378

Table S3. Cartesian coordinates (Å) and transition moments of optimized structure of (R)-**6'** in the lowest-energy excited state (S_1) calculated at the CAM-B3LYP-D3(BJ)/def2-SV(P) level of theory.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-0.060218	-1.415137	-1.457782
2	6	0	-1.213233	-0.651903	-1.590963
3	6	0	-1.178236	0.753859	-1.590900
4	6	0	0.060223	1.414945	-1.457756
5	6	0	1.213237	0.651712	-1.590947
6	6	0	1.178241	-0.754049	-1.590912
7	1	0	-2.185530	-1.145974	-1.537666
8	1	0	2.185533	1.145782	-1.537620
9	6	0	-0.149039	-2.802460	-0.870888
10	1	0	0.553748	-3.492564	-1.362364
11	1	0	-1.164618	-3.193014	-1.034989
12	6	0	0.160275	-2.805837	0.685144
13	1	0	1.173380	-3.203608	0.845858
14	1	0	-0.547226	-3.493920	1.174427
15	6	0	-0.084645	1.423152	1.280660
16	6	0	-1.219817	0.668920	1.419166

17	6	0	-1.187049	-0.762244	1.426652
18	6	0	0.084643	-1.423408	1.280636
19	6	0	1.219810	-0.669179	1.419204
20	6	0	1.187042	0.761986	1.426718
21	1	0	-2.195336	1.152448	1.334171
22	1	0	2.195332	-1.152707	1.334244
23	6	0	-0.160258	2.805596	0.685196
24	6	0	0.149052	2.802257	-0.870835
25	1	0	-0.553726	3.492378	-1.362299
26	1	0	1.164636	3.192801	-1.034922
27	1	0	0.547248	3.493664	1.174496
28	1	0	-1.173359	3.203373	0.845919
29	6	0	2.403416	-1.479615	-1.521668
30	6	0	3.442186	-2.103333	-1.438778
31	6	0	-2.403412	1.479429	-1.521729
32	6	0	-3.442172	2.103186	-1.438988
33	6	0	2.375511	1.479582	1.386851
34	6	0	3.429218	2.114961	1.318110
35	6	0	-2.375517	-1.479839	1.386702
36	6	0	-3.429206	-2.115237	1.317883
37	6	0	7.068091	-4.224310	-1.276607
38	6	0	5.867851	-4.915201	-1.173988
39	6	0	4.668999	-4.215394	-1.221549
40	6	0	4.670619	-2.825016	-1.363426
41	1	0	7.997676	-4.791130	-1.237249
42	1	0	5.868654	-6.001822	-1.064620
43	1	0	3.711798	-4.736694	-1.157178
44	6	0	7.124451	-2.831677	-1.417813
45	6	0	5.900155	-2.119938	-1.450037
46	7	0	5.880670	-0.745110	-1.560208
47	6	0	8.412612	-2.113103	-1.514590
48	1	0	4.951249	-0.336382	-1.578099
49	5	0	7.072318	0.032255	-1.629426
50	6	0	8.405764	-0.705766	-1.617501
51	6	0	9.602884	0.037294	-1.687133
52	7	0	7.094692	1.448562	-1.692284
53	1	0	6.252849	2.012903	-1.659146
54	6	0	9.529794	1.509899	-1.770262
55	6	0	8.278202	2.170303	-1.762694
56	6	0	8.224775	3.570876	-1.816788
57	6	0	9.381965	4.327403	-1.877281
58	6	0	10.625164	3.691606	-1.890653
59	6	0	10.682047	2.308294	-1.839175
60	1	0	7.246816	4.059138	-1.799800
61	1	0	9.315836	5.417961	-1.916818
62	1	0	11.546979	4.275665	-1.941749
63	1	0	11.661285	1.829121	-1.846559
64	6	0	-7.067926	4.224393	-1.276411
65	6	0	-4.670555	2.824937	-1.363457
66	6	0	-4.668831	4.215307	-1.221496
67	6	0	-5.867632	4.915194	-1.173813
68	1	0	-7.997469	4.791275	-1.236959
69	1	0	-3.711591	4.736538	-1.157169
70	1	0	-5.868353	6.001809	-1.064381

71	6	0	-5.900145	2.119950	-1.450029
72	6	0	-7.124389	2.831773	-1.417706
73	6	0	-8.412604	2.113299	-1.514488
74	5	0	-7.072471	-0.032153	-1.629424
75	6	0	-8.405863	0.705965	-1.617436
76	6	0	-9.603040	-0.037005	-1.687052
77	6	0	-8.278520	-2.170113	-1.762631
78	6	0	-9.530063	-1.509616	-1.770166
79	6	0	-10.682378	-2.307929	-1.839011
80	6	0	-10.625600	-3.691246	-1.890459
81	6	0	-9.382447	-4.327135	-1.877125
82	6	0	-8.225199	-3.570692	-1.816696
83	1	0	-11.661581	-1.828684	-1.846350
84	1	0	-11.547459	-4.275239	-1.941499
85	1	0	-9.316400	-5.417699	-1.916643
86	1	0	-7.247275	-4.059027	-1.799733
87	6	0	-4.632653	-2.828241	1.280573
88	6	0	-4.648643	-4.231443	1.128541
89	6	0	-5.848755	-4.916331	1.127458
90	6	0	-7.052427	-4.224411	1.279879
91	1	0	-5.860311	-6.002704	1.013001
92	1	0	-7.981267	-4.793188	1.271757
93	1	0	-3.698026	-4.757176	1.022118
94	6	0	-7.103012	-2.833997	1.428913
95	6	0	-5.876277	-2.122354	1.416645
96	7	0	-5.848094	-0.758105	1.528904
97	6	0	-8.382369	-2.111671	1.574789
98	1	0	-4.917150	-0.350749	1.502464
99	6	0	-8.368212	-0.704060	1.678914
100	5	0	-7.036797	0.029086	1.640680
101	7	0	-7.045360	1.442934	1.704654
102	6	0	-9.558902	0.043600	1.791197
103	1	0	-6.203160	2.003056	1.629230
104	6	0	-8.222007	2.170159	1.816630
105	6	0	-9.475609	1.514830	1.870530
106	6	0	-10.620942	2.319317	1.979823
107	6	0	-10.554755	3.701908	2.026920
108	6	0	-9.309460	4.332323	1.967531
109	6	0	-8.159173	3.570704	1.866770
110	1	0	-11.601602	1.845055	2.022846
111	1	0	-11.471131	4.290831	2.109858
112	1	0	-9.237343	5.422608	2.002483
113	1	0	-7.180153	4.053994	1.812303
114	6	0	7.052331	4.224324	1.280133
115	6	0	4.632627	2.828028	1.280813
116	6	0	4.648541	4.231241	1.128870
117	6	0	5.848617	4.916191	1.127801
118	1	0	7.981140	4.793151	1.272024
119	1	0	3.697895	4.756935	1.022517
120	1	0	5.860112	6.002574	1.013423
121	6	0	5.876297	2.122194	1.416798
122	6	0	7.102995	2.833903	1.429064
123	6	0	8.382394	2.111636	1.574852
124	7	0	5.848191	0.757939	1.528997

125	1	0	4.917267	0.350535	1.502590
126	5	0	7.036939	-0.029195	1.640718
127	6	0	8.368317	0.704020	1.678926
128	6	0	9.559050	-0.043581	1.791138
129	7	0	7.045576	-1.443043	1.704684
130	1	0	6.203403	-2.003208	1.629282
131	6	0	9.475836	-1.514815	1.870471
132	6	0	8.222264	-2.170207	1.816620
133	6	0	8.159504	-3.570755	1.866780
134	6	0	9.309832	-4.332315	1.967515
135	6	0	10.555097	-3.701836	2.026863
136	6	0	10.621213	-2.319242	1.979746
137	1	0	7.180507	-4.054096	1.812346
138	1	0	9.237772	-5.422603	2.002478
139	1	0	11.471505	-4.290711	2.109792
140	1	0	11.601849	-1.844928	2.022757
141	7	0	-5.880762	0.745125	-1.560254
142	1	0	-4.951372	0.336331	-1.578208
143	7	0	-7.094953	-1.448459	-1.692273
144	1	0	-6.253151	-2.012862	-1.659169
145	6	0	-9.644878	2.773759	-1.490153
146	6	0	-10.817056	0.659232	-1.654949
147	6	0	-10.826177	2.045230	-1.559654
148	1	0	-11.769426	0.130524	-1.696081
149	1	0	-11.782209	2.574471	-1.528413
150	1	0	-9.705086	3.857826	-1.400224
151	6	0	-10.776224	-0.648478	1.802273
152	6	0	-9.617405	-2.767501	1.594351
153	6	0	-10.792911	-2.034444	1.706653
154	1	0	-11.724769	-0.116613	1.877199
155	1	0	-9.684383	-3.851218	1.505141
156	1	0	-11.751204	-2.560444	1.708843
157	6	0	9.617397	2.767528	1.594379
158	6	0	10.776338	0.648560	1.802169
159	6	0	10.792948	2.034529	1.706590
160	1	0	11.724914	0.116741	1.877036
161	1	0	11.751214	2.560579	1.708749
162	1	0	9.684315	3.851252	1.505199
163	6	0	10.816953	-0.658850	-1.655049
164	6	0	9.644937	-2.773469	-1.490282
165	6	0	10.826180	-2.044849	-1.559772
166	1	0	11.769282	-0.130070	-1.696184
167	1	0	11.782252	-2.574018	-1.528547
168	1	0	9.705229	-3.857533	-1.400371

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	-4.2775	-0.8492	-0.0000	19.0177	1.3426
2	-3.4389	0.5677	0.0000	12.1484	0.9696

```
Ground to excited state transition velocity dipole moments (Au):
    state          X           Y           Z        Dip. S.      Osc.
      1         0.4494      0.0887      0.0000      0.2098      1.3208
      2         0.4094     -0.0670     -0.0000      0.1721      0.9583
Ground to excited state transition magnetic dipole moments (Au):
    state          X           Y           Z
      1        -0.4936      1.8472      0.0001
      2        -0.5891     -1.9763      0.0001
Ground to excited state transition velocity quadrupole moments (Au):
    state          XX          YY          ZZ          XY          XZ          YZ
      1      0.0001     -0.0000      0.0000     -0.0000      1.2536      0.3217
      2     -0.0000     -0.0000     -0.0000      0.0001     -1.2439      0.2935

 <0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>
 Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX          YY          ZZ     R(velocity)    E-M Angle
      1       175.8249   -257.8060   -304.7649   -128.9154       93.79
      2       144.9696   -357.3841   -429.8890   -214.1011       97.30

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]
 Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX          YY          ZZ     R(length)
      1     -1492.9938   1109.2624      0.0000   -127.9105
      2     -1432.6739    793.3931     -0.0000   -213.0936

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)
    state          X           Y           Z        Dip. S.   Osc.(frdel)
      1        -1.9222     -0.0753     -0.0000      1.9975      1.3317
      2        -1.4078     -0.0380     -0.0000      1.4459      0.9639

 ---------------------------------------------------------------------
 Excitation energies and oscillator strengths:
 ---------------------------------------------------------------------
 Excited State   1:      Singlet-A      2.8816 eV  430.26 nm  f=1.3426  <S**2>=0.000
     352 -> 357        -0.13727
     354 -> 357         0.30319
     356 -> 357         0.55195
     356 -> 358        -0.16533

 Excited State   2:      Singlet-A      3.2577 eV  380.59 nm  f=0.9696  <S**2>=0.000
     351 -> 357        -0.28324
     351 -> 358        -0.16491
     352 -> 357        -0.22298
     352 -> 358        -0.18410
     354 -> 357        -0.25191
     354 -> 358        -0.13510
     356 -> 357         0.25540
     356 -> 358         0.32068
```

Summary of chiroptical properties of (R)-6' (CAM-B3LYP-D3(BJ)/def2-SV(P))

state	$\lvert\mu_e\rvert$ /10^{-20} esu-cm	$\lvert\mu_m\rvert$ /10^{-20} erg/Gauss	cosθ (E-M Angle)	$g_{lum,calcd.}$ (4R/(D+G))	E_{ex} /nm
1	1109	1.773	-0.065	-0.000416	430
2	887	1.913	-0.126	-0.001090	381

Table S4. Cartesian coordinates (Å) and transition moments of optimized structure of (R)-**6'** in the lowest-energy excited state (S_1) calculated at the ωB97XD/def2-SV(P) level of theory.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.062984	-1.416820	-1.456158
2	6	0	-1.216066	-0.649938	-1.592985
3	6	0	-1.176824	0.756161	-1.590002
4	6	0	0.062950	1.416932	-1.456142
5	6	0	1.216031	0.650056	-1.592972
6	6	0	1.176791	-0.756043	-1.589995
7	1	0	-2.191292	-1.141753	-1.539751
8	1	0	2.191255	1.141873	-1.539735
9	6	0	-0.155189	-2.804015	-0.864076
10	1	0	0.538298	-3.501312	-1.361796
11	1	0	-1.176013	-3.188886	-1.017778
12	6	0	0.168699	-2.807434	0.689811
13	1	0	1.187249	-3.199043	0.840298
14	1	0	-0.529423	-3.503108	1.185067
15	6	0	-0.089288	1.425486	1.290730
16	6	0	-1.223821	0.667464	1.433704
17	6	0	-1.185193	-0.764947	1.437753
18	6	0	0.089238	-1.425404	1.290708
19	6	0	1.223768	-0.667387	1.433712
20	6	0	1.185141	0.765023	1.437770
21	1	0	-2.202705	1.147742	1.348392
22	1	0	2.202654	-1.147662	1.348416
23	6	0	-0.168745	2.807523	0.689850
24	6	0	0.155151	2.804119	-0.864037
25	1	0	-0.538335	3.501423	-1.361751
26	1	0	1.175974	3.188992	-1.017731
27	1	0	0.529381	3.503182	1.185119
28	1	0	-1.187293	3.199138	0.840342
29	6	0	2.402602	-1.484041	-1.508693
30	6	0	3.440178	-2.111395	-1.404945
31	6	0	-2.402629	1.484166	-1.508692
32	6	0	-3.440177	2.111563	-1.404932
33	6	0	2.372614	1.485465	1.384888
34	6	0	3.425639	2.125100	1.293394
35	6	0	-2.372661	-1.485396	1.384866
36	6	0	-3.425665	-2.125069	1.293390

