Supporting Information

Role of Exciton Delocalization in Chiroptical Properties of Benzothiadiazole Carbon Nanohoops

Kovida Kovida[1], Juraj Malinčík[1,3], Carlos M. Cruz[2], Araceli G. Campaña[2], Tomáš Šolomek[1,3*]

[1]Van't Hoff Institute for Molecular Sciences (HIMS), University of Amsterdam, PO Box 94157, 1090 GD Amsterdam, The Netherlands

[2]Department of Organic Chemistry, University of Granada, Avda Fuentenueva, s/n, 18071 Granada, Spain

[3]Prievidza Chemical Society, M. Hodžu 10/16, 971 01 Prievidza, Slovakia

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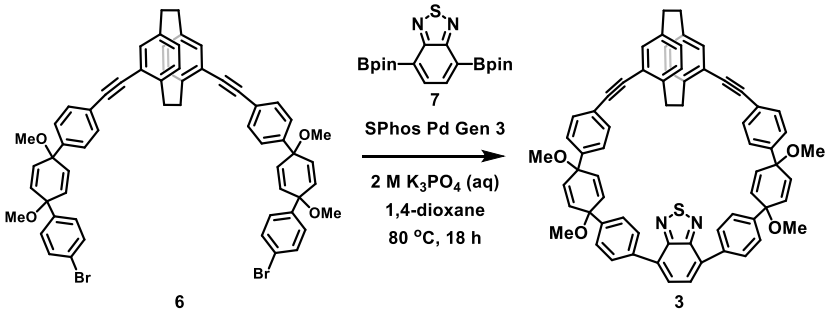
1. General Experimental Details

All reagents and solvents were used as received without further purification, unless stated otherwise. All commercially available reagents and chemicals were purchased from Sigma Aldrich, TCI, Fluorochem and Fisher Scientific and, if applicable, kept under argon atmosphere. Anhydrous solvents were purchased from Acros and stored under molecular sieves (4 Å). Technical solvents were bought from VWR International and Biosolve, and were used as received. All glassware were oven dried and cooled under an inert atmosphere using Schlenk techniques. Column chromatography was performed using silica (60, F254, Merck™). TLC analysis was performed using Silica TLC plates (F254, Supelco Sigma-Aldrich™) with visualization under ultraviolet light (254 nm and 365 nm). Recycling gel permeation chromatography (GPC) and chiral high-performance liquid chromatography (HPLC) were performed on LaboAce 5060 from Japan Analytical Industry using JAIGEL-2HR Plus (20x600mm) and Chiralpak IG (20x250mm) as columns, respectively, and an appropriate solvent. Analytical HPLC analysis was performed on a Shimadzu Prominence LC10-AT system equipped with a diode array detector (DAD) and Chiralpak IG column (4.6x250mm). ^{1}H (400 MHz), ^{13}C (100 MHz) spectra were recorded unless stated otherwise at ambient temperature using a Bruker AV II 400 spectrometer and analysed using MestReNova software. Chemical shifts (δ) in the ^{1}H NMR spectra are reported in parts per million (ppm) relative to $CDCl_3$ (7.26 ppm) and all ^{13}C NMR spectra are reported in ppm relative to $CDCl_3$ (77.16 ppm) unless stated otherwise. High resolution mass spectra (HRMS) were collected on an AccuTOF LC, JMS-T100LP Mass spectrometer (JEOL, Japen). UV-Vis absorption spectra were recorded on the spectrophotometer Shimadzu UV2700 equipped with a deuterium lamp (190-350 nm), a halogen lamp (330-900 nm) and a photomultiplier (Hamamatsu R928). Emission spectra were recorded with Horiba Jobin Vyon Fluorolog-3 spectrofluorometer in an appropriate solvent.

2. Synthetic Procedures and Characterization

Compounds **4-6** were synthesized following the literature protocols.[1,2] Spectral data matched the values reported in the literature. Compound **7** is commercially available.

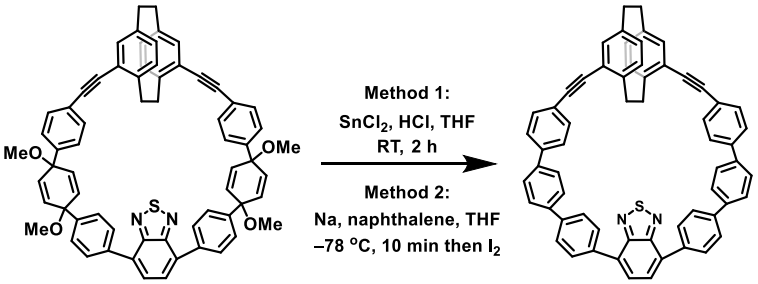


Experimental procedure for 3: To a 500 ml round-bottom flask, **6** (153 mg, 0.154 mmol, 1 equiv), **7** (63 mg, 0.161 mmol, 1.05 equiv) and SPhos Pd Gen 3 (12 mg, 0.015 mmol, 0.1 equiv) were added. The flask was evacuated and backfilled with argon five times. 1,4-dioxane and 2 M aq K_3PO_4 solution were sparged with Ar for 2 hours prior to use. To the reaction mixture, dioxane (200 ml) was added and the solution was sparged with Ar for another 1 hour. The reaction mixture was heated to 80 °C at which point the degassed K_3PO_4 solution (20 ml) was added dropwise. The reaction mixture was allowed to stir overnight at 80 °C. The solution was cooled down and filtered through celite and the flask was rinsed using ethyl acetate. The filtrate was washed with brine, dried over sodium sulfate and volatiles were removed under reduced pressure. The product was purified using silica gel chromatography (30% ethyl acetate in petroleum ether) and gel permeation chromatography (chloroform) to afford the product **4** as a green crystalline solid (34 mg, 23%).

^{1}H NMR (400 MHz, $CDCl_3$, 298 K, δ/ppm): 7.97 (d, *J* = 8.5 Hz, 4H), 7.84 (s, 2H), 7.56 (d, *J* = 8.4 Hz, 4H), 7.38 (d, *J* = 8.5 Hz, 4H), 7.24 (d, *J* = 8.3 Hz, 4H), 6.91 (d, *J* = 7.9 Hz, 2H), 6.59 (d, *J* = 1.8 Hz, 2H), 6.47 (dd, *J* = 7.9, 1.8 Hz, 2H), 6.33 (ddd, *J* = 10.4, 3.8, 2.4 Hz, 4H), 6.18 – 6.06 (m, 4H), 3.54 (m, 2H), 3.51 (s, 6H), 3.48 (s, 6H), 3.23 – 3.10 (m, 2H), 3.08 – 2.96 (m, 2H), 2.93 – 2.79 (m, 2H)**.**

^{13}C NMR (101 MHz, $CDCl_3$, 298 K, δ/ppm): 154.25, 142.78, 142.67, 139.56, 137.01, 135.80, 134.30, 134.22, 133.15, 132.93, 132.84, 132.18, 131.16, 131.05, 129.43, 128.35, 126.72, 126.32, 124.94, 122.98, 93.16, 89.81, 75.50, 75.26, 52.25, 52.06, 35.03, 33.48, 29.72.

HRMS (FD+): *m/z* calculated for $C_{66}H_{52}N_2O_4S$**:** 968.3648, found 968.3645.



3 2

Experimental procedure for 2:

Method 1: An H_2SnCl_4 solution was freshly prepared: $SnCl_2 \cdot 2H_2O$ (147 mg, 138 µmol) was suspended in THF (5 mL) and 37% aqueous HCl (100 µL) was added and the resulting mixture was stirred for 30 min. To a 50 ml round bottom flask, **3** (7 mg, 0.007 mmol, 1 equiv) was dissolved in 7 ml THF and H_2SnCl_4 solution (2 ml, 0.21 mmol, 0.122 M, 30 equiv) was added dropwise. The fluorescence of the solution changes from bright green to bright yellow. After completion of the reaction, the reaction mixture was quenched with 2M aqueous NaOH solution. The aqueous layer was extracted with dichloromethane and organic layers were combined and dried over sodium sulfate. The crude mixture was purified by column chromatography (SiO_2, 100% toluene) followed by gel permeation chromatography (Chloroform) to get an orange solid (3 mg, 60%).

Method 2: A 1 M sodium naphthalide solution was freshly prepared: naphthalene (473 mg, 3.8 mmol) was added in 3.8 ml of THF. To this, sodium (125 mg, 5.56 mmol) was added under argon and this was allowed to stir for 18 h. A dark green solution (sodium naphthalide, 1 M) is formed. To a 50 ml round bottom flask, **3** (6 mg, 0.006 mmol) was dissolved in 4 ml THF and was cooled to –78 °C and sodium naphthalide solution (0.4 ml, 1 M, 60 equiv) was added dropwise at this temperature. This was allowed to stir for 10 min before quenching it with 1 M solution of iodine in THF followed by sodium thiosulfate solution. The reaction mixture was extracted using dichloromethane and organic layers were combined and dried over sodium sulfate. The solvents were solvents were removed under reduced pressure. The crude was The crude mixture was purified by column chromatography (SiO_2, 100% toluene) followed by gel permeation chromatography (Chloroform) to get an orange solid (3.5 mg, 70%).