37	6	0	7.050224	-4.260509	-1.187759
38	6	0	5.842216	-4.939422	-1.075588
39	6	0	4.649142	-4.228682	-1.141778
40	6	0	4.665636	-2.839729	-1.309364
41	1	0	7.973818	-4.838274	-1.133284
42	1	0	5.832496	-6.024338	-0.945597
43	1	0	3.686024	-4.740427	-1.072426
44	6	0	7.121577	-2.869814	-1.355105
45	6	0	5.902807	-2.145314	-1.402495
46	7	0	5.896953	-0.771907	-1.532888
47	6	0	8.420013	-2.166067	-1.460589
48	1	0	4.973647	-0.350260	-1.559761
49	5	0	7.098989	-0.005404	-1.603631
50	6	0	8.428629	-0.758645	-1.578169
51	6	0	9.633973	-0.026989	-1.651234
52	7	0	7.136082	1.412038	-1.682585
53	1	0	6.299342	1.983835	-1.653252
54	6	0	9.574439	1.447897	-1.746644
55	6	0	8.327739	2.121016	-1.752385
56	6	0	8.287857	3.523657	-1.818551
57	6	0	9.453978	4.269493	-1.874409
58	6	0	10.692323	3.621437	-1.874365
59	6	0	10.735702	2.236416	-1.813681
60	1	0	7.314496	4.023669	-1.812903
61	1	0	9.398092	5.360967	-1.922550
62	1	0	11.620592	4.196682	-1.922699
63	1	0	11.712925	1.750379	-1.810759
64	6	0	-7.050322	4.260535	-1.187971
65	6	0	-4.665671	2.839849	-1.309427
66	6	0	-4.649240	4.228812	-1.141932
67	6	0	-5.842345	4.939507	-1.075830
68	1	0	-7.973940	4.838275	-1.133610
69	1	0	-3.686145	4.740603	-1.072588
70	1	0	-5.832673	6.024436	-0.945944
71	6	0	-5.902811	2.145372	-1.402528
72	6	0	-7.121615	2.869823	-1.355185
73	6	0	-8.420020	2.166011	-1.460595
74	5	0	-7.098901	0.005410	-1.603679
75	6	0	-8.428573	0.758595	-1.578263
76	6	0	-9.633886	0.026881	-1.651289
77	6	0	-8.327552	-2.121065	-1.752434
78	6	0	-9.574282	-1.448001	-1.746747
79	6	0	-10.735507	-2.236570	-1.813872
80	6	0	-10.692062	-3.621590	-1.874548
81	6	0	-9.453687	-4.269592	-1.874500
82	6	0	-8.287603	-3.523705	-1.818581
83	1	0	-11.712751	-1.750576	-1.811035
84	1	0	-11.620301	-4.196876	-1.922951
85	1	0	-9.397749	-5.361064	-1.922623
86	1	0	-7.314220	-4.023674	-1.812874
87	6	0	-4.626376	-2.843819	1.232658
88	6	0	-4.627621	-4.246123	1.056231
89	6	0	-5.822927	-4.941840	1.033262
90	6	0	-7.033997	-4.261201	1.190202

91	1	0	-5.824616	-6.026689	0.899600
92	1	0	-7.957530	-4.840599	1.164856
93	1	0	-3.670771	-4.762418	0.949031
94	6	0	-7.099083	-2.872285	1.363603
95	6	0	-5.877588	-2.148157	1.369111
96	7	0	-5.862464	-0.784430	1.499060
97	6	0	-8.389045	-2.164833	1.514803
98	1	0	-4.937319	-0.363987	1.483813
99	6	0	-8.390186	-0.757060	1.634338
100	5	0	-7.061951	-0.008322	1.610674
101	7	0	-7.085259	1.406861	1.689872
102	6	0	-9.589349	-0.020986	1.748647
103	1	0	-6.248228	1.974839	1.618020
104	6	0	-8.270589	2.121045	1.801945
105	6	0	-9.519563	1.452763	1.841645
106	6	0	-10.674216	2.246992	1.950079
107	6	0	-10.621632	3.631443	2.008052
108	6	0	-9.380900	4.274340	1.963023
109	6	0	-8.221241	3.523585	1.865925
110	1	0	-11.653138	1.765561	1.982615
111	1	0	-11.544784	4.211212	2.089089
112	1	0	-9.318818	5.365567	2.008113
113	1	0	-7.246430	4.018912	1.824067
114	6	0	7.033992	4.261187	1.190094
115	6	0	4.626359	2.843831	1.232615
116	6	0	4.627615	4.246134	1.056173
117	6	0	5.822927	4.941838	1.033159
118	1	0	7.957534	4.840565	1.164684
119	1	0	3.670767	4.762440	0.948997
120	1	0	5.824627	6.026683	0.899461
121	6	0	5.877560	2.148161	1.369076
122	6	0	7.099060	2.872276	1.363554
123	6	0	8.389012	2.164817	1.514798
124	7	0	5.862418	0.784436	1.499041
125	1	0	4.937267	0.364006	1.483819
126	5	0	7.061900	0.008314	1.610627
127	6	0	8.390143	0.757039	1.634275
128	6	0	9.589299	0.020957	1.748602
129	7	0	7.085194	-1.406867	1.689867
130	1	0	6.248153	-1.974839	1.618074
131	6	0	9.519502	-1.452795	1.841564
132	6	0	8.270518	-2.121061	1.801933
133	6	0	8.221154	-3.523597	1.865996
134	6	0	9.380806	-4.274365	1.963062
135	6	0	10.621551	-3.631486	2.007960
136	6	0	10.674152	-2.247038	1.949929
137	1	0	7.246332	-4.018910	1.824224
138	1	0	9.318711	-5.365589	2.008224
139	1	0	11.544701	-4.211266	2.088948
140	1	0	11.653083	-1.765622	1.982366
141	7	0	-5.896900	0.771958	-1.532849
142	1	0	-4.973577	0.350343	-1.559666
143	7	0	-7.135929	-1.412034	-1.682602
144	1	0	-6.299170	-1.983796	-1.653118

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    145          6           0       -9.646566    2.839760   -1.428763
    146          6           0      -10.841945    0.736241   -1.609808
    147          6           0      -10.836321    2.122816   -1.502856
    148          1           0      -11.802633    0.220411   -1.653355
    149          1           0      -11.787346    2.661914   -1.465235
    150          1           0       -9.699317    3.924602   -1.328570
    151          6           0      -10.800822   -0.726528    1.747599
    152          6           0       -9.618486   -2.834305    1.524059
    153          6           0      -10.802653   -2.113085    1.639217
    154          1           0      -11.757932   -0.207804    1.823473
    155          1           0       -9.678075   -3.918764    1.423733
    156          1           0      -11.756090   -2.649148    1.632736
    157          6           0        9.618452    2.834289    1.524173
    158          6           0       10.800772    0.726497    1.747655
    159          6           0       10.802611    2.113061    1.639357
    160          1           0       11.757877    0.207769    1.823563
    161          1           0       11.756048    2.649123    1.632973
    162          1           0        9.678046    3.918758    1.423950
    163          6           0       10.842000   -0.736412   -1.609881
    164          6           0        9.646526   -2.839888   -1.428958
    165          6           0       10.836312   -2.122998   -1.503073
    166          1           0       11.802711   -0.220629   -1.653478
    167          1           0       11.787314   -2.662150   -1.465616
    168          1           0        9.699227   -3.924751   -1.328980
---------------------------------------------------------------------

---------------------------------------------------------------------
Ground to excited state transition electric dipole moments (Au):
    state          X           Y           Z        Dip. S.      Osc.
      1        -4.2147     -0.8917      0.0000     18.5590      1.3402
      2         3.8703     -0.5248      0.0000     15.2543      1.2543
Ground to excited state transition velocity dipole moments (Au):
    state          X           Y           Z        Dip. S.      Osc.
      1         0.4526      0.0954     -0.0000      0.2140      1.3170
      2        -0.4742      0.0641     -0.0000      0.2290      1.2375
Ground to excited state transition magnetic dipole moments (Au):
    state          X           Y           Z
      1        -0.5161      1.9401     -0.0000
      2         0.6639      1.9720      0.0001
Ground to excited state transition velocity quadrupole moments (Au):
    state       XX          YY          ZZ          XY          XZ          YZ
      1      -0.0000     -0.0000     -0.0000     -0.0000      1.2630      0.3146
      2      -0.0000     -0.0000      0.0000      0.0000      1.1984     -0.3249

 <0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>
 Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX          YY          ZZ     R(velocity)    E-M Angle
      1       210.8727   -297.7534   -229.9387   -105.6065       93.00
      2       142.1189   -460.8494   -761.7129   -360.1478      100.91
```

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1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]
 Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX           YY           ZZ     R(length)
      1     -1538.3005   1223.4136      0.0000   -104.9623
      2     -1817.0467    731.8549     -0.0000   -361.7306

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)
    state          X            Y            Z        Dip. S.   Osc.(frdel)
      1         -1.9078      -0.0851      -0.0000      1.9929      1.3286
      2         -1.8352      -0.0336      -0.0000      1.8688      1.2459

 ---------------------------------------------------------------------
 Excitation energies and oscillator strengths:
 ---------------------------------------------------------------------
 Excited State 1:      Singlet-A    2.9476 eV 420.62 nm f=1.3402 <S**2>=0.000
     352 -> 357         0.14771
     354 -> 357        -0.30994
     356 -> 357        -0.52810
     356 -> 358         0.17158

Excited State 2:      Singlet-A    3.3562 eV 369.42 nm f=1.2543 <S**2>=0.000
     351 -> 357         0.27573
     351 -> 358         0.19887
     352 -> 357        -0.22756
     352 -> 358        -0.19830
     354 -> 357        -0.20470
     354 -> 358        -0.17264
     356 -> 357         0.23680
     356 -> 358         0.29177
```

Summary of chiroptical properties of (R)-6' (ωB97XD/def2-SV(P))

state	$\lvert\mu_e\rvert$ /10^{-20} esu-cm	$\lvert\mu_m\rvert$ /10^{-20} erg/Gauss	$\cos\theta$ (E-M Angle)	$g_{lum,calcd.}$ (4R/(D+G))	E_{ex} /nm
1	1096	1.862	-0.051	-0.000350	421
2	993	0.449	-0.189	-0.001467	369

Table S5. Cartesian coordinates (Å) and transition moments of optimized structure of (R)-Ph-PCP[30] in the lowest-energy excited state (S_1) calculated at the M06-2X/def2-SV(P) level of theory.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.100446	-1.416466	-1.451732
2	6	0	-1.236438	-0.621283	-1.559951
3	6	0	-1.162096	0.794226	-1.583323
4	6	0	0.100507	1.416365	-1.451810
5	6	0	1.236498	0.621178	-1.559985

6	6	0	1.162155	-0.794335	-1.583281
7	1	0	-2.224168	-1.085019	-1.490089
8	1	0	2.224229	1.084915	-1.490152
9	6	0	-0.207329	-2.802373	-0.861195
10	1	0	0.432729	-3.521639	-1.397022
11	1	0	-1.249704	-3.148447	-0.944726
12	6	0	0.221824	-2.809006	0.664668
13	1	0	1.261415	-3.161254	0.749404
14	1	0	-0.425584	-3.521788	1.201804
15	6	0	-0.131252	1.426982	1.257992
16	6	0	-1.248377	0.642932	1.386062
17	6	0	-1.159043	-0.791822	1.398258
18	6	0	0.131305	-1.426918	1.258079
19	6	0	1.248427	-0.642860	1.386099
20	6	0	1.159092	0.791896	1.398212
21	1	0	-2.241674	1.090586	1.300489
22	1	0	2.241726	-1.090513	1.300541
23	6	0	-0.221787	2.809035	0.664498
24	6	0	0.207380	2.802307	-0.861360
25	1	0	-0.432675	3.521539	-1.397238
26	1	0	1.249754	3.148386	-0.944903
27	1	0	0.425608	3.521860	1.201590
28	1	0	-1.261386	3.161268	0.749202
29	6	0	2.362113	-1.559908	-1.516289
30	6	0	3.392908	-2.206097	-1.435866
31	6	0	-2.362061	1.559789	-1.516348
32	6	0	-3.392871	2.205954	-1.435919
33	6	0	2.327193	1.558433	1.408794
34	6	0	3.362651	2.223640	1.399237
35	6	0	-2.327155	-1.558339	1.408862
36	6	0	-3.362639	-2.223507	1.399320
37	6	0	4.570263	-4.360253	-1.212179
38	6	0	4.605006	-2.958655	-1.331962
39	6	0	5.751975	-5.086545	-1.103798
40	6	0	6.985053	-4.431806	-1.114053
41	6	0	7.029323	-3.041341	-1.233579
42	6	0	5.852512	-2.307299	-1.341171
43	6	0	-5.852476	2.307081	-1.341391
44	6	0	-4.604991	2.958476	-1.332020
45	6	0	-7.029320	3.041070	-1.233796
46	6	0	-6.985103	4.431524	-1.114111
47	6	0	-5.752047	5.086301	-1.103697
48	6	0	-4.570303	4.360062	-1.212075
49	6	0	-4.513276	-4.391339	1.277110
50	6	0	-4.555822	-2.981501	1.383927
51	6	0	-5.690097	-5.127158	1.258519
52	6	0	-6.928254	-4.482189	1.344590
53	6	0	-6.982534	-3.088495	1.450269
54	6	0	-5.813789	-2.340049	1.470246
55	6	0	5.813797	2.340327	1.470380
56	6	0	4.555801	2.981688	1.383843
57	6	0	6.982497	3.088842	1.450408
58	6	0	6.928142	4.482517	1.344516
59	6	0	5.689956	5.127398	1.258231