^{1}H NMR: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, δ/ppm): 7.99 (d, *J* = 8.5 Hz, 4H), 7.67 – 7.45 (m, 22H), 6.93 (d, *J* = 7.8 Hz, 2H), 6.54 (d, *J* = 1.8 Hz, 2H), 6.50 (dd, *J* = 7.8, 1.8 Hz, 2H), 3.34 – 3.21 (m, 2H), 3.19 – 3.04 (m, 2H), 2.90 – 2.71 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$, 298 K, δ/ppm): δ 154.82, 145.03, 140.37, 139.82, 139.47, 138.68, 138.60, 136.41, 133.84, 132.42, 131.79, 131.67, 131.57, 130.61, 127.97, 127.72, 127.42, 127.35, 127.25, 124.62, 122.64, 94.71, 92.99, 35.47, 33.51. (The nanohoop sample was kept at high vacuum for 8 h, however the solvent peaks could still not be removed leading to the visible signals in up field region of the spectrum, therefore, only the chemical shifts for the signals that belong to the compound are mentioned here)

HRMS (FD+): calculated for $C_{62}H_{40}N_2S$: 844.2912, found 844.2921

3. NMR and HRMS spectra

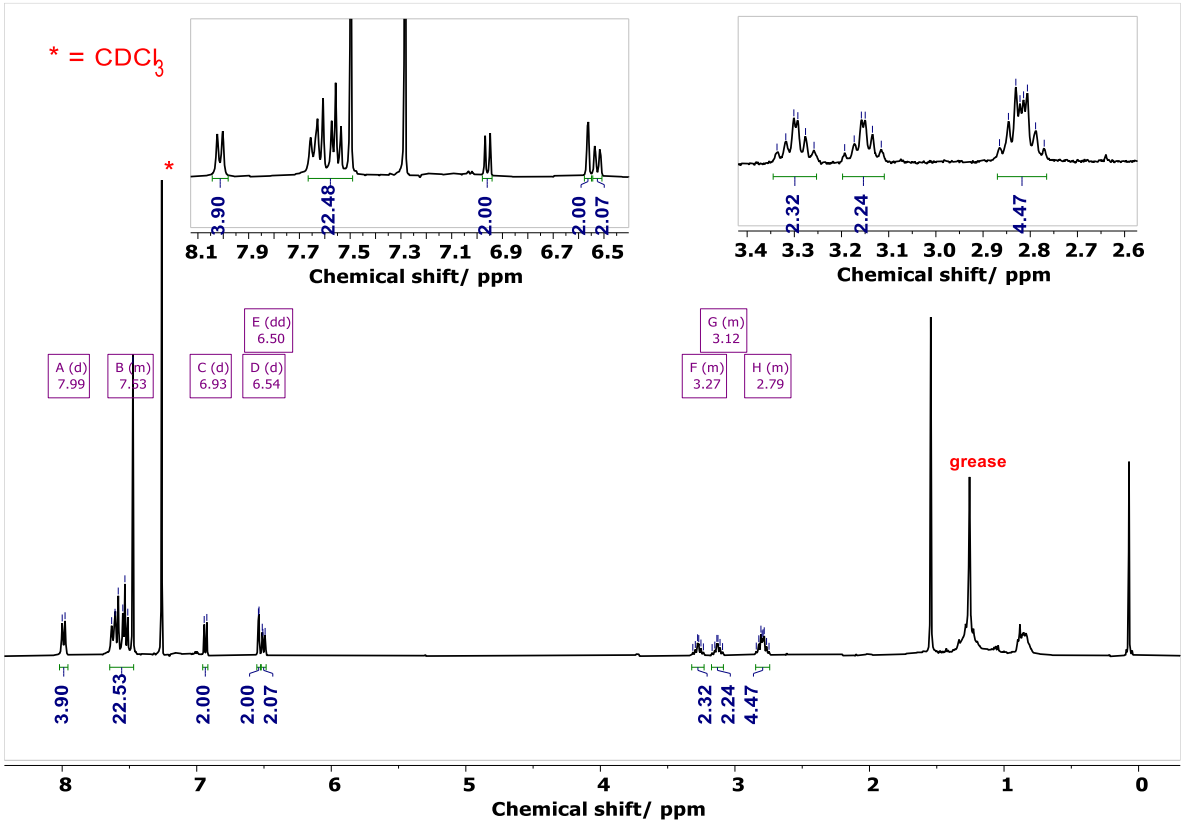


Figure S1. ^{1}H NMR spectrum of compound **2** in $CDCl_3$ recorded at 298 K.

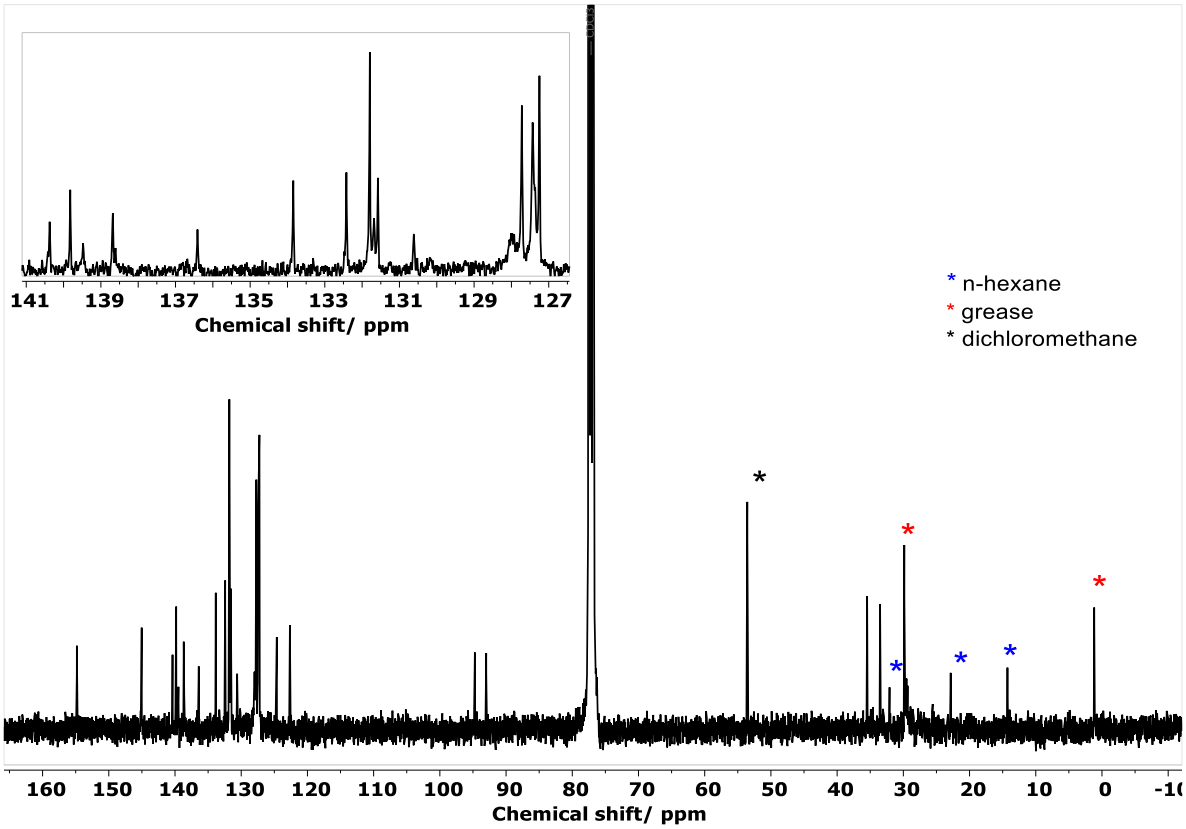


Figure S2. ^{13}C NMR spectrum of compound **2** in $CDCl_3$ recorded at 298 K.