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     60          6           0        4.513178    4.391508    1.276818
     61          1           0       -7.851376   -5.066212    1.329137
     62          1           0       -5.646204   -6.215760    1.175937
     63          1           0       -3.543145   -4.888938    1.210112
     64          1           0       -7.911317    5.004753   -1.030008
     65          1           0       -5.711366    6.174360   -1.011551
     66          1           0       -3.603643    4.868867   -1.207169
     67          1           0        3.543023    4.889040    1.209656
     68          1           0        5.646002    6.215985    1.175484
     69          1           0        7.851232    5.066593    1.329065
     70          1           0        3.603586   -4.869027   -1.207407
     71          1           0        5.711250   -6.174613   -1.011778
     72          1           0        7.911243   -5.005074   -1.029949
     73          1           0       -7.991831    2.523797   -1.244335
     74          1           0       -5.881934    1.219371   -1.435609
     75          1           0       -5.848504   -1.251548    1.551987
     76          1           0       -7.949119   -2.583543    1.517943
     77          1           0        5.882013   -1.219579   -1.435261
     78          1           0        7.991853   -2.524099   -1.243994
     79          1           0        5.848570    1.251840    1.552291
     80          1           0        7.949106    2.583960    1.518256
---------------------------------------------------------------------

---------------------------------------------------------------------
Ground to excited state transition electric dipole moments (Au):
    state          X           Y           Z        Dip. S.      Osc.
      1        -3.2564     -1.5752      0.0000     13.0852      0.9860
      2         1.8144     -1.6384      0.0000      5.9764      0.4915
Ground to excited state transition velocity dipole moments (Au):
    state          X           Y           Z        Dip. S.      Osc.
      1         0.3761      0.1821     -0.0000      0.1746      1.0301
      2        -0.2286      0.2073     -0.0000      0.0952      0.5147
Ground to excited state transition magnetic dipole moments (Au):
    state          X           Y           Z
      1        -1.1141      1.1558      0.0000
      2         0.8139      1.4921      0.0000
Ground to excited state transition velocity quadrupole moments (Au):
    state        XX          YY          ZZ          XY          XZ          YZ
      1      -0.0000      0.0001     -0.0000      0.0001      0.9199      0.7766
      2      -0.0000     -0.0001      0.0000      0.0001      1.0001     -0.4454

<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX          YY          ZZ     R(velocity)    E-M Angle
      1       134.3857   -397.0606  -1042.1667   -434.9472      108.11
      2       292.3826   -241.3887    656.1075    235.7005       76.40

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]
 Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX          YY          ZZ     R(length)
      1     -2565.5117   1287.5598     -0.0000   -425.9840
      2     -1044.2456   1728.7961     -0.0000    228.1835
```

```
1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)
    state          X           Y           Z        Dip. S.   Osc.(frdel)
      1        -1.2248     -0.2869     -0.0000      1.5117      1.0078
      2        -0.4147     -0.3397     -0.0000      0.7544      0.5030

 ----------------------------------------------------------------------
 Excitation energies and oscillator strengths:
 ----------------------------------------------------------------------
 Excited State   1:      Singlet-A      3.0758 eV  403.10 nm  f=0.9860  <S**2>=0.000
     160 ->161        -0.68673

 Excited State   2:      Singlet-A      3.3569 eV  369.34 nm  f=0.4915  <S**2>=0.000
     155 ->161        -0.12775
     159 ->161         0.66390
     159 ->162         0.11116
```

Summary of chiroptical properties of (R)-Ph-NBN (M06-2X/def2-SV(P))

state	$\lvert\mu_e\rvert$ /10^{-20} esu-cm	$\lvert\mu_m\rvert$ /10^{-20} erg/Gauss	$\cos\theta$ (E-M Angle)	$g_{lum,calcd.}$ (4R/(D+G))	E_{ex} /nm
1	-401	1.489	-0.311	-0.002014	403
2	-417	1.576	0.233	0.002362	369

Table S6. Cartesian coordinates (Å) and transition moments of optimized structure of (R)-Naph-PCP[30] in the lowest-energy excited state (S_1) calculated at the M06-2X/def2-SV(P) level of theory.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.150058	-1.413935	1.403890
2	6	0	1.100762	-0.831907	1.556976
3	6	0	1.279623	0.567008	1.533657
4	6	0	0.149927	1.413817	1.404071
5	6	0	-1.100881	0.831767	1.557168
6	6	0	-1.279758	-0.567153	1.533704
7	1	0	1.996527	-1.459106	1.506836
8	1	0	-1.996646	1.458976	1.507195
9	6	0	-0.247949	-2.794149	0.792511
10	1	0	-1.295313	-3.131634	0.822748
11	1	0	0.347226	-3.524988	1.364682
12	6	0	0.260047	-2.793872	-0.705238
13	1	0	-0.327695	-3.535232	-1.271021
14	1	0	1.311124	-3.120492	-0.738054
15	6	0	-0.141240	1.420409	-1.328652
16	6	0	1.098142	0.853391	-1.490682
17	6	0	1.293031	-0.565127	-1.473949
18	6	0	0.141331	-1.420320	-1.328812
19	6	0	-1.098065	-0.853285	-1.490789

20	6	0	-1.292942	0.565233	-1.473922
21	1	0	1.993252	1.479728	-1.416362
22	1	0	-1.993186	-1.479621	-1.416624
23	6	0	-0.259963	2.793898	-0.704998
24	6	0	0.247848	2.794112	0.792821
25	1	0	1.295200	3.131611	0.823199
26	1	0	-0.347431	3.524878	1.364958
27	1	0	-1.311016	3.120589	-0.737931
28	1	0	0.327872	3.535270	-1.270685
29	6	0	-2.616371	-1.050445	1.440044
30	6	0	-3.784897	-1.381416	1.329503
31	6	0	2.616226	1.050328	1.440080
32	6	0	3.784681	1.381496	1.329432
33	6	0	-2.601298	1.043365	-1.408616
34	6	0	-3.784670	1.382796	-1.316921
35	6	0	2.601404	-1.043217	-1.408601
36	6	0	3.784782	-1.382652	-1.316865
37	6	0	-5.484919	-3.073452	0.889958
38	6	0	-5.154876	-1.767532	1.227431
39	6	0	-6.831443	-3.473079	0.781603
40	6	0	-7.844089	-2.569736	1.016006
41	6	0	-7.553383	-1.227422	1.374991
42	6	0	-6.196138	-0.807061	1.479334
43	6	0	-8.589200	-0.286856	1.632712
44	6	0	-5.919354	0.541855	1.825318
45	6	0	-6.942812	1.428155	2.067079
46	6	0	-8.293035	1.009242	1.975983
47	1	0	-9.627784	-0.619500	1.550816
48	1	0	-4.877296	0.864725	1.889178
49	1	0	-6.713949	2.464944	2.324728
50	1	0	-9.096025	1.724339	2.171105
51	6	0	5.919339	-0.541491	1.825560
52	6	0	6.195960	0.807370	1.479235
53	6	0	5.154614	1.767765	1.227312
54	6	0	7.553164	1.227810	1.374641
55	6	0	7.843737	2.570117	1.015532
56	6	0	6.831009	3.473387	0.781203
57	6	0	5.484524	3.073684	0.889728
58	6	0	6.942907	-1.427649	2.067386
59	6	0	8.589099	0.287355	1.632306
60	6	0	8.293087	-1.008687	1.975893
61	1	0	4.877317	-0.864414	1.889724
62	1	0	6.714153	-2.464373	2.325382
63	1	0	9.627644	0.620064	1.550157
64	1	0	9.096159	-1.723694	2.171008
65	6	0	5.476286	-3.085132	-0.906675
66	6	0	5.132771	-1.763716	-1.238215
67	6	0	6.815462	-3.478489	-0.816769
68	6	0	7.834223	-2.570976	-1.058648
69	6	0	7.542245	-1.229453	-1.411952
70	6	0	6.184339	-0.802436	-1.501319
71	6	0	8.576736	-0.291676	-1.682882
72	6	0	5.910022	0.540519	-1.847876
73	6	0	6.934941	1.428223	-2.105560

74	6	0	8.281503	1.006605	-2.027802
75	1	0	9.615298	-0.627219	-1.612415
76	1	0	4.868212	0.866539	-1.904839
77	1	0	6.703848	2.463642	-2.366749
78	1	0	9.085698	1.717227	-2.234517
79	6	0	-5.909505	-0.540792	-1.847847
80	6	0	-6.184094	0.802188	-1.501607
81	6	0	-5.132726	1.763673	-1.238523
82	6	0	-7.542080	1.228984	-1.412438
83	6	0	-7.834332	2.570514	-1.059360
84	6	0	-6.815747	3.478214	-0.817444
85	6	0	-5.476491	3.085069	-0.907168
86	6	0	-6.934240	-1.428755	-2.105357
87	6	0	-8.576382	0.290953	-1.683204
88	6	0	-8.280886	-1.007371	-2.027757
89	1	0	-4.867629	-0.866631	-1.904656
90	1	0	-6.702944	-2.464194	-2.366286
91	1	0	-9.615007	0.626327	-1.612874
92	1	0	-9.084933	-1.718194	-2.234356
93	1	0	8.880724	-2.879970	-0.987867
94	1	0	7.055502	-4.511679	-0.554116
95	1	0	4.675935	-3.803458	-0.717337
96	1	0	8.890677	2.875207	0.932653
97	1	0	7.065591	4.505809	0.511720
98	1	0	4.682434	3.792147	0.708328
99	1	0	-4.676280	3.803554	-0.717835
100	1	0	-7.055984	4.511399	-0.554950
101	1	0	-8.880894	2.879336	-0.988729
102	1	0	-4.682898	-3.792000	0.708575
103	1	0	-7.066115	-4.505504	0.512207
104	1	0	-8.891058	-2.874767	0.933292

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	-2.8704	0.8257	-0.0002	8.9207	0.6378
2	3.5305	0.1928	-0.0001	12.5013	0.9985

Ground to excited state transition velocity dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	0.3194	-0.0927	0.0000	0.1106	0.6874
2	-0.4388	-0.0228	0.0000	0.1931	1.0743

Ground to excited state transition magnetic dipole moments (Au):

state	X	Y	Z
1	-0.3281	-2.4501	-0.0000
2	0.5740	-1.1205	0.0003

Ground to excited state transition velocity quadrupole moments (Au):

state	XX	YY	ZZ	XY	XZ	YZ
1	0.0002	0.0000	-0.0000	-0.0001	-1.3794	0.1711
2	0.0003	-0.0001	0.0000	-0.0000	-0.3972	-0.2903

```
<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>
 Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX           YY           ZZ      R(velocity)    E-M Angle
      1       327.2468    -165.3496     644.8904     268.9292        81.44
      2        48.5907    -367.3629   -1017.2880    -445.3534       114.15

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]
 Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX           YY           ZZ     R(length)
      1      -666.0223    1430.6567      -0.0000    254.8781
      2     -1432.9903     152.7632       0.0000   -426.7424

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)
    state          X            Y            Z         Dip. S.   Osc.(frdel)
      1        -0.9167      -0.0766      -0.0000       0.9932      0.6622
      2        -1.5492      -0.0044      -0.0000       1.5536      1.0357

---------------------------------------------------------------------
Excitation energies and oscillator strengths:
---------------------------------------------------------------------
Excited State 1:     Singlet-A    2.9183 eV 424.84 nm f=0.6378 <S**2>=0.000
     211 ->214         -0.14711
     212 ->213          0.65949

Excited State 2:     Singlet-A    3.2602 eV 380.30 nm f=0.9985 <S**2>=0.000
     211 ->214         -0.23896
     212 ->213         -0.14288
     212 ->214         -0.62158
```

Summary of chiroptical properties of (R)-Naph-PCP (M06-2X/def2-SV(P))

state	$\|\mu_e\|$ /10^{-20} esu-cm	$\|\mu_m\|$ /10^{-20} erg/Gauss	$\cos\theta$ (E-M Angle)	$g_{lum,calcd.}$ (4R/(D+G))	E_{ex} /nm
1	-760	2.293	0.146	0.001768	425
2	-899	1.168	-0.407	-0.002112	380

Table S7. Cartesian coordinates (Å) and transition moments of optimized structure of (R)-Anth-PCP'[30] in the lowest-energy excited state (S_1) calculated at the M06-2X/def2-SV(P) level of theory.