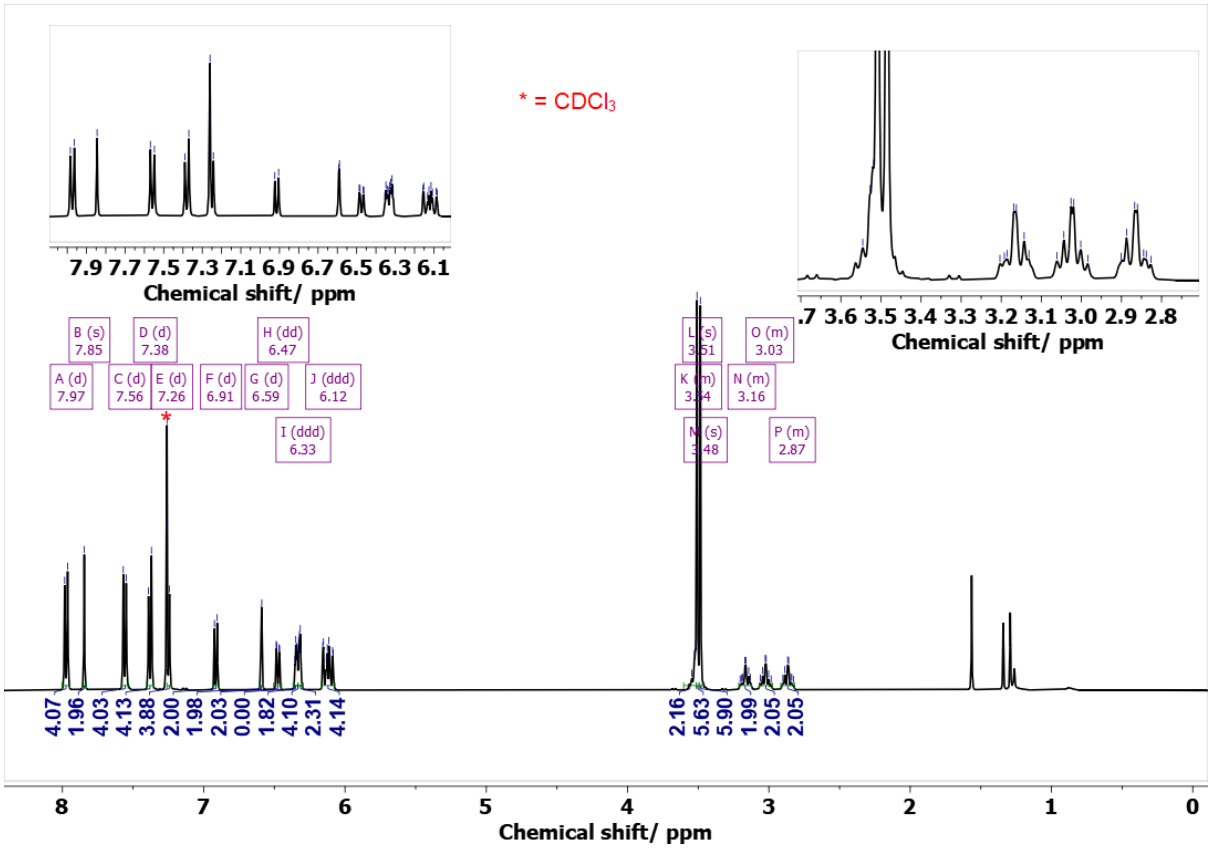


Figure S3. ^{1}H NMR spectrum of compound **3** in $CDCl_3$ recorded at 298 K.

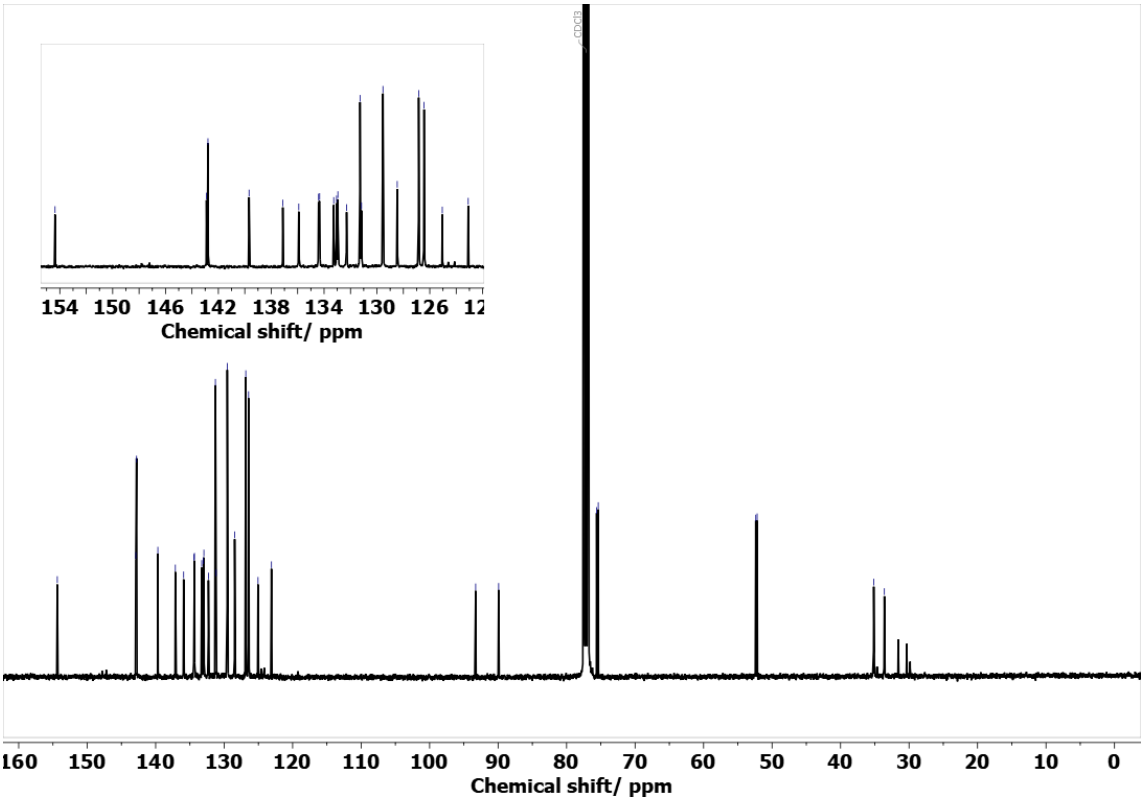


Figure S4. ^{13}C NMR spectrum of compound **3** in $CDCl_3$ recorded at 298 K.

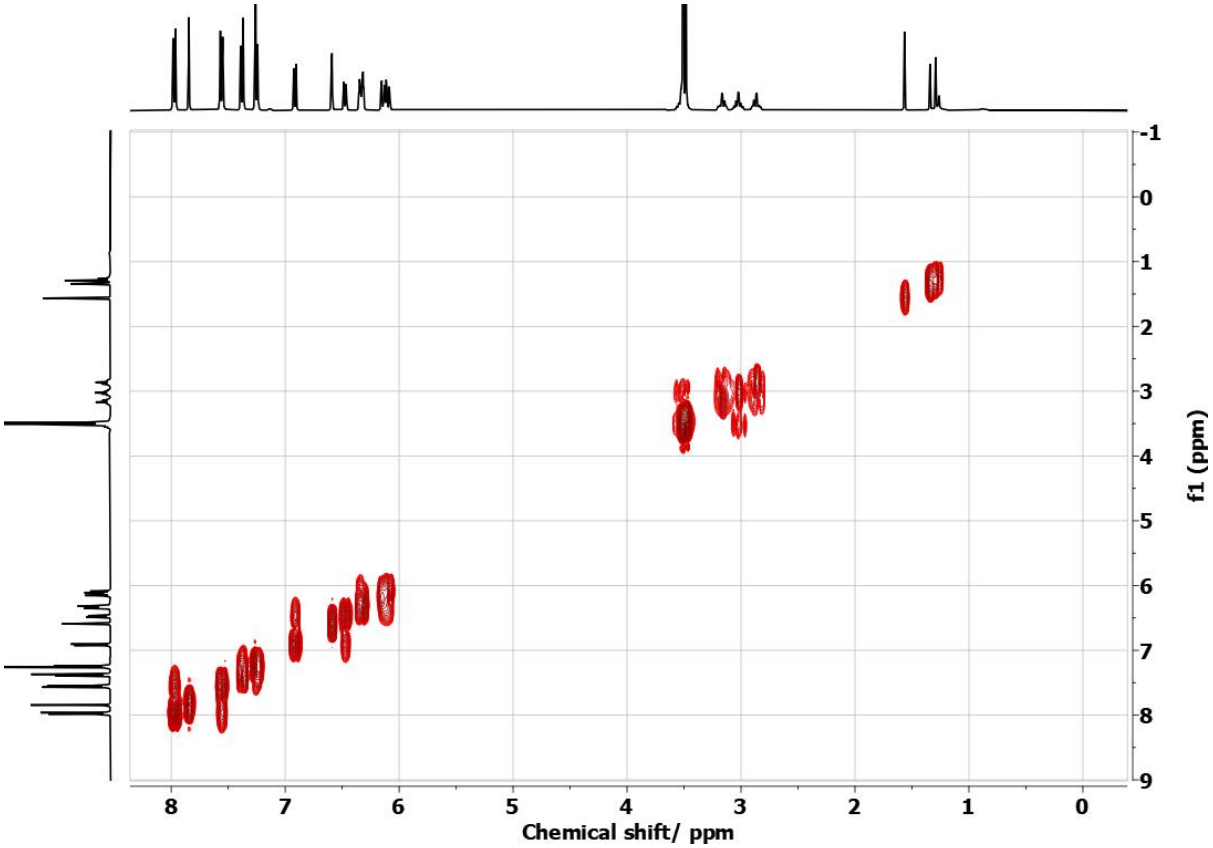


Figure S5. ^{1}H-^{1}H COSY spectrum of compound **3** in $CDCl_3$ recorded at 298 K.

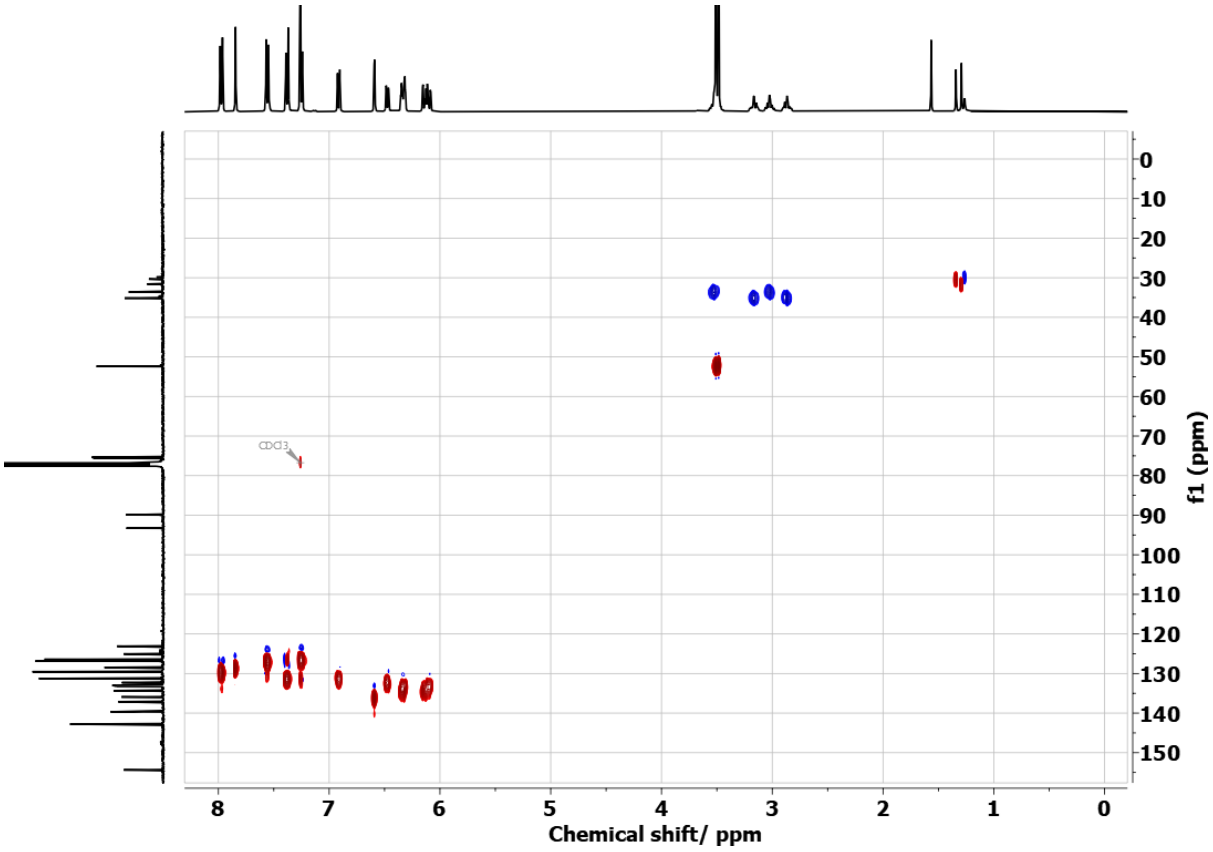


Figure S6. ^{1}H-^{13}C HSQC spectrum of compound **3** in $CDCl_3$ recorded at 298 K.

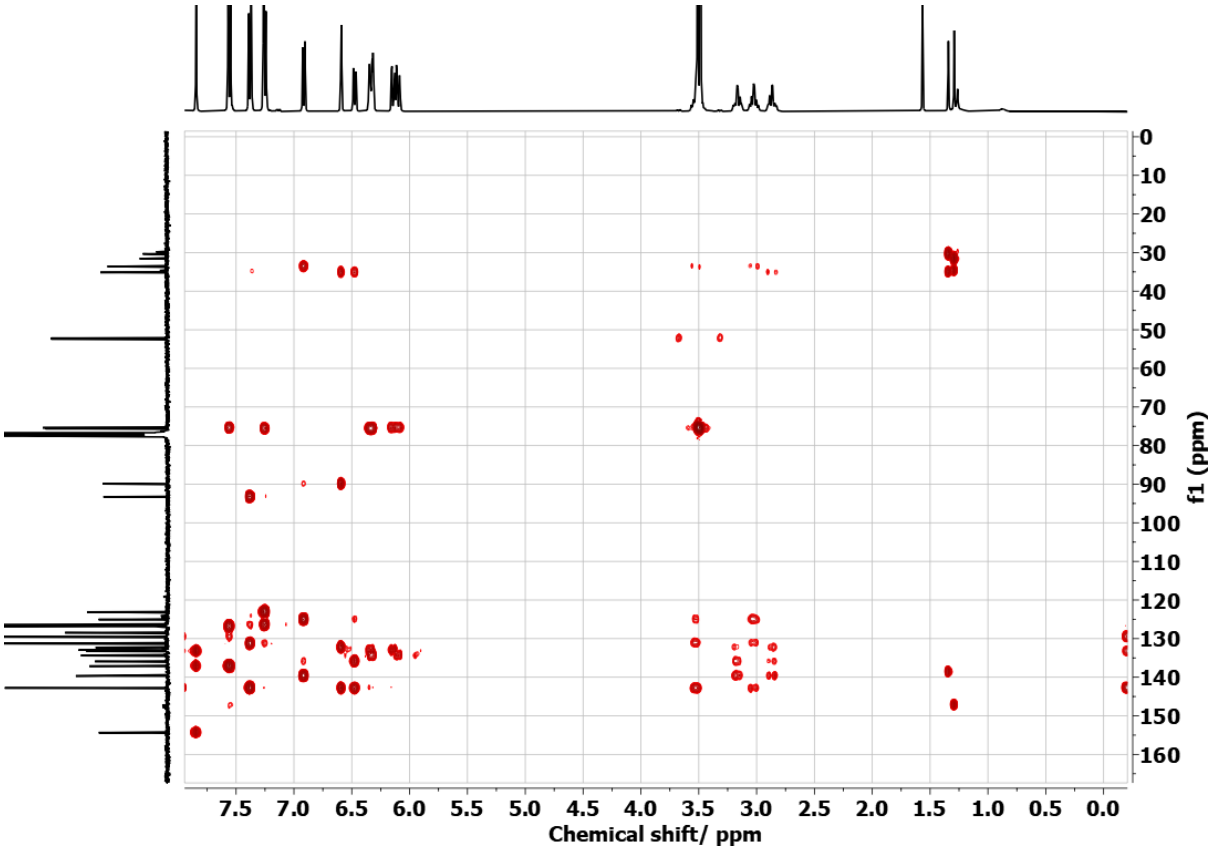


Figure S7. ^{1}H-^{13}C HMBC spectrum of compound **3** in $CDCl_3$ recorded at 298 K.

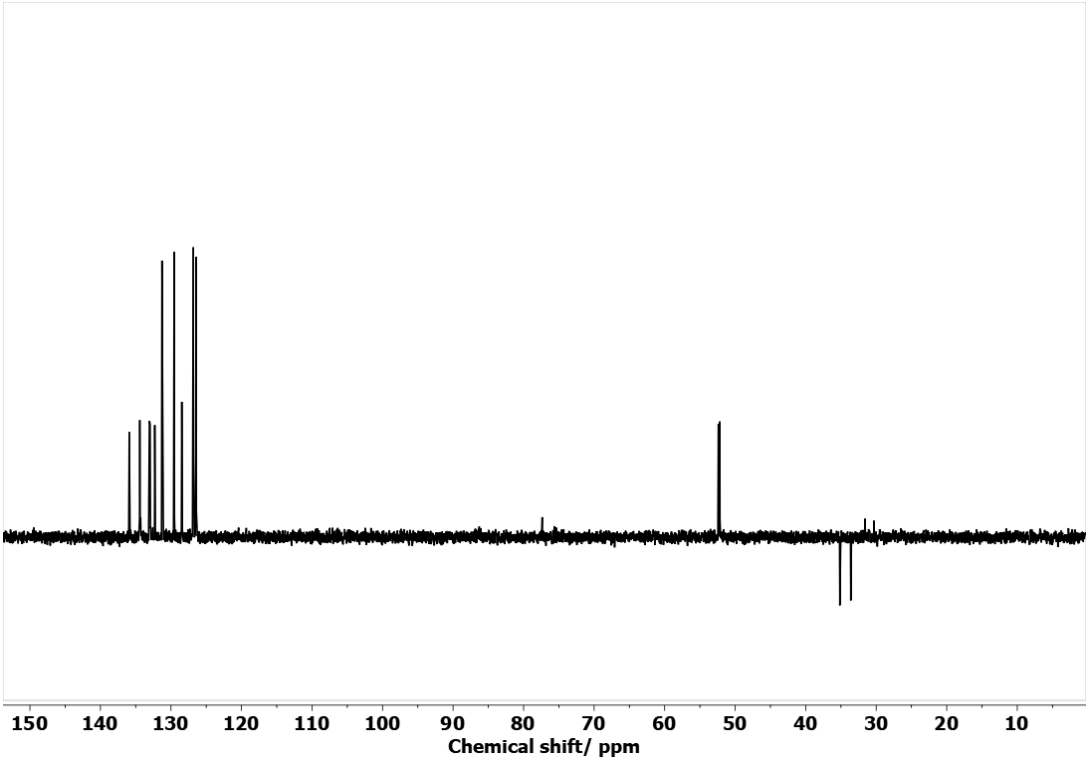


Figure S8. DEPT ^{13}C NMR spectrum of compound **3** in $CDCl_3$ recorded at 298 K.