```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
      1          6           0       -0.034669   -1.395691    1.292878
      2          6           0        1.200831   -0.778732    1.434715
      3          6           0        1.334685    0.627786    1.386280
      4          6           0        0.174461    1.436050    1.262871
      5          6           0       -1.053667    0.818445    1.446764
      6          6           0       -1.186099   -0.585624    1.429548
```

7	1	0	2.111246	-1.382871	1.387004
8	1	0	-1.968878	1.417545	1.399809
9	6	0	-0.117713	-2.788747	0.715088
10	1	0	-1.066494	-3.260412	1.013904
11	1	0	0.698412	-3.408260	1.118695
12	6	0	-0.015834	-2.794819	-0.875775
13	1	0	-0.835873	-3.412121	-1.275515
14	1	0	0.930442	-3.275657	-1.168962
15	6	0	-0.251200	1.426927	-1.475415
16	6	0	0.968115	0.789643	-1.658345
17	6	0	1.080519	-0.616124	-1.613282
18	6	0	-0.086210	-1.407000	-1.467541
19	6	0	-1.310825	-0.769271	-1.612393
20	6	0	-1.420669	0.636614	-1.573977
21	1	0	1.890491	1.377841	-1.621792
22	1	0	-2.231952	-1.356230	-1.551743
23	6	0	-0.267752	2.812314	-0.869125
24	6	0	0.226244	2.813414	0.641003
25	1	0	1.259240	3.192662	0.685250
26	1	0	-0.402671	3.518773	1.208125
27	1	0	-1.289519	3.218644	-0.918438
28	1	0	0.379871	3.494230	-1.443352
29	6	0	-2.506106	-1.114921	1.317645
30	6	0	-3.664553	-1.462301	1.165471
31	6	0	2.657031	1.127625	1.269219
32	6	0	3.855119	1.368543	1.170563
33	6	0	-2.730393	1.176366	-1.394830
34	6	0	-3.880619	1.522692	-1.188643
35	6	0	2.395897	-1.135936	-1.487221
36	6	0	3.586599	-1.376915	-1.330718
37	6	0	-4.353980	-3.987278	-0.062683
38	6	0	-5.355566	-3.091544	0.425252
39	6	0	-5.030280	-1.841452	1.009091
40	6	0	-6.732775	-3.471792	0.298126
41	6	0	-7.732369	-2.606889	0.756037
42	6	0	-7.425811	-1.362080	1.313211
43	6	0	-6.054716	-0.957423	1.434588
44	6	0	-4.696315	-5.177228	-0.645592
45	6	0	-7.050801	-4.728115	-0.310828
46	6	0	-8.455051	-0.469676	1.756395
47	6	0	-5.771599	0.337716	1.970836
48	6	0	-6.782506	1.169423	2.369284
49	6	0	-8.144970	0.756755	2.271393
50	1	0	-9.495362	-0.793893	1.664940
51	1	0	-4.729240	0.656863	2.043231
52	1	0	-6.546991	2.163257	2.759082
53	1	0	-8.937147	1.433931	2.600403
54	6	0	-6.066049	-5.555643	-0.772702
55	1	0	-3.304851	-3.697312	0.035544
56	1	0	-3.916845	-5.846722	-1.016954
57	1	0	-8.103904	-5.008662	-0.400529
58	1	0	-6.321536	-6.510064	-1.238811
59	6	0	5.541695	-0.773971	2.053326
60	6	0	6.079173	0.434250	1.559751

61	6	0	5.252482	1.520625	1.113755
62	6	0	7.507580	0.571445	1.489459
63	6	0	8.065446	1.744110	0.963478
64	6	0	7.266261	2.836734	0.554990
65	6	0	5.842659	2.737118	0.632752
66	6	0	6.362082	-1.803862	2.501871
67	6	0	8.318861	-0.513141	1.922910
68	6	0	7.841696	4.023905	0.032664
69	6	0	5.057373	3.833879	0.203469
70	6	0	5.646607	4.982044	-0.288328
71	6	0	7.052383	5.077463	-0.379795
72	1	0	8.931475	4.089436	-0.033648
73	1	0	3.969012	3.753887	0.267090
74	1	0	5.022711	5.818593	-0.611476
75	1	0	7.512703	5.986060	-0.774753
76	6	0	7.757720	-1.666225	2.447221
77	1	0	4.456239	-0.886092	2.095889
78	1	0	5.916533	-2.725487	2.883573
79	1	0	9.405739	-0.403647	1.865326
80	1	0	8.399682	-2.480609	2.791600
81	6	0	4.699257	-3.821137	-0.224953
82	6	0	5.523596	-2.749620	-0.645684
83	6	0	4.978997	-1.535811	-1.183935
84	6	0	6.940758	-2.873273	-0.498478
85	6	0	7.777637	-1.806044	-0.892176
86	6	0	7.264251	-0.625423	-1.444706
87	6	0	5.842116	-0.464809	-1.585209
88	6	0	5.244619	-4.965437	0.324668
89	6	0	7.469118	-4.057059	0.079046
90	6	0	8.116704	0.442681	-1.839220
91	6	0	5.352095	0.756079	-2.099415
92	6	0	6.212614	1.772944	-2.499344
93	6	0	7.601380	1.608957	-2.382530
94	1	0	9.197318	0.310106	-1.734721
95	1	0	4.271947	0.888626	-2.191762
96	1	0	5.804074	2.705086	-2.895975
97	1	0	8.273027	2.413451	-2.691386
98	6	0	6.642521	-5.085849	0.481509
99	1	0	3.616386	-3.725365	-0.341123
100	1	0	4.590248	-5.781024	0.641372
101	1	0	8.553453	-4.138691	0.197391
102	1	0	7.066428	-5.992007	0.920225
103	6	0	-5.982933	-0.313998	-1.898478
104	6	0	-6.268375	0.973903	-1.344979
105	6	0	-5.244139	1.881482	-0.972499
106	6	0	-7.640159	1.344740	-1.148926
107	6	0	-7.946775	2.582815	-0.577070
108	6	0	-6.944986	3.471894	-0.173823
109	6	0	-5.567715	3.123724	-0.372884
110	6	0	-6.992567	-1.171233	-2.241035
111	6	0	-8.669310	0.424461	-1.531880
112	6	0	-7.259838	4.720695	0.452220
113	6	0	-4.563079	4.040745	0.066685
114	6	0	-4.901875	5.221865	0.668995

```
    115          6           0       -6.271710    5.569668    0.865129
    116          1           0       -8.313020    4.977337    0.596001
    117          1           0       -3.514181    3.773960   -0.084192
    118          1           0       -4.119958    5.908110    1.002588
    119          1           0       -6.524637    6.517849    1.345219
    120          6           0       -8.357645   -0.794468   -2.063418
    121          1           0       -4.938867   -0.605340   -2.033313
    122          1           0       -6.753696   -2.157300   -2.647900
    123          1           0       -9.710979    0.722127   -1.383039
    124          1           0       -9.150022   -1.491281   -2.348082
    125          1           0        9.154164    1.835912    0.904011
    126          1           0        8.860759   -1.917892   -0.788184
    127          1           0       -8.781160   -2.904327    0.660079
    128          1           0       -8.995692    2.855094   -0.424649
---------------------------------------------------------------------

---------------------------------------------------------------------
Ground to excited state transition electric dipole moments (Au):
    state          X           Y           Z        Dip. S.      Osc.
      1         3.6384      0.0121      0.0176     13.2387      0.8511
      2        -0.8751     -0.9667     -0.1887      1.7358      0.1218
Ground to excited state transition velocity dipole moments (Au):
    state          X           Y           Z        Dip. S.      Osc.
      2        -0.3813      0.0005     -0.0024      0.1454      1.0050
      3         0.0981      0.1108      0.0229      0.0224      0.1421
Ground to excited state transition magnetic dipole moments (Au):
    state          X           Y           Z
      2         0.3382      0.1776     -0.0598
      3        -0.1420      1.6575      0.8639
Ground to excited state transition velocity quadrupole moments (Au):
    state          XX          YY          ZZ          XY          XZ          YZ
      2       -2.0411      0.0110     -0.0360     -0.1026     -0.0198      0.1131
      3        0.2541     -0.0276     -0.0260     -0.7523      0.8747     -0.0076

<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>
 Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX          YY          ZZ     R(velocity)    E-M Angle
      2         1.7939   -631.1657   -314.3922   -314.5880      150.82
      3       300.0291     75.2066    898.3812    424.5390       47.54

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]
 Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
    state          XX          YY          ZZ     R(length)
      1      -870.0823     -1.5194      0.7443   -290.2858
      2       -87.8666   1133.0738    115.2533    386.8202

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)
    state          X           Y           Z        Dip. S.   Osc.(frdel)
      1        -1.3872      0.0000     -0.0000      1.3872      0.9248
      2        -0.0859     -0.1071     -0.0043      0.1973      0.1315
```

```
----------------------------------------------------------------------
Excitation energies and oscillator strengths:
----------------------------------------------------------------------
Excited State 1:     Singlet-A   2.6240 eV 472.49 nm f=0.8511 <S**2>=0.000
     261 -> 265        0.20709
     261 -> 267       -0.11026
     263 -> 265       -0.65655

Excited State 2:     Singlet-A   2.8638 eV 432.93 nm f=0.1218 <S**2>=0.000
     261 -> 266        0.18710
     261 -> 268        0.13972
     262 -> 265        0.21709
     262 -> 267        0.17388
     263 -> 266        0.51958
     264 -> 266       -0.16434
     264 -> 267       -0.19964
```

Summary of chiroptical properties of (R)-Anth-PCP (M06-2X/def2-SV(P))

state	$\lvert\mu_e\rvert$ /10^{-20} esu-cm	$\lvert\mu_m\rvert$ /10^{-20} erg/Gauss	cosθ (E-M Angle)	$g_{lum,calcd.}$ (4R/(D+G))	E_{ex} /nm
1	101	0.359	-0.876	-0.001357	472
2	335	1.738	0.665	0.013787	433

Adiabatic Ionization Energies

The structures of neutral **6'**, radical cation **6'$^{+}$**, and diradical dication **6'$^{2+}$** were optimized using the TPSS[9] meta functional in conjunction and the resolution of the identity approximation. The geometry optimizations were performed using the def2-TZVP basis set along with the recommended fitting bases required for the RI approximation.[11,12] In addition, dispersion interactions between the NBN-moieties were dealt with using Grimme's D3 scheme along with Becke-Johnson damping.[13,14] Subsequently, harmonic vibrational frequencies were computed by finite differences of analytical gradients.

Energies were refined by single point computations at the M06-2X/def2-TZVP//RI-TPSS-D3(BJ)/def2-TZVP level of theory. To speed up the M06-2X computation, with the Coulomb and HF exchange resolution of identity (RI) approximation RIJCOSX[31] was used in conjunction with the general def2/J[12] auxiliary basis set. The solvation model based on density (SMD)[32] was used to simulate the solvation energies in CH_2Cl_2 for geometry optimizations as well as single point calculations. The *Lebedev* numerical quadrature grid6 was employed. These computations were done with Orca 4.2.1.[33,34]

Table S8. Total energies and thermal contributions at 298 K at the M06-2X/def2-TZVP level of theory in dichloromethane (SMD method).

compound	E_{el} /Hartree	ZPE /eV	E_{solv} /eV	H^{0} /eV	G^{0} /eV
6'	-4232.15973	35.12	-3.10	-115125.63	-115130.43
6'$^{+}$	-4231.95113	35.20	-4.23	-115119.89	-115124.67
6'$^{2+}$	-4231.73535	35.21	-6.27	-115114.00	-115118.80

Electronic energy is the dispersion and solvation corrected total energy from the electronic structure calculation $E_{el} = E_{kin\text{-}el} + E_{nuc\text{-}el} + E_{el\text{-}el} + E_{nuc\text{-}nuc} + E_{disp} + E_{solv}$. Enthalpy is defined as $H^0 = U + k_bT$ at 298 K, with $U = E_{ZPE} + E_{vib} + E_{rot} + E_{trans}$ and zero-point energy corrected electronic energy $E_{ZPE} = E_{el} + ZPE$. The Gibbs free energy is $G^0 = H^0 - T{\cdot}S$ with the entropy contributions $T{\cdot}S = T{\cdot}(S_{el}+S_{vib}+S_{rot}+S_{trans})$ at T = 298 K.

Table S9. Zero-point energy corrected electronic energy ΔE_{ZPE}, enthalpy ΔH^0 (at 298 K) and Gibbs free energy ΔG^0 (at 298 K) in solution (SMD method in CH_2Cl_2, M06-2X/def2-TZVP//TPSS-D3(BJ)/def2-TZVP) for the adiabatic oxidation steps of 6' to the radical cation $6'^{+}$ and the diradical dication $6'^{2+}$.

oxidation step	ΔE_{ZPE} /eV	ΔH^0 /eV	ΔG^0 /eV
$6' \rightarrow 6'^{+}$	5.76	5.74	5.75
$6'^{+} \rightarrow 6'^{2+}$	5.89	5.89	5.87

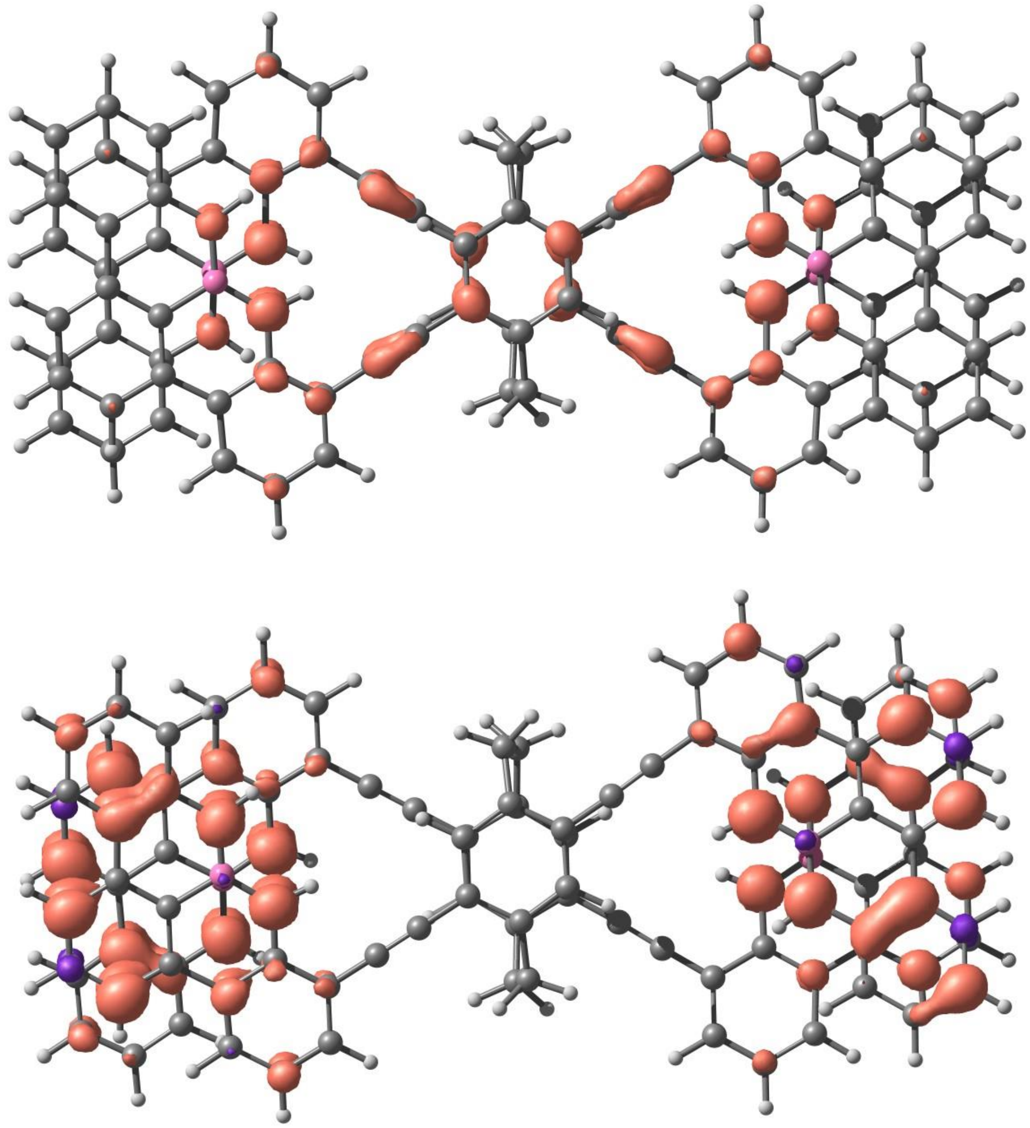

Figure S66. Spin densities (contour value 0.002) of the radical **6'⁺** (top) and the triplet diradical **6'²⁺** (bottom) as computed at the M06-2X/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level of theory.

6. Cartesian Coordinates

Conformer Analysis and Frontier Molecular Orbitals

All Cartesian coordinates given below were computed at the RI-TPSS-D3(BJ)/def2-QZVP level of theory and are given in Å and absolute energies are given in atomic units.