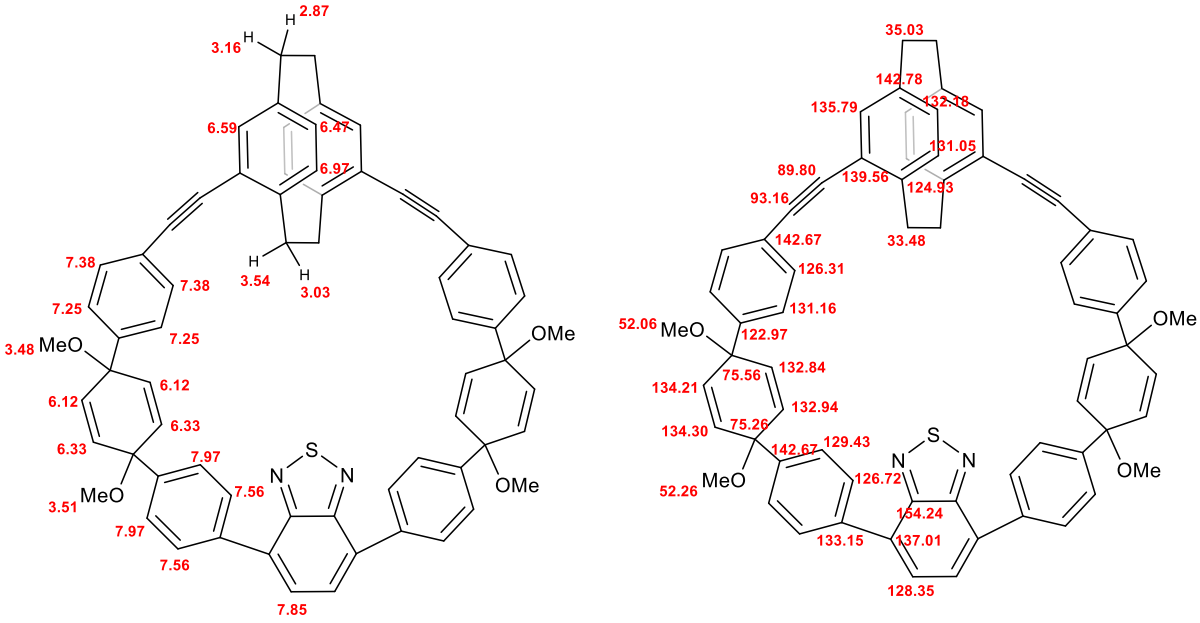


Figure S9. ^{1}H and ^{13}C NMR chemical shifts assignments of compound **3**

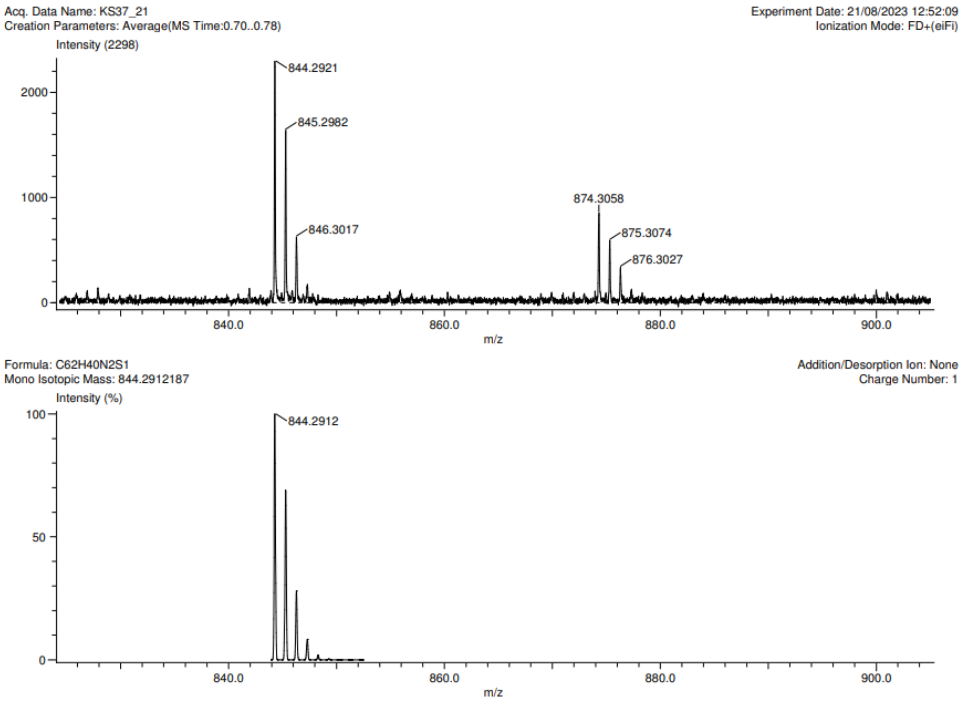


Figure S10. HRMS for compound **2**.

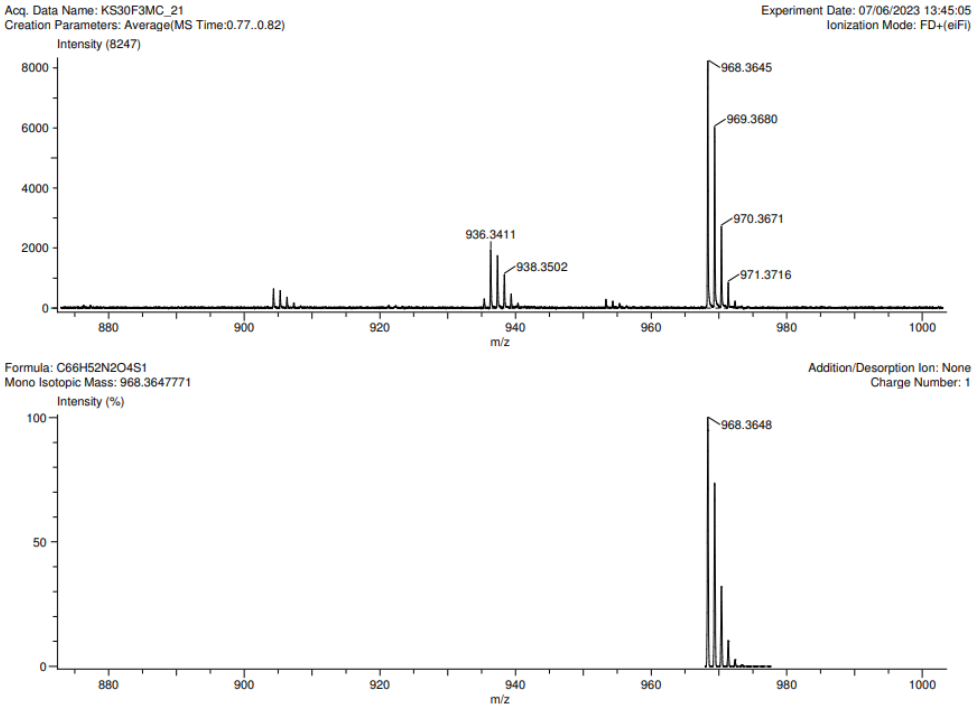


Figure S11. HRMS for compound **3**.

4. Photophysical Properties

We measured the photophysical properties of **2** and **3**. Excitation wavelength for all fluorescence measurements was 350 nm.

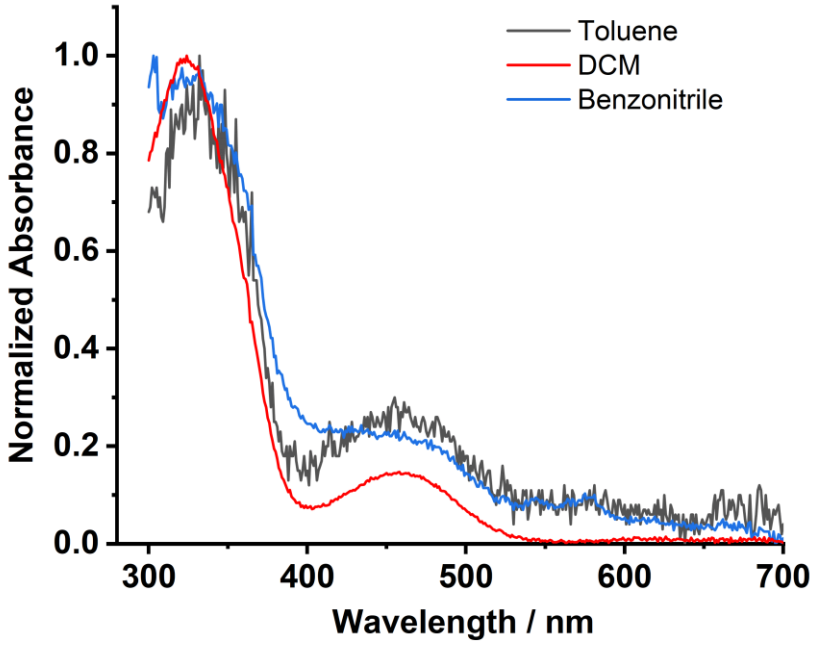


Figure S12. Absorption spectra of **2** in toluene (black), benzonitrile (blue) and dichloromethane (red).