```
168
D2 isomer A, -4235.06445
6       -0.065852000      1.415424000      1.372302000
6       -1.216199000      0.652941000      1.520384000
6       -1.182902000     -0.756302000      1.511454000
6        0.065852000     -1.415424000      1.372302000
6        1.216199000     -0.652941000      1.520384000
6        1.182902000      0.756302000      1.511454000
1       -2.182103000      1.143723000      1.467963000
1        2.182103000     -1.143723000      1.467963000
6       -0.158832000      2.801400000      0.784647000
1        0.539568000      3.491644000      1.263515000
1       -1.171562000      3.181895000      0.931843000
6        0.158832000      2.801400000     -0.784647000
1        1.171562000      3.181895000     -0.931843000
1       -0.539568000      3.491644000     -1.263515000
6       -0.065852000     -1.415424000     -1.372302000
6       -1.216199000     -0.652941000     -1.520384000
6       -1.182902000      0.756302000     -1.511454000
6        0.065852000      1.415424000     -1.372302000
6        1.216199000      0.652941000     -1.520384000
6        1.182902000     -0.756302000     -1.511454000
1       -2.182103000     -1.143723000     -1.467963000
1        2.182103000      1.143723000     -1.467963000
6       -0.158832000     -2.801400000     -0.784647000
6        0.158832000     -2.801400000      0.784647000
1       -0.539568000     -3.491644000      1.263515000
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6       -2.389783000     -1.484090000      1.437353000
6       -3.415355000     -2.136897000      1.340301000
6        2.389783000     -1.484090000     -1.437353000
6        3.415355000     -2.136897000     -1.340301000
6       -2.389783000      1.484090000     -1.437353000
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6        7.015733000      4.290421000      1.157775000
6        5.807076000      4.965109000      1.022748000
6        4.611311000      4.259735000      1.078382000
6        4.621062000      2.868033000      1.259964000
1        7.935760000      4.858263000      1.109029000
1        5.798835000      6.039783000      0.880843000
```

1	3.658070000	4.768145000	0.990226000
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6	5.863851000	2.177808000	1.380962000
7	5.851191000	0.806920000	1.531980000
6	8.373609000	2.200815000	1.475887000
1	4.918348000	0.405653000	1.549250000
5	7.057504000	0.039243000	1.613448000
6	8.378119000	0.789227000	1.597894000
6	9.589614000	0.061956000	1.698321000
7	7.095357000	-1.380295000	1.717225000
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6	9.536037000	-1.402432000	1.800111000
6	8.290670000	-2.085790000	1.801252000
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6	10.659320000	-3.570675000	1.957563000
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6	-10.789279000	-2.162818000	1.573492000
1	-11.748369000	-0.262518000	1.746331000
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1	11.732350000	-2.699621000	-1.556997000
1	9.646353000	-3.954511000	-1.373249000
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6	9.600488000	2.877765000	1.472474000
6	10.789279000	2.162818000	1.573492000
1	11.748369000	0.262518000	1.746331000
1	11.732350000	2.699621000	1.556997000
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168
C1 isomer B, -4235.05362

6	-0.633456000	2.960374000	1.542574000
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6	-1.876296000	0.861591000	1.752749000
6	-0.673031000	0.127742000	1.606821000
6	0.525404000	0.824098000	1.713402000
6	0.577729000	2.230635000	1.669536000
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6	-0.656252000	4.340692000	0.935671000
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1	-1.631786000	4.794213000	1.120321000
6	-0.409410000	4.299853000	-0.648630000
1	0.587522000	4.694860000	-0.853608000
1	-1.142253000	4.962448000	-1.115061000
6	-0.649016000	0.063889000	-1.140470000
6	-1.792174000	0.831687000	-1.280802000
6	-1.760027000	2.242387000	-1.294192000
6	-0.510124000	2.898683000	-1.196931000
6	0.635864000	2.125513000	-1.347278000
6	0.601139000	0.716190000	-1.305309000
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1	0.275954000	-1.767875000	1.354450000
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6	2.850173000	3.528545000	1.410673000
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6	-4.337784000	-0.051950000	1.773107000
6	1.805105000	-0.017087000	-1.237149000
6	2.823943000	-0.681923000	-1.151391000
6	-3.004113000	2.901741000	-1.180694000
6	-4.143692000	3.302139000	-1.006318000
6	6.417596000	5.714503000	1.039746000
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6	4.047636000	4.264520000	1.268361000
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1	5.167328000	7.438344000	0.749772000
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6	6.513403000	4.332160000	1.265695000
6	5.302832000	3.594737000	1.365915000
7	5.314878000	2.228367000	1.553998000
6	7.814187000	3.654662000	1.378350000
1	4.389235000	1.814302000	1.611485000
5	6.534500000	1.479758000	1.613324000
6	7.843019000	2.246946000	1.535118000
6	9.067746000	1.539379000	1.614661000
7	6.596552000	0.063986000	1.750455000
1	5.775866000	-0.528803000	1.759745000
6	9.038868000	0.077013000	1.749790000
6	7.804151000	-0.623029000	1.808354000
6	7.790777000	-2.022486000	1.916279000
6	8.972163000	-2.743694000	1.963911000
6	10.197799000	-2.072036000	1.912790000
6	10.215982000	-0.689874000	1.809889000
1	6.833063000	-2.533092000	1.948392000
1	8.940546000	-3.825253000	2.043512000
1	11.129272000	-2.625776000	1.951378000
1	11.173377000	-0.185265000	1.764450000
6	-8.433063000	-0.931611000	2.066312000
6	-5.715955000	-0.354511000	1.857629000
6	-6.636221000	0.663859000	2.149620000
6	-7.989345000	0.370308000	2.257153000
1	-9.494697000	-1.130846000	2.132263000
1	-6.272038000	1.675378000	2.280973000
1	-8.700281000	1.159789000	2.469065000
6	-6.175100000	-1.685884000	1.657222000
6	-7.557881000	-1.986715000	1.760851000
6	-8.042949000	-3.357030000	1.539235000
5	-5.637994000	-4.018747000	1.095167000
6	-7.113186000	-4.368607000	1.195903000
6	-7.529103000	-5.699290000	0.946912000
6	-5.149110000	-6.349971000	0.459308000
6	-6.526000000	-6.694512000	0.540563000
6	-6.880288000	-8.010052000	0.190483000

6	-5.945165000	-8.951462000	-0.213008000
6	-4.593866000	-8.596777000	-0.278112000
6	-4.206262000	-7.309098000	0.055450000
1	-7.923708000	-8.298760000	0.228416000
1	-6.262930000	-9.953857000	-0.476661000
1	-3.849272000	-9.320882000	-0.591058000
1	-3.159115000	-7.021723000	0.003389000
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6	-6.103354000	4.716658000	-0.445045000
6	-7.475241000	4.805086000	-0.230608000
6	-8.278673000	3.678141000	-0.374156000
1	-7.920078000	5.752572000	0.051179000
1	-9.342872000	3.776309000	-0.196213000
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6	-7.760691000	2.424459000	-0.739591000
6	-6.361513000	2.338398000	-0.965711000
7	-5.774163000	1.148868000	-1.328595000
6	-8.610453000	1.228010000	-0.870134000
1	-4.768102000	1.217778000	-1.443413000
6	-8.012933000	-0.006842000	-1.225456000
5	-6.514932000	-0.063596000	-1.459804000
7	-5.931589000	-1.318191000	-1.796364000
6	-8.774241000	-1.196780000	-1.338861000
1	-4.940502000	-1.443821000	-1.957987000
6	-6.688857000	-2.479362000	-1.909987000
6	-8.093726000	-2.447824000	-1.702967000
6	-8.790585000	-3.661491000	-1.848316000
6	-8.154579000	-4.849218000	-2.169923000
6	-6.768864000	-4.864622000	-2.355951000
6	-6.049476000	-3.689003000	-2.225482000
1	-9.861470000	-3.674042000	-1.689989000
1	-8.727528000	-5.764859000	-2.255693000
1	-6.255247000	-5.791327000	-2.585137000
1	-4.971510000	-3.688124000	-2.364536000
6	6.417975000	-2.851657000	-1.047824000
6	4.027142000	-1.419570000	-1.095670000
6	4.018502000	-2.805449000	-0.874214000
6	5.212362000	-3.515727000	-0.846892000
1	7.336747000	-3.422802000	-1.018547000
1	3.067483000	-3.305950000	-0.733051000
1	5.205114000	-4.585992000	-0.674809000
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6	6.487429000	-1.467703000	-1.273240000
6	7.771645000	-0.777627000	-1.470207000
7	5.253867000	0.625561000	-1.475099000
1	4.322850000	1.031316000	-1.466211000
5	6.459346000	1.385871000	-1.614943000
6	7.777009000	0.630717000	-1.624998000
6	8.986993000	1.350495000	-1.781878000
7	6.497849000	2.802168000	-1.754549000
1	5.672816000	3.387075000	-1.707834000
6	8.934901000	2.812607000	-1.913420000

6	7.692333000	3.500768000	-1.890967000
6	7.658447000	4.900023000	-1.997807000
6	8.827253000	5.632505000	-2.122543000
6	10.059934000	4.972689000	-2.151233000
6	10.098079000	3.590815000	-2.049792000
1	6.695705000	5.401444000	-1.968205000
1	8.780082000	6.713631000	-2.200444000
1	10.981493000	5.535249000	-2.250875000
1	11.061098000	3.095412000	-2.066944000
7	-5.250988000	-2.668333000	1.356363000
1	-4.294470000	-2.328941000	1.326007000
7	-4.722676000	-5.062247000	0.764795000
1	-3.723621000	-4.920212000	0.685511000
6	-9.399228000	-3.701797000	1.641559000
6	-8.891839000	-6.008050000	1.076176000
6	-9.803517000	-5.014777000	1.417914000
1	-9.253837000	-7.015262000	0.909153000
1	-10.854923000	-5.268718000	1.510179000
1	-10.145826000	-2.959989000	1.897001000
6	-10.151673000	-1.131232000	-1.077141000
6	-9.992532000	1.252903000	-0.629184000
6	-10.739210000	0.082333000	-0.730324000
1	-10.772465000	-2.016473000	-1.137685000
1	-10.496305000	2.172023000	-0.354683000
1	-11.806315000	0.117076000	-0.533635000
6	8.995510000	-1.459739000	-1.493807000
6	10.191796000	0.631311000	-1.789430000
6	10.182726000	-0.752344000	-1.651014000
1	11.142213000	1.139582000	-1.897531000
1	11.123867000	-1.292691000	-1.654769000
1	9.040804000	-2.534263000	-1.372541000
6	10.263488000	2.270221000	1.544619000
6	9.030354000	4.348594000	1.321561000
6	10.232088000	3.653330000	1.404136000
1	11.223731000	1.771234000	1.592761000
1	11.166106000	4.202854000	1.346572000
1	9.057136000	5.423133000	1.195471000

168
C2 isomer C, -4235.04450

6	0.801970000	1.166447000	1.306301000
6	-0.574094000	1.255255000	1.460026000
6	-1.400158000	0.111257000	1.459382000
6	-0.801970000	-1.166447000	1.306301000
6	0.574094000	-1.255255000	1.460026000
6	1.400158000	-0.111257000	1.459382000
1	-1.056312000	2.225982000	1.421161000
1	1.056312000	-2.225982000	1.421161000
6	1.572543000	2.323682000	0.719489000
1	2.642212000	2.155109000	0.865232000
1	1.312638000	3.263538000	1.213069000

6	1.289152000	2.496054000	-0.849102000
1	2.240256000	2.713728000	-1.343168000
1	0.634813000	3.357446000	-0.992821000
6	-0.640705000	-1.266967000	-1.438765000
6	-1.372134000	-0.098510000	-1.586737000
6	-0.768028000	1.177065000	-1.569338000
6	0.640705000	1.266967000	-1.438765000
6	1.372134000	0.098510000	-1.586737000
6	0.768028000	-1.177065000	-1.569338000
1	-2.454518000	-0.147182000	-1.522841000
1	2.454518000	0.147182000	-1.522841000
6	-1.289152000	-2.496054000	-0.849102000
6	-1.572543000	-2.323682000	0.719489000
1	-2.642212000	-2.155109000	0.865232000
1	-1.312638000	-3.263538000	1.213069000
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1	-2.240256000	-2.713728000	-1.343168000
6	2.799883000	-0.307690000	1.475155000
6	3.977815000	-0.614774000	1.557848000
6	-2.799883000	0.307690000	1.475155000
6	-3.977815000	0.614774000	1.557848000
6	1.624846000	-2.295644000	-1.470065000
6	2.463128000	-3.169334000	-1.320777000
6	-1.624846000	2.295644000	-1.470065000
6	-2.463128000	3.169334000	-1.320777000
6	7.992026000	-1.734198000	2.070586000