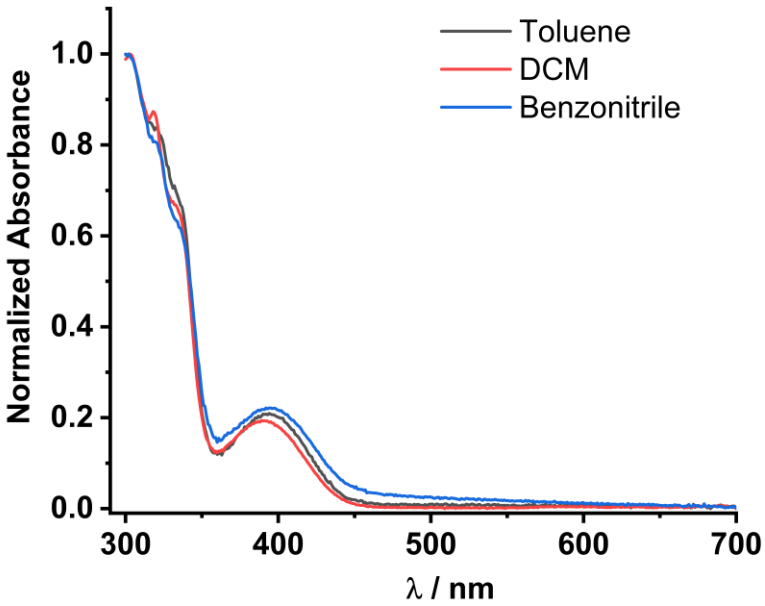


Figure S13. Absorption spectra of **3** in toluene (black), benzonitrile (blue) and dichloromethane (red).

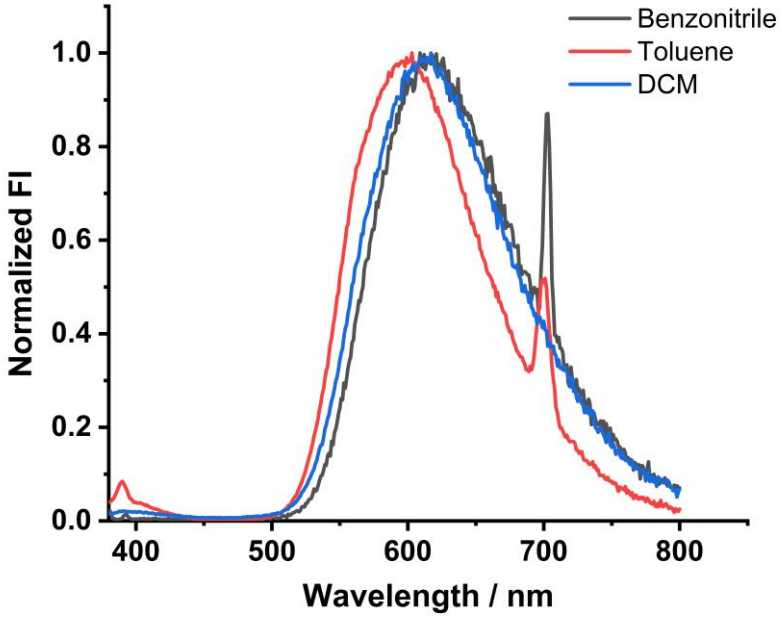


Figure S14. Fluorescence spectra of **2** in toluene (black), benzonitrile (blue) and dichloromethane (red).

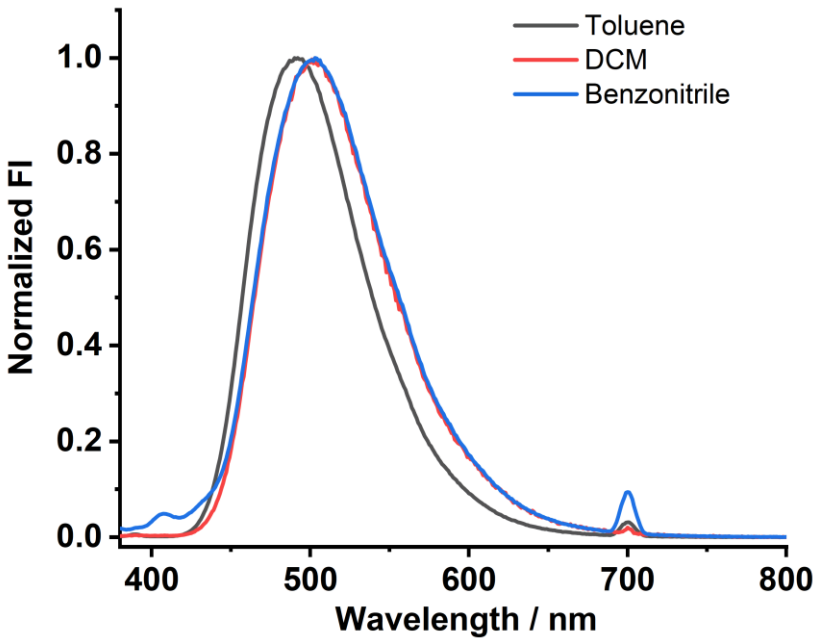


Figure S15. Fluorescence spectra of **3** in toluene (black), benzonitrile (blue) and dichloromethane (red).

Luminescence quantum yield measurements

Quantum yield of **2** (0.48) and **3** (0.70) was measured in dichloromethane using a relative quantum yield measurement method. [10]CPP in THF was used as a standard (QY = 0.46).[3] Excitation wavelength was 350 nm. The integrated fluorescence region for all three molecules was 450-900 nm. Gradient of the plot of integrated fluorescence intensity against absorbance was incorporated in the equation for the quantum yield calculation.

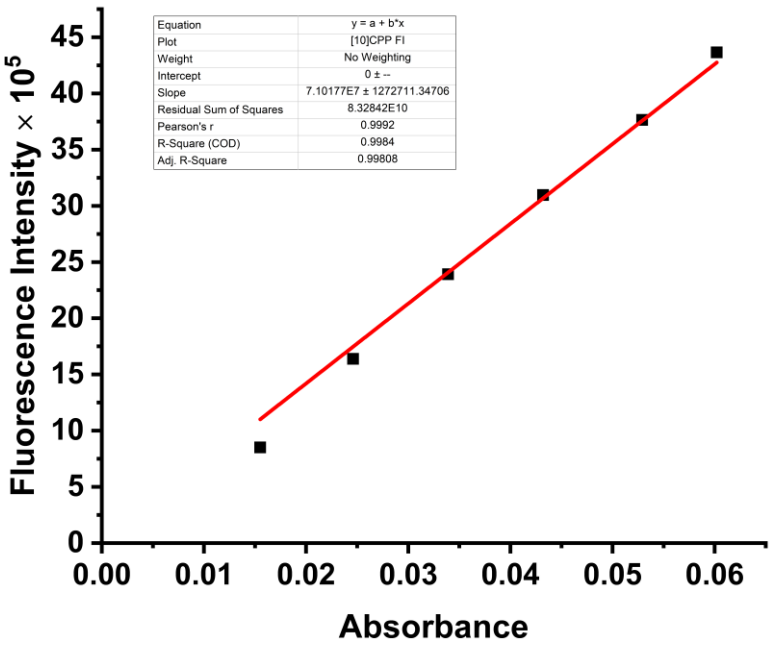


Figure S16. Integrated fluorescence intensity vs absorbance for [10]CPP.

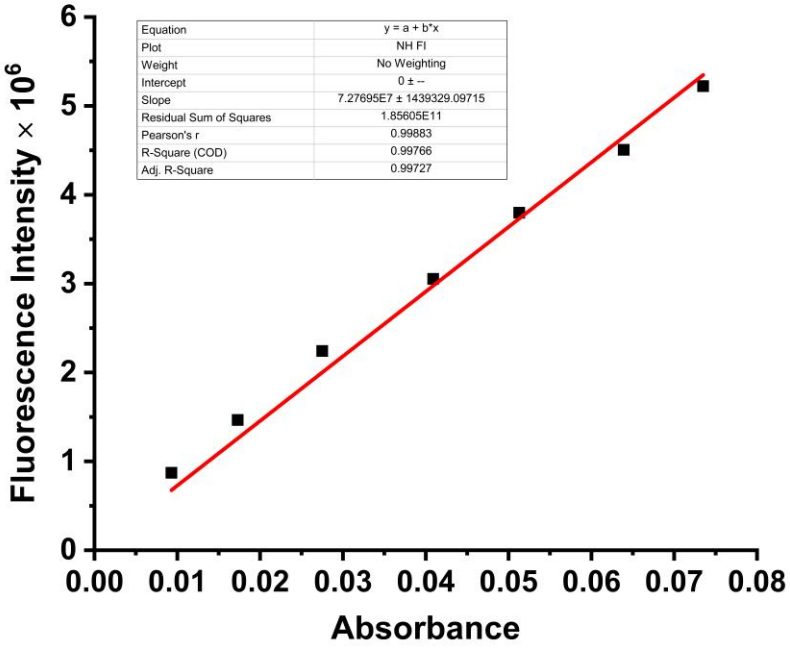


Figure S17. Integrated fluorescence intensity vs absorbance for **2**.