6	6.993867000	-2.696731000	2.141976000
6	5.665481000	-2.334185000	1.960315000
6	5.330184000	-0.994757000	1.712639000
1	9.020801000	-2.046378000	2.193092000
1	7.252803000	-3.733810000	2.318453000
1	4.874443000	-3.073371000	1.998604000
6	7.714594000	-0.381316000	1.816137000
6	6.356680000	-0.011558000	1.637175000
7	6.001464000	1.299607000	1.384583000
6	8.781296000	0.626698000	1.724348000
1	4.998970000	1.437246000	1.299312000
5	6.973975000	2.337160000	1.250311000
6	8.436456000	1.969421000	1.433571000
6	9.424943000	2.976149000	1.313730000
7	6.655141000	3.699825000	0.973896000
1	5.708044000	4.032983000	0.845470000
6	9.011129000	4.341836000	0.959166000
6	7.637112000	4.667359000	0.795524000
6	7.260455000	5.972084000	0.438417000
6	8.210116000	6.959920000	0.234354000
6	9.567043000	6.657098000	0.385419000
6	9.944952000	5.371125000	0.741565000
1	6.203284000	6.195637000	0.319354000
1	7.897219000	7.960581000	-0.043613000
1	10.320775000	7.419836000	0.225231000
1	11.000899000	5.152555000	0.848044000

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6	-5.330184000	0.994757000	1.712639000
6	-5.665481000	2.334185000	1.960315000
6	-6.993867000	2.696731000	2.141976000
1	-9.020801000	2.046378000	2.193092000
1	-4.874443000	3.073371000	1.998604000
1	-7.252803000	3.733810000	2.318453000
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6	-9.424943000	-2.976149000	1.313730000
6	-7.637112000	-4.667359000	0.795524000
6	-9.011129000	-4.341836000	0.959166000
6	-9.944952000	-5.371125000	0.741565000
6	-9.567043000	-6.657098000	0.385419000
6	-8.210116000	-6.959920000	0.234354000
6	-7.260455000	-5.972084000	0.438417000
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1	-10.320775000	-7.419836000	0.225231000
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1	-6.203284000	-6.195637000	0.319354000
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6	-4.676348000	6.091894000	-0.612714000
6	-5.918784000	5.471148000	-0.692713000
1	-4.614642000	7.148176000	-0.377143000
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1	-2.538937000	5.824490000	-0.758424000
6	-6.061540000	4.107300000	-0.996080000
6	-4.875242000	3.364141000	-1.233908000
7	-4.926864000	2.025566000	-1.545401000
6	-7.375824000	3.443610000	-1.035054000
1	-4.010131000	1.605579000	-1.662723000
6	-7.438964000	2.056668000	-1.317399000
5	-6.153173000	1.296573000	-1.584334000
7	-6.238709000	-0.099086000	-1.851979000
6	-8.669532000	1.353956000	-1.322099000
1	-5.428889000	-0.680468000	-2.025713000
6	-7.451595000	-0.779947000	-1.853311000
6	-8.667384000	-0.088284000	-1.606445000
6	-9.852269000	-0.846659000	-1.628562000
6	-9.856438000	-2.210596000	-1.870355000
6	-8.648931000	-2.877385000	-2.099255000
6	-7.462597000	-2.163741000	-2.089464000
1	-10.795766000	-0.352465000	-1.434068000
1	-10.790408000	-2.760145000	-1.860386000
1	-8.635590000	-3.948253000	-2.267219000
1	-6.516801000	-2.671058000	-2.259976000
6	5.918784000	-5.471148000	-0.692713000
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6	4.875242000	-3.364141000	-1.233908000
6	6.061540000	-4.107300000	-0.996080000
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7	4.926864000	-2.025566000	-1.545401000
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6	7.438964000	-2.056668000	-1.317399000
6	8.669532000	-1.353956000	-1.322099000
7	6.238709000	0.099086000	-1.851979000
1	5.428889000	0.680468000	-2.025713000
6	8.667384000	0.088284000	-1.606445000
6	7.451595000	0.779947000	-1.853311000
6	7.462597000	2.163741000	-2.089464000
6	8.648931000	2.877385000	-2.099255000
6	9.856438000	2.210596000	-1.870355000
6	9.852269000	0.846659000	-1.628562000
1	6.516801000	2.671058000	-2.259976000
1	8.635590000	3.948253000	-2.267219000
1	10.790408000	2.760145000	-1.860386000
1	10.795766000	0.352465000	-1.434068000
7	-6.001464000	-1.299607000	1.384583000
1	-4.998970000	-1.437246000	1.299312000
7	-6.655141000	-3.699825000	0.973896000
1	-5.708044000	-4.032983000	0.845470000
6	-10.135580000	-0.308342000	1.903010000
6	-10.767183000	-2.620781000	1.516681000
6	-11.104429000	-1.302691000	1.805212000
1	-11.556794000	-3.359214000	1.446924000
1	-12.147796000	-1.042962000	1.955293000
1	-10.445787000	0.706224000	2.119669000
6	-9.842587000	2.067220000	-1.030889000
6	-8.573257000	4.122917000	-0.764792000
6	-9.781442000	3.431751000	-0.762376000
1	-10.804932000	1.570640000	-1.008003000
1	-8.577476000	5.183518000	-0.543907000
1	-10.698491000	3.969757000	-0.542710000
6	8.573257000	-4.122917000	-0.764792000
6	9.842587000	-2.067220000	-1.030889000
6	9.781442000	-3.431751000	-0.762376000
1	10.804932000	-1.570640000	-1.008003000
1	10.698491000	-3.969757000	-0.542710000
1	8.577476000	-5.183518000	-0.543907000
6	10.767183000	2.620781000	1.516681000
6	10.135580000	0.308342000	1.903010000
6	11.104429000	1.302691000	1.805212000
1	11.556794000	3.359214000	1.446924000
1	12.147796000	1.042962000	1.955293000

1	10.445787000	-0.706224000	2.119669000

168

C2 isomer D, -4235.03511

6	1.794303000	0.880341000	-1.318253000
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6	-0.923777000	1.739545000	-1.311942000
6	-0.197528000	1.661551000	-0.118047000
6	1.143085000	1.201427000	-0.088630000
1	1.663417000	1.063794000	-3.462529000
1	-0.723484000	1.781931000	0.835286000
6	2.941912000	-0.103739000	-1.363953000
1	3.649306000	0.070793000	-0.533876000
1	3.492480000	0.038934000	-2.310706000
6	2.434173000	-1.627522000	-1.278927000
1	2.813154000	-2.065532000	-0.338474000
1	2.884262000	-2.190340000	-2.117701000
6	-1.794303000	-0.880341000	-1.318253000
6	-1.165638000	-1.253700000	-2.505352000
6	0.198403000	-1.644054000	-2.535748000
6	0.923777000	-1.739545000	-1.311942000
6	0.197528000	-1.661551000	-0.118047000
6	-1.143085000	-1.201427000	-0.088630000
1	-1.663417000	-1.063794000	-3.462529000
1	0.723484000	-1.781931000	0.835286000
6	-2.941912000	0.103739000	-1.363953000
6	-2.434173000	1.627522000	-1.278927000
1	-2.884262000	2.190340000	-2.117701000
1	-2.813154000	2.065532000	-0.338474000
1	-3.649306000	-0.070793000	-0.533876000
1	-3.492480000	-0.038934000	-2.310706000
6	1.757238000	0.857400000	1.143421000
6	2.320286000	0.467227000	2.167553000
6	-0.827582000	1.678763000	-3.808582000
6	-1.237757000	1.542333000	-4.962150000
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6	4.286110000	-0.758217000	5.699334000
6	4.806931000	-1.131443000	4.454476000
6	4.160812000	-0.729491000	3.282527000
6	2.975116000	0.035221000	3.351031000
1	4.812132000	-1.077912000	6.603761000
1	5.725051000	-1.727781000	4.401426000
1	4.561068000	-0.993722000	2.297515000
6	3.107409000	0.007949000	5.829384000
6	2.429574000	0.390132000	4.629501000
7	1.247290000	1.102524000	4.676303000
6	2.571618000	0.394623000	7.150154000

1	0.849570000	1.313995000	3.756601000
5	0.618129000	1.462421000	5.917495000
6	1.336443000	1.100249000	7.212401000
6	0.751217000	1.469038000	8.457011000
7	-0.632546000	2.148022000	6.007455000
1	-1.199982000	2.380697000	5.190772000
6	-0.542674000	2.177174000	8.457241000
6	-1.203736000	2.493259000	7.229418000
6	-2.450487000	3.156677000	7.245943000
6	-3.060675000	3.507515000	8.449184000
6	-2.424864000	3.206275000	9.666710000
6	-1.190628000	2.556055000	9.655313000
1	-2.935988000	3.385818000	6.289008000
1	-4.030790000	4.019595000	8.439031000
1	-2.892727000	3.477540000	10.620409000
1	-0.713283000	2.324325000	10.612507000
6	-2.797364000	0.670784000	-8.786915000
6	-1.755402000	1.293439000	-6.260623000
6	-0.957781000	1.444886000	-7.413183000
6	-1.484418000	1.138668000	-8.672355000
1	-3.180474000	0.428276000	-9.783159000
1	0.074539000	1.790736000	-7.302575000
1	-0.863298000	1.254642000	-9.567585000
6	-3.102866000	0.818408000	-6.383138000
6	-3.639185000	0.491366000	-7.665222000
6	-5.016986000	-0.031638000	-7.789153000
5	-5.197025000	0.147425000	-5.256018000
6	-5.795848000	-0.220923000	-6.610139000
6	-7.122234000	-0.740763000	-6.664509000
6	-7.289661000	-0.573679000	-4.147629000
6	-7.873461000	-0.924987000	-5.405741000
6	-9.185919000	-1.453886000	-5.382755000
6	-9.900684000	-1.635574000	-4.198150000
6	-9.309839000	-1.284840000	-2.971124000
6	-8.018499000	-0.760138000	-2.952089000
1	-9.661608000	-1.734383000	-6.328066000
1	-10.914917000	-2.050299000	-4.228162000
1	-9.856162000	-1.422455000	-2.030133000
1	-7.546155000	-0.485478000	-1.999331000
6	1.755402000	-1.293439000	-6.260623000
6	0.957781000	-1.444886000	-7.413183000
6	1.484418000	-1.138668000	-8.672355000
6	2.797364000	-0.670784000	-8.786915000
1	0.863298000	-1.254642000	-9.567585000
1	3.180474000	-0.428276000	-9.783159000
1	-0.074539000	-1.790736000	-7.302575000
6	3.639185000	-0.491366000	-7.665222000
6	3.102866000	-0.818408000	-6.383138000
7	3.857788000	-0.662030000	-5.233160000
6	5.016986000	0.031638000	-7.789153000
1	3.363388000	-0.938163000	-4.379564000
6	5.795848000	0.220923000	-6.610139000

5	5.197025000	-0.147425000	-5.256018000
7	6.000149000	0.047410000	-4.087633000
6	7.122234000	0.740763000	-6.664509000
1	5.675772000	-0.178462000	-3.145761000
6	7.289661000	0.573679000	-4.147629000
6	7.873461000	0.924987000	-5.405741000
6	9.185919000	1.453886000	-5.382755000
6	9.900684000	1.635574000	-4.198150000
6	9.309839000	1.284840000	-2.971124000
6	8.018499000	0.760138000	-2.952089000
1	9.661608000	1.734383000	-6.328066000
1	10.914917000	2.050299000	-4.228162000
1	9.856162000	1.422455000	-2.030133000
1	7.546155000	0.485478000	-1.999331000
6	-4.286110000	0.758217000	5.699334000
6	-2.975116000	-0.035221000	3.351031000
6	-4.160812000	0.729491000	3.282527000
6	-4.806931000	1.131443000	4.454476000
1	-4.812132000	1.077912000	6.603761000
1	-4.561068000	0.993722000	2.297515000
1	-5.725051000	1.727781000	4.401426000
6	-2.429574000	-0.390132000	4.629501000
6	-3.107409000	-0.007949000	5.829384000
6	-2.571618000	-0.394623000	7.150154000
7	-1.247290000	-1.102524000	4.676303000
1	-0.849570000	-1.313995000	3.756601000
5	-0.618129000	-1.462421000	5.917495000
6	-1.336443000	-1.100249000	7.212401000
6	-0.751217000	-1.469038000	8.457011000
7	0.632546000	-2.148022000	6.007455000
1	1.199982000	-2.380697000	5.190772000
6	0.542674000	-2.177174000	8.457241000
6	1.203736000	-2.493259000	7.229418000
6	2.450487000	-3.156677000	7.245943000
6	3.060675000	-3.507515000	8.449184000
6	2.424864000	-3.206275000	9.666710000
6	1.190628000	-2.556055000	9.655313000
1	2.935988000	-3.385818000	6.289008000
1	4.030790000	-4.019595000	8.439031000
1	2.892727000	-3.477540000	10.620409000
1	0.713283000	-2.324325000	10.612507000
7	-3.857788000	0.662030000	-5.233160000
1	-3.363388000	0.938163000	-4.379564000
7	-6.000149000	-0.047410000	-4.087633000
1	-5.675772000	0.178462000	-3.145761000
6	-5.596146000	-0.363370000	-9.032693000
6	-7.661127000	-1.061527000	-7.929582000
6	-6.900713000	-0.868791000	-9.088617000
1	-8.675423000	-1.461871000	-8.025143000
1	-7.336324000	-1.120820000	-10.063686000
1	-5.041600000	-0.232535000	-9.967506000
6	7.661127000	1.061527000	-7.929582000

6	5.596146000	0.363370000	-9.032693000
6	6.900713000	0.868791000	-9.088617000
1	8.675423000	1.461871000	-8.025143000
1	5.041600000	0.232535000	-9.967506000
1	7.336324000	1.120820000	-10.063686000
6	-3.227263000	-0.077579000	8.357323000
6	-1.434682000	-1.123726000	9.642347000
6	-2.655040000	-0.442633000	9.580694000
1	-1.021761000	-1.377420000	10.623876000
1	-3.170253000	-0.177793000	10.511903000
1	-4.176253000	0.465717000	8.361656000
6	1.434682000	1.123726000	9.642347000
6	3.227263000	0.077579000	8.357323000
6	2.655040000	0.442633000	9.580694000
1	1.021761000	1.377420000	10.623876000
1	3.170253000	0.177793000	10.511903000
1	4.176253000	-0.465717000	8.361656000

72
“monomer”, C1, -1752.14796

C	3.336877000	-1.575664000	-1.409804000
C	2.274375000	-0.683363000	-1.462938000
C	2.462272000	0.707835000	-1.349946000
C	3.774866000	1.216169000	-1.193331000
C	4.833348000	0.347515000	-1.437006000
C	4.642433000	-1.043385000	-1.542694000
H	1.261383000	-1.069994000	-1.423088000
H	5.849867000	0.721162000	-1.381716000
C	3.096559000	-2.983999000	-0.926571000
H	3.733858000	-3.703137000	-1.445165000
H	2.054606000	-3.251296000	-1.114757000
C	3.376834000	-3.131040000	0.644675000
H	4.335450000	-3.636642000	0.774608000
H	2.593599000	-3.767045000	1.062638000
C	3.596891000	1.029172000	1.547638000
C	2.374212000	0.377910000	1.675915000
C	2.267770000	-1.021538000	1.572220000
C	3.431910000	-1.790694000	1.333551000
C	4.660083000	-1.161034000	1.507705000
C	4.766266000	0.235955000	1.617799000
H	1.461244000	0.962206000	1.703624000
H	5.572130000	-1.738087000	1.401915000
C	3.651969000	2.456220000	1.061243000
C	4.011735000	2.533655000	-0.496896000
H	3.409478000	3.334639000	-0.932592000
H	5.064408000	2.804163000	-0.596154000
H	4.403266000	3.037979000	1.600206000
H	2.678017000	2.923412000	1.217580000
C	5.769457000	-1.905468000	-1.588623000
C	6.727287000	-2.644292000	-1.611032000
C	1.334633000	1.538046000	-1.167276000
C	0.360504000	2.236141000	-0.943252000

C	6.050009000	0.843496000	1.609342000
C	7.141956000	1.363220000	1.589649000
C	0.978056000	-1.617855000	1.549460000
C	-0.127777000	-2.110195000	1.549215000
C	-3.278899000	4.145389000	-0.083756000
C	-0.847185000	2.909359000	-0.656057000
C	-0.925076000	4.305357000	-0.567537000
C	-2.140036000	4.918273000	-0.281321000
H	-4.212971000	4.648332000	0.135584000
H	-0.028483000	4.892054000	-0.730389000
H	-2.201366000	5.998481000	-0.214863000
C	-2.017259000	2.119210000	-0.446630000
C	-3.259760000	2.742388000	-0.157644000
C	-4.469559000	1.929682000	0.056126000
B	-3.032805000	-0.116429000	-0.351212000
C	-4.376040000	0.517833000	-0.035276000
C	-5.506839000	-0.314921000	0.159105000
C	-4.080895000	-2.346903000	-0.254715000
C	-5.345580000	-1.774049000	0.052994000
C	-6.420866000	-2.660581000	0.246855000
C	-6.279072000	-4.036466000	0.146450000
C	-5.027728000	-4.580934000	-0.158996000
C	-3.943917000	-3.740866000	-0.356500000
H	-7.397751000	-2.256756000	0.484178000
H	-7.135154000	-4.682891000	0.303634000
H	-4.900602000	-5.654864000	-0.243045000
H	-2.967550000	-4.153254000	-0.598254000
N	-1.910909000	0.747026000	-0.530245000
H	-0.966281000	0.422209000	-0.715152000
N	-2.967915000	-1.536853000	-0.454165000
H	-2.113976000	-2.032723000	-0.677710000
C	-5.719780000	2.496893000	0.346098000
C	-6.738840000	0.293371000	0.445308000
C	-6.830106000	1.679114000	0.534853000
H	-7.632319000	-0.299754000	0.598396000
H	-7.790533000	2.133356000	0.756736000
H	-5.841907000	3.570212000	0.426372000
H	8.106302000	1.812929000	1.581216000
H	-1.104339000	-2.530670000	1.603354000
H	7.574898000	-3.286826000	-1.640618000

104
"dimer through space", C2, -2579.79545

C	-0.988966000	1.689026000	5.198185000
C	-0.203796000	1.639714000	6.344280000
C	1.154276000	1.274446000	6.297988000
C	1.742893000	0.953583000	5.051007000
C	1.037616000	1.290431000	3.902675000
C	-0.323564000	1.650730000	3.946617000
H	-0.677636000	1.727214000	7.315858000
H	1.489602000	1.105255000	2.934240000

C	-2.481952000	1.493814000	5.297037000
H	-3.021183000	2.154851000	4.614251000
H	-2.801065000	1.720435000	6.315941000
C	-2.915001000	-0.009301000	4.956613000
H	-3.311737000	-0.034470000	3.939682000
H	-3.715964000	-0.285392000	5.645919000
C	0.988966000	-1.689026000	5.198185000
C	0.203796000	-1.639714000	6.344280000
C	-1.154276000	-1.274446000	6.297988000
C	-1.742893000	-0.953583000	5.051007000
C	-1.037616000	-1.290431000	3.902675000
C	0.323564000	-1.650730000	3.946617000
H	0.677636000	-1.727214000	7.315858000
H	-1.489602000	-1.105255000	2.934240000
C	2.481952000	-1.493814000	5.297037000
C	2.915001000	0.009301000	4.956613000
H	3.715964000	0.285392000	5.645919000
H	3.311737000	0.034470000	3.939682000
H	3.021183000	-2.154851000	4.614251000
H	2.801065000	-1.720435000	6.315941000
C	-1.055270000	1.767248000	2.744453000
C	-1.722020000	1.837017000	1.726127000
C	1.860991000	1.046716000	7.507861000
C	2.461166000	0.838392000	8.537522000
C	1.055270000	-1.767248000	2.744453000
C	1.722020000	-1.837017000	1.726127000
C	-1.860991000	-1.046716000	7.507861000
C	-2.461166000	-0.838392000	8.537522000
C	-3.865452000	2.181520000	-1.867890000
C	-4.549494000	2.221055000	-0.657491000
C	-3.849063000	2.105418000	0.536991000
C	-2.455911000	1.937443000	0.523532000
H	-4.430228000	2.271571000	-2.786710000
H	-5.625948000	2.348499000	-0.646885000
H	-4.360889000	2.148834000	1.491486000
C	-2.473022000	2.017766000	-1.941868000
C	-1.760449000	1.879655000	-0.720662000
N	-0.395095000	1.686293000	-0.710293000
C	-1.764574000	1.972403000	-3.230346000
H	-0.000311000	1.606100000	0.222071000
B	0.366465000	1.573487000	-1.917658000
C	-0.366465000	1.742556000	-3.237043000
C	0.361254000	1.659936000	-4.449571000
N	1.767358000	1.322546000	-1.957275000
H	2.323634000	1.148967000	-1.129366000
C	1.805696000	1.397701000	-4.397925000
C	2.469970000	1.229701000	-3.153516000
C	3.846734000	0.958472000	-3.119299000
C	4.579278000	0.847810000	-4.289389000
C	3.944421000	1.016082000	-5.524075000
C	2.585492000	1.286503000	-5.562718000
H	4.327187000	0.823238000	-2.154894000

H	5.641951000	0.634348000	-4.241671000
H	4.508054000	0.934463000	-6.446762000
H	2.107291000	1.407251000	-6.527016000
C	3.865452000	-2.181520000	-1.867890000
C	2.455911000	-1.937443000	0.523532000
C	3.849063000	-2.105418000	0.536991000
C	4.549494000	-2.221055000	-0.657491000
H	4.430228000	-2.271571000	-2.786710000
H	4.360889000	-2.148834000	1.491486000
H	5.625948000	-2.348499000	-0.646885000
C	1.760449000	-1.879655000	-0.720662000
C	2.473022000	-2.017766000	-1.941868000
C	1.764574000	-1.972403000	-3.230346000
N	0.395095000	-1.686293000	-0.710293000
H	0.000311000	-1.606100000	0.222071000
B	-0.366465000	-1.573487000	-1.917658000
C	0.366465000	-1.742556000	-3.237043000
C	-0.361254000	-1.659936000	-4.449571000
N	-1.767358000	-1.322546000	-1.957275000
H	-2.323634000	-1.148967000	-1.129366000
C	-1.805696000	-1.397701000	-4.397925000
C	-2.469970000	-1.229701000	-3.153516000
C	-3.846734000	-0.958472000	-3.119299000
C	-4.579278000	-0.847810000	-4.289389000
C	-3.944421000	-1.016082000	-5.524075000
C	-2.585492000	-1.286503000	-5.562718000
H	-4.327187000	-0.823238000	-2.154894000
H	-5.641951000	-0.634348000	-4.241671000
H	-4.508054000	-0.934463000	-6.446762000
H	-2.107291000	-1.407251000	-6.527016000
C	2.423529000	-2.134940000	-4.456228000
C	0.337445000	-1.818826000	-5.655992000
C	1.707633000	-2.055739000	-5.646110000
H	-0.175088000	-1.754170000	-6.608092000
H	2.233515000	-2.171182000	-6.588397000
H	3.491614000	-2.304057000	-4.500325000
C	-0.337445000	1.818826000	-5.655992000
C	-2.423529000	2.134940000	-4.456228000
C	-1.707633000	2.055739000	-5.646110000
H	0.175088000	1.754170000	-6.608092000
H	-2.233515000	2.171182000	-6.588397000
H	-3.491614000	2.304057000	-4.500325000
H	2.985160000	0.666276000	9.447452000
H	-2.985160000	-0.666276000	9.447452000

104
“dimer through bond”, C2, -2579.76947

C	1.416564000	-0.059092000	-1.298967000
C	0.657412000	-1.211977000	-1.446297000
C	-0.752509000	-1.185593000	-1.438437000
C	-1.416564000	0.059092000	-1.298967000

C	-0.657412000	1.211977000	-1.446297000
C	0.752509000	1.185593000	-1.438437000
H	1.152188000	-2.176141000	-1.394012000
H	-1.152188000	2.176141000	-1.394012000
C	2.800974000	-0.142345000	-0.706191000
H	3.489025000	0.558140000	-1.185210000
H	3.187739000	-1.153089000	-0.849012000
C	2.799181000	0.180253000	0.862918000
H	3.170933000	1.196104000	1.006795000
H	3.494509000	-0.511956000	1.342944000
C	-1.414171000	-0.076912000	1.450546000
C	-0.640214000	-1.222718000	1.604298000
C	0.765134000	-1.170617000	1.611141000
C	1.414171000	0.076912000	1.450546000
C	0.640214000	1.222718000	1.604298000
C	-0.765134000	1.170617000	1.611141000
H	-1.118770000	-2.195239000	1.572212000
H	1.118770000	2.195239000	1.572212000
C	-2.799181000	-0.180253000	0.862918000
C	-2.800974000	0.142345000	-0.706191000
H	-3.489025000	-0.558140000	-1.185210000
H	-3.187739000	1.153089000	-0.849012000
H	-3.494509000	0.511956000	1.342944000
H	-3.170933000	-1.196104000	1.006795000
C	1.463605000	2.400872000	-1.339663000
C	2.072407000	3.446925000	-1.189740000
C	-1.463605000	-2.400872000	-1.339663000
C	-2.072407000	-3.446925000	-1.189740000
C	-1.505506000	2.383157000	1.630840000
C	-2.123216000	3.422985000	1.677050000
C	1.505506000	-2.383157000	1.630840000
C	2.123216000	-3.422985000	1.677050000
C	3.683909000	7.263538000	-0.503766000
C	4.541291000	6.210650000	-0.803028000
C	4.026992000	4.939782000	-1.035189000
C	2.644834000	4.719259000	-0.970381000
H	4.110370000	8.243266000	-0.325820000
H	5.610300000	6.382060000	-0.855773000
H	4.680162000	4.107968000	-1.271669000
C	2.290645000	7.100640000	-0.422608000
C	1.768059000	5.802784000	-0.663341000
N	0.412267000	5.558025000	-0.602221000
C	1.389281000	8.218292000	-0.093879000
H	0.165656000	4.587125000	-0.770979000
B	-0.534111000	6.583451000	-0.302995000
C	-0.006674000	7.980245000	-0.025421000
C	-0.921309000	9.015717000	0.292443000
N	-1.943600000	6.375560000	-0.252063000
H	-2.373088000	5.479300000	-0.444923000
C	-2.358493000	8.704559000	0.355222000
C	-2.832745000	7.393291000	0.076659000
C	-4.207643000	7.113186000	0.136308000

C	-5.122953000	8.098317000	0.470099000
C	-4.675206000	9.392958000	0.750517000
C	-3.319096000	9.676468000	0.689762000
H	-4.545672000	6.104493000	-0.088422000
H	-6.180554000	7.860913000	0.511334000
H	-5.381096000	10.172606000	1.013481000
H	-2.990199000	10.684861000	0.909895000
C	-3.683909000	-7.263538000	-0.503766000
C	-2.644834000	-4.719259000	-0.970381000
C	-4.026992000	-4.939782000	-1.035189000
C	-4.541291000	-6.210650000	-0.803028000
H	-4.110370000	-8.243266000	-0.325820000
H	-4.680162000	-4.107968000	-1.271669000
H	-5.610300000	-6.382060000	-0.855773000
C	-1.768059000	-5.802784000	-0.663341000
C	-2.290645000	-7.100640000	-0.422608000
C	-1.389281000	-8.218292000	-0.093879000
B	0.534111000	-6.583451000	-0.302995000
C	0.006674000	-7.980245000	-0.025421000
C	0.921309000	-9.015717000	0.292443000
C	2.832745000	-7.393291000	0.076659000
C	2.358493000	-8.704559000	0.355222000
C	3.319096000	-9.676468000	0.689762000
C	4.675206000	-9.392958000	0.750517000
C	5.122953000	-8.098317000	0.470099000
C	4.207643000	-7.113186000	0.136308000
H	2.990199000	-10.684861000	0.909895000
H	5.381096000	-10.172606000	1.013481000
H	6.180554000	-7.860913000	0.511334000
H	4.545672000	-6.104493000	-0.088422000
N	-0.412267000	-5.558025000	-0.602221000
H	-0.165656000	-4.587125000	-0.770979000
N	1.943600000	-6.375560000	-0.252063000
H	2.373088000	-5.479300000	-0.444923000
C	-1.856351000	-9.517291000	0.157887000
C	0.412267000	-10.300502000	0.536804000
C	-0.957749000	-10.534327000	0.466734000
H	1.070984000	-11.125351000	0.780229000
H	-1.334924000	-11.534059000	0.657877000
H	-2.913688000	-9.749673000	0.117056000
C	-0.412267000	10.300502000	0.536804000
C	1.856351000	9.517291000	0.157887000
C	0.957749000	10.534327000	0.466734000
H	-1.070984000	11.125351000	0.780229000
H	1.334924000	11.534059000	0.657877000
H	2.913688000	9.749673000	0.117056000
H	-2.651658000	4.341990000	1.775053000
H	2.651658000	-4.341990000	1.775053000