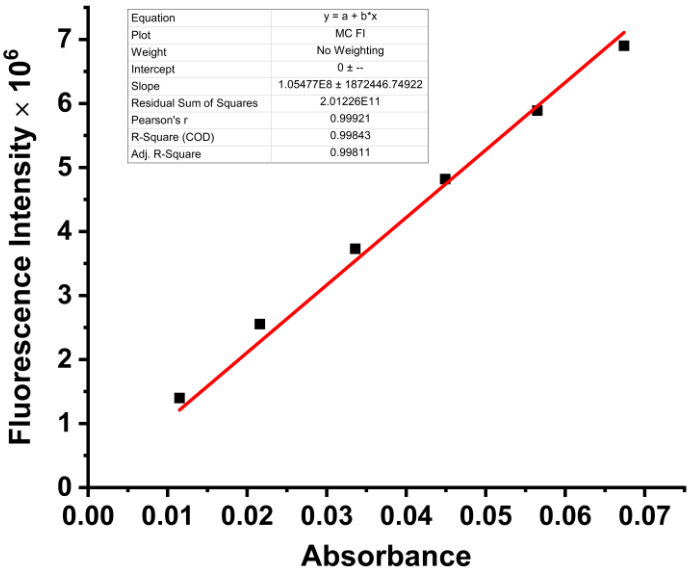


Figure S18. Integrated fluorescence intensity vs absorbance for **3**.

5. Chiral HPLC

Enantiomers of **2** and **3** were resolved on a preparative scale using recycling HPLC equipped with a Chiralpak IG (20x250mm) column by Daicel. For **2**, 50% DCM in *n*-heptane was used as an eluent at 20 mL min^{-1} flow rate. For **3**, toluene/TBME/*n*-heptane (v/v, 1:7:2) was used as an eluent at 15 mL min^{-1} flow rate. Due to poor enantiomer separation for **3** (Figure S20), both enantiomers were individually reinjected after the 1st run (Figure S21 and S22).

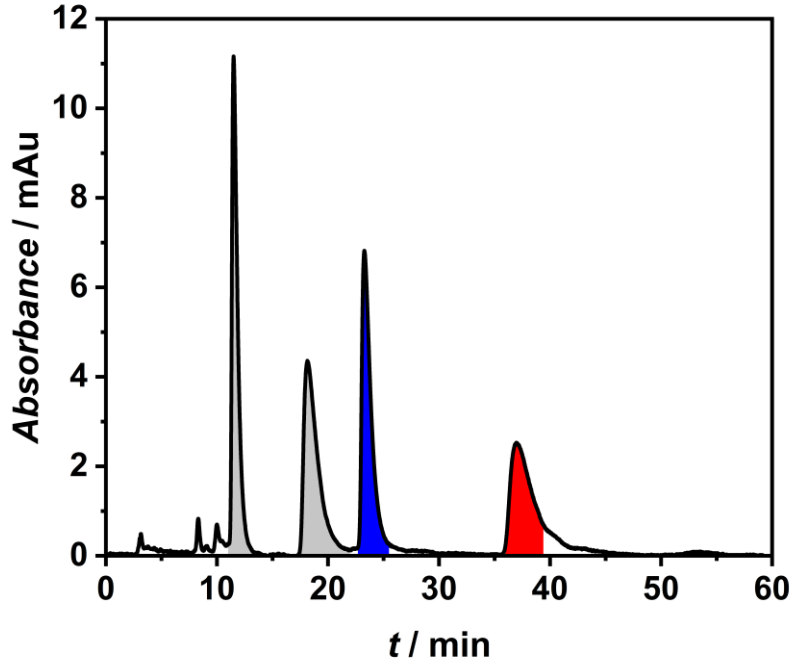


Figure S19. HPLC chromatogram of **2**. A racemate was injected and recycled (grey) until peak separation. Enantiomer 1 (blue) and enantiomer 2 (red) were collected in the 2nd cycle and correspond to (S_P)- and (R_P)-enantiomers, respectively.

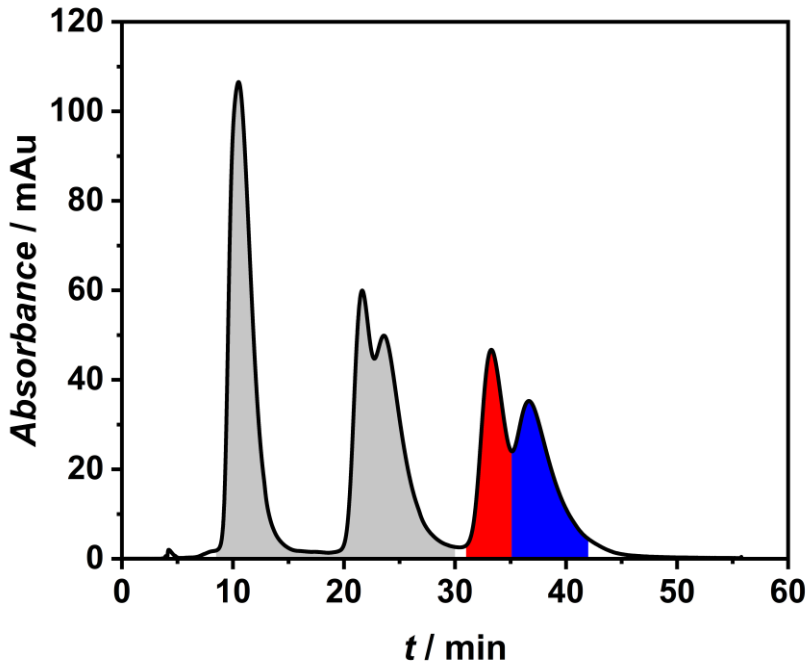


Figure S20. HPLC chromatogram of **3**. A racemate was injected and recycled (grey) until peak separation. Enantiomer 1 (red) and enantiomer 2 (blue) were collected in the 3rd cycle and correspond to (R_P)- and (S_P)-enantiomers, respectively.

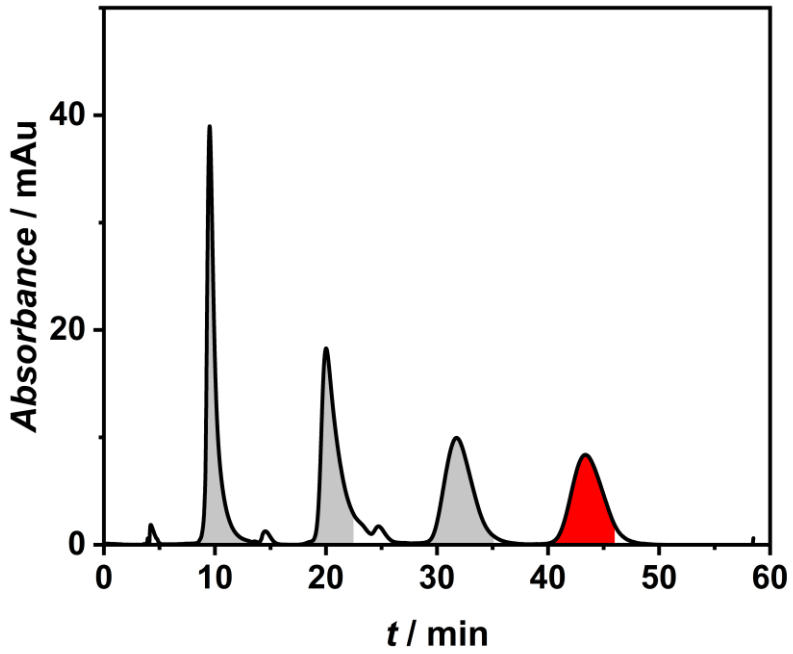


Figure S21. HPLC chromatogram of enantiomer 1 reinjection for **3**. The peak was recycled (grey) for 3 times before collection (red) and corresponds to (R_P)-enantiomer. The sample was then reinjected to analytical HPLC to confirm its purity.