Adiabatic Ionization Energies

All Cartesian coordinates given below were computed at the RI-TPSS-D3(BJ)/def2-TZVP level of theory and are given in Å and absolute energies are given in atomic units.

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168
neutral 6′, -4234.93592
6        0.059573267      1.430576032     -1.370437850
6        1.213541409      0.670428883     -1.519792690
6        1.182396224     -0.740230518     -1.511412679
6       -0.065345330     -1.405107795     -1.371670651
6       -1.219713047     -0.644840219     -1.516656230
6       -1.188590587      0.765840090     -1.506976505
1        2.179843556      1.164002128     -1.474611587
1       -2.185742682     -1.138768789     -1.469712867
6        0.151407643      2.817752617     -0.784606656
1       -0.555915609      3.506525198     -1.255017711
1        1.160824308      3.204376768     -0.945217494
6       -0.148810067      2.817094643      0.788005540
1       -1.157794594      3.204619338      0.949282043
1        0.559309200      3.504744968      1.258851540
6        0.064023876     -1.406603097      1.370688342
6        1.219111216     -0.647543101      1.516434726
6        1.189212722      0.763171661      1.508107392
6       -0.058345053      1.429215382      1.372372898
6       -1.212976774      0.669958199      1.521084933
6       -1.183105302     -0.740690340      1.511232038
1        2.184714936     -1.142304157      1.469008547
1       -2.178907767      1.164369941      1.477054581
6        0.152646338     -2.793803995      0.784350124
6       -0.155352399     -2.792798220     -0.786728988
1        0.549171564     -3.481692433     -1.261161058
1       -1.165882996     -3.178280119     -0.942986329
1       -0.552555747     -3.482524098      1.258044157
1        1.162799246     -3.180498786      0.940130065
6       -2.398728805      1.491286909     -1.420398709
6       -3.426442828      2.140617762     -1.301818404
6        2.392130556     -1.466733383     -1.428995899
6        3.418064030     -2.119306843     -1.313217336
6       -2.393461321     -1.466169010      1.428775466
6       -3.419320795     -2.118230784      1.309343609
6        2.399906540      1.487754427      1.422387493
6        3.427543906      2.136593747      1.300518293
6       -6.987829390      4.348052462     -0.955150724
6       -5.762369402      4.993813706     -0.816262005
6       -4.580671106      4.269354379     -0.929886048
6       -4.621058359      2.885725025     -1.171181383
1       -7.895542887      4.934200207     -0.868297214
1       -5.730136130      6.062033150     -0.624295812
1       -3.615783445      4.757881136     -0.836098490
6       -7.087680009      2.967571047     -1.199483257
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6	-5.879259560	2.221970793	-1.292958956
7	-5.898571221	0.859259067	-1.500261413
6	-8.392286864	2.300553576	-1.346798658
1	-4.978504696	0.428889018	-1.555079801
5	-7.121407209	0.122533560	-1.616727431
6	-8.426786866	0.898006757	-1.551313039
6	-9.654558438	0.202013501	-1.690166010
7	-7.186026841	-1.286190014	-1.811034200
1	-6.361637369	-1.875402591	-1.861152251
6	-9.628203801	-1.254010085	-1.893900404
6	-8.393401238	-1.959313333	-1.946683697
6	-8.383831191	-3.353120867	-2.129905619
6	-9.567964522	-4.061389471	-2.261867444
6	-10.792835775	-3.384020346	-2.215701209
6	-10.808662282	-2.008358725	-2.033917981
1	-7.426503367	-3.867495960	-2.157405758
1	-9.539179904	-5.139227987	-2.397202885
1	-11.726818256	-3.929480703	-2.314902188
1	-11.766578355	-1.500449776	-1.991691767
6	6.966725554	-4.347176517	-0.967033695
6	4.608706493	-2.870850871	-1.183667009
6	4.560014528	-4.254906188	-0.946309435
6	5.737343257	-4.986452286	-0.832707330
1	7.871162482	-4.938291251	-0.880033083
1	3.592098079	-4.738106410	-0.856143642
1	5.698377907	-6.055087486	-0.644168366
6	5.870764812	-2.213965867	-1.301817787
6	7.074731350	-2.966604014	-1.207160390
6	8.383423407	-2.306594075	-1.349139136
5	7.125343772	-0.121486920	-1.621612092
6	8.426233852	-0.904179766	-1.552944524
6	9.658245655	-0.214866768	-1.687281785
6	8.409583047	1.953390296	-1.948221317
6	9.640408690	1.241297472	-1.891099037
6	10.825491087	1.989069898	-2.027272483
6	10.817881691	3.364760371	-2.209435071
6	9.596886192	4.048829271	-2.260033235
6	8.408365011	3.347186991	-2.131906838
1	11.780455601	1.475890840	-1.981667908
1	11.755249898	3.904981509	-2.305244468
1	9.574675017	5.126795118	-2.395608288
1	7.454071619	3.866949184	-2.163022365
6	4.622166357	2.881804216	1.170892996
6	4.581584192	4.265357577	0.929226212
6	5.763149501	4.990136635	0.816587460
6	6.988620852	4.344643695	0.956483908
1	5.730880079	6.058286811	0.624284081
1	7.895908692	4.931383400	0.869353403
1	3.616652664	4.753570210	0.834253196
6	7.088795109	2.964252867	1.201117507
6	5.880435043	2.218327238	1.293919253
7	5.899828867	0.855734474	1.501385088

6	8.393470185	2.297522167	1.349419285
1	4.979860981	0.424994194	1.555601913
6	8.428044653	0.894911715	1.553802721
5	7.122713996	0.119171844	1.618157352
7	7.187341756	-1.289617435	1.811576603
6	9.655808594	0.198938591	1.693078826
1	6.362608214	-1.878644776	1.859000990
6	8.394664818	-1.962716152	1.947020648
6	9.629457267	-1.257221549	1.895775559
6	10.809976093	-2.011505118	2.035752565
6	10.794236382	-3.387375235	2.215855256
6	9.569415786	-4.064982687	2.260190877
6	8.385231869	-3.356799792	2.128378892
1	11.767809065	-1.503339308	1.994845190
1	11.728217518	-3.932824162	2.315161979
1	9.540750452	-5.143030416	2.393933681
1	7.428025537	-3.871481267	2.154254102
6	-6.968367500	-4.345398303	0.963806206
6	-4.610144171	-2.869542615	1.180212209
6	-4.561744354	-4.253232271	0.940609063
6	-5.739190181	-4.984583916	0.827309820
1	-7.872923896	-4.936277512	0.876524364
1	-3.593972598	-4.736320146	0.848449384
1	-5.700496693	-6.052908642	0.637012441
6	-5.872026579	-2.212756329	1.300780403
6	-7.076096257	-2.965165985	1.206031522
6	-8.384677718	-2.305288995	1.349644729
7	-5.899166807	-0.850109551	1.507710398
1	-4.981591375	-0.414450202	1.563961090
5	-7.126367633	-0.120297876	1.622306964
6	-8.427292775	-0.903003694	1.554228992
6	-9.659242534	-0.213707670	1.689169220
7	-7.199185961	1.288094604	1.816195998
1	-6.378028667	1.881827932	1.866749802
6	-9.641366176	1.242378926	1.893183582
6	-8.410587347	1.954532581	1.948889014
6	-8.409220349	3.348407975	2.132063469
6	-9.597615011	4.050061360	2.261087742
6	-10.818600637	3.365889704	2.212151375
6	-10.826334555	1.990124928	2.030535724
1	-7.454909406	3.868246463	2.162117045
1	-9.575328706	5.128076357	2.396224288
1	-11.755903381	3.906053177	2.308989684
1	-11.781361561	1.476924955	1.986358305
7	5.898267464	-0.851161403	-1.506947066
1	4.981149801	-0.414522539	-1.563043192
7	7.198150103	1.286847623	-1.816100242
1	6.376480781	1.879662890	-1.870513576
6	9.594167521	-3.012525319	-1.279772455
6	10.848885278	-0.956048676	-1.606358166
6	10.803232579	-2.333256683	-1.406591738
1	11.815810541	-0.470727564	-1.686711987

1	11.733680984	-2.890475503	-1.335518308
1	9.610893912	-4.083653376	-1.112943752
6	10.850771113	0.933750530	1.617727188
6	9.608390298	2.996781532	1.285938277
6	10.813307600	2.311191161	1.418292662
1	11.814699938	0.443263149	1.702561704
1	9.632577515	4.067818199	1.119682130
1	11.746946137	2.863708538	1.352382898
6	-9.595449510	-3.011205899	1.280589371
6	-10.849939423	-0.954811313	1.608331775
6	-10.804435348	-2.331942716	1.408122594
1	-11.816855421	-0.469486733	1.688756926
1	-11.734944921	-2.889061624	1.337081332
1	-9.612332671	-4.082254357	1.113287089
6	-10.849489031	0.936751179	-1.613783070
6	-9.607119548	2.999851572	-1.282132929
6	-10.812043407	2.314156571	-1.413817756
1	-11.813482586	0.446298970	-1.698252387
1	-11.745740496	2.866477844	-1.347000205
1	-9.630512252	4.070898896	-1.115858701

168
radical cation **6′**$^{+}$, -4234.74934

6	0.044001477	1.520921251	-1.317455953
6	1.198800767	0.775671281	-1.506571417
6	1.171300837	-0.635070575	-1.564424749
6	-0.073695852	-1.315304819	-1.462791577
6	-1.229579070	-0.553069813	-1.576390842
6	-1.201721456	0.857028109	-1.498565021
1	2.163046359	1.269481433	-1.438320589
1	-2.193866343	-1.052301569	-1.571807856
6	0.128422833	2.868692618	-0.647093290
1	-0.582416727	3.582816820	-1.070966390
1	1.135669637	3.269771957	-0.782665104
6	-0.171584544	2.759321599	0.922134079
1	-1.181049208	3.131965552	1.110140102
1	0.534381840	3.415397288	1.438534501
6	0.058702638	-1.498592000	1.270732665
6	1.209104058	-0.745464279	1.454577269
6	1.172309133	0.665093927	1.512799129
6	-0.077472334	1.336975134	1.416358063
6	-1.227658489	0.566955652	1.535168601
6	-1.190471305	-0.842987836	1.457826157
1	2.176356554	-1.232847064	1.382680382
1	-2.195440282	1.059311884	1.534545946
6	0.149648621	-2.845760431	0.600120305
6	-0.156078789	-2.738331657	-0.968188462
1	0.552722226	-3.389255403	-1.487194048
1	-1.163359772	-3.118597365	-1.152686489
1	-0.555295549	-3.564366002	1.026226423
1	1.159866811	-3.240342736	0.732723781

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6	-3.421434530	2.260331088	-1.315929900
6	2.387172028	-1.344890675	-1.492033081
6	3.432475992	-1.962016977	-1.352479795
6	-2.390611671	-1.579549241	1.377336924
6	-3.402746669	-2.260089471	1.293067164
6	2.384394625	1.381044830	1.437481816
6	3.429508102	1.998683206	1.298744556
6	-6.996671621	4.470897556	-1.078830328
6	-5.771886588	5.119381100	-0.942989445
6	-4.581573779	4.401823418	-1.020235282
6	-4.609505221	3.014740097	-1.225601332
1	-7.904144821	5.059722850	-1.014632266
1	-5.746115480	6.192028966	-0.778668231
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6	-7.090646089	3.085974979	-1.288327901
6	-5.870442351	2.346561516	-1.349236955
7	-5.878698569	0.986275772	-1.519696879
6	-8.382911352	2.402133683	-1.429500194
1	-4.953207638	0.565653269	-1.592563072
5	-7.093334353	0.235747675	-1.617862704
6	-8.402584704	0.992687224	-1.560929963
6	-9.619272973	0.275275030	-1.672036160
7	-7.130512662	-1.178727623	-1.786608637
1	-6.293374667	-1.747708067	-1.873192848
6	-9.572584499	-1.183885698	-1.790450954
6	-8.319895628	-1.874558522	-1.862459464
6	-8.283432042	-3.276150579	-1.995163704
6	-9.453812981	-4.007774551	-2.031101257
6	-10.693226989	-3.349863833	-1.944570329
6	-10.739956346	-1.970027305	-1.833092572
1	-7.316769047	-3.768836293	-2.052861476
1	-9.413661310	-5.089316300	-2.120616862
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1	-11.707393532	-1.485358670	-1.763954643
6	7.045080209	-4.054334217	-0.821833391
6	4.638208655	-2.669737288	-1.171590165
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6	5.832137413	-4.723688108	-0.698736385
1	7.961642794	-4.615331562	-0.686500118
1	3.681322039	-4.556673627	-0.792269648
1	5.821707275	-5.784100667	-0.467944597
6	5.886884385	-1.976174978	-1.284504959
6	7.116699128	-2.682210365	-1.115690495
6	8.399629406	-1.984828104	-1.247659358
5	7.083644145	0.128301272	-1.694353063
6	8.403040151	-0.601855849	-1.548586437
6	9.613217733	0.119063054	-1.699843184
6	8.298249487	2.219250173	-2.121579648
6	9.554872325	1.546147819	-2.010481450
6	10.719514577	2.317615955	-2.208898068
6	10.664732541	3.672740606	-2.483321080

6	9.420851787	4.321215497	-2.569039861
6	8.254603083	3.601390374	-2.390412358
1	11.689186987	1.837722254	-2.140241347
1	11.582872695	4.233170796	-2.628970636
1	9.371901561	5.385518667	-2.778477881
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168
diradical dication **6′**$^{2+}$, -4234.57581

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