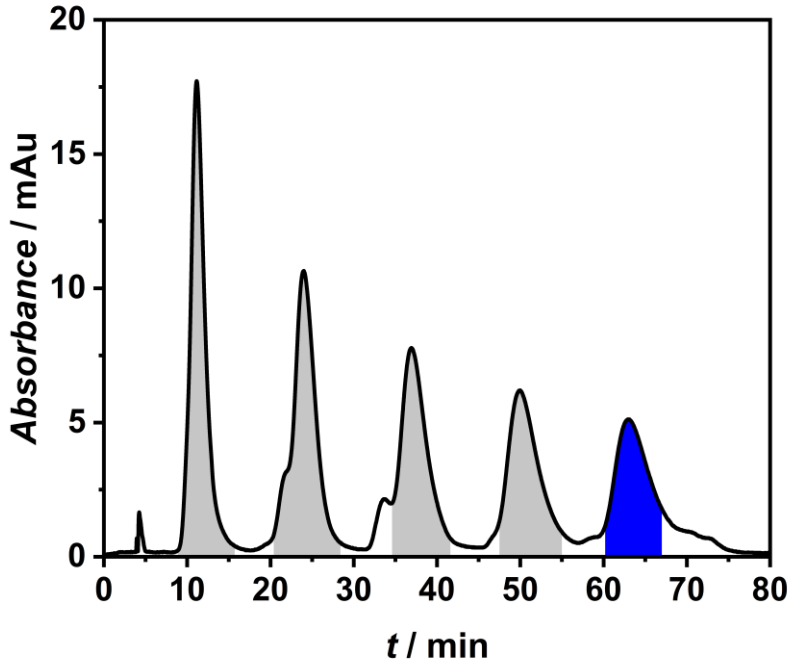


Figure S22. HPLC chromatogram of enantiomer 2 reinjection for **3**. The peak was recycled (grey) for 4 times before collection (blue) and corresponds to (S_P)-enantiomer. Two fractions of the blue region were collected, the second when the UV intensity reached the maximum to ensure the enantiomeric purity of the sample. The second collected sample was reinjected on analytical HPLC to confirm purity (see Figure S58–S61) and was used for the measurements of the chiroptical properties.

6. Chiroptical Properties

Circular dichroism (CD) and circularly polarized luminescence (CPL) spectra of **2** and **3** were measured in dichloromethane. CPL signal of **3** was too weak to measure spectra of higher quality as it was close to detection limit of the instrument.

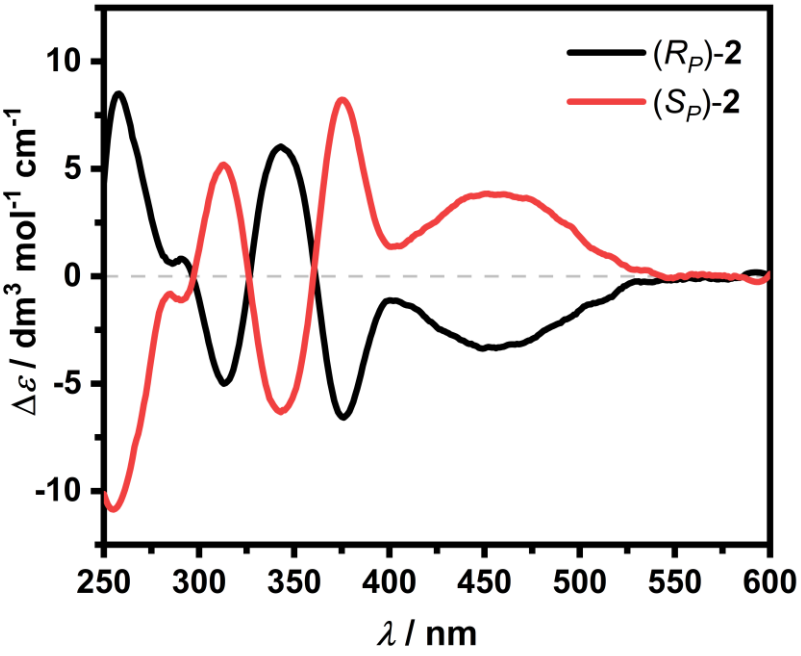


Figure S23. CD spectra of **2**.

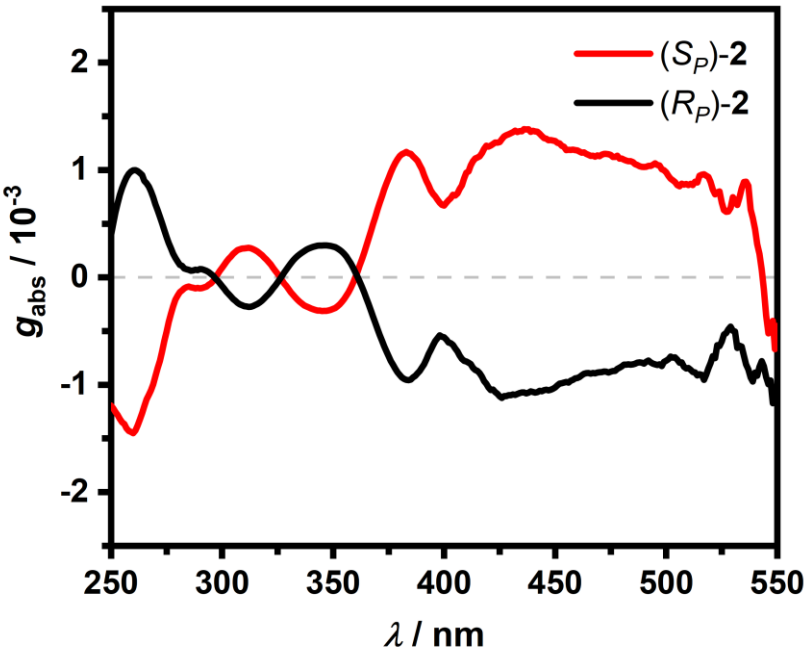


Figure S24. g_{abs} plot of **2**.

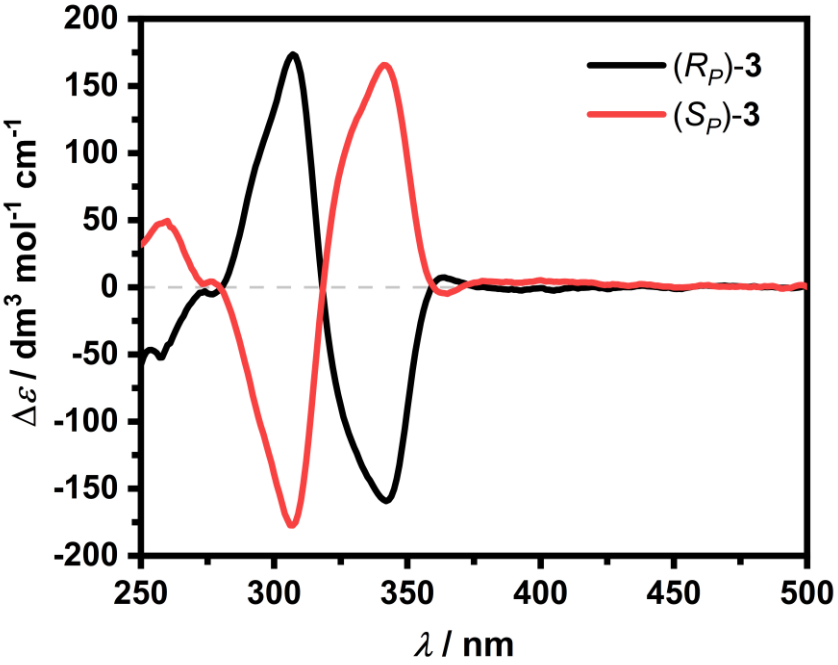


Figure S25. CD spectra of **3**.

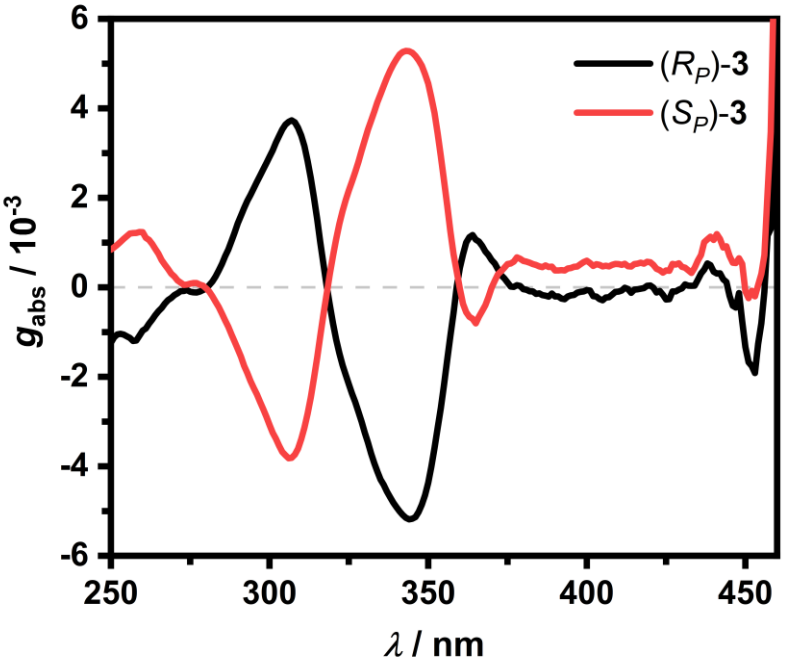


Figure S26. g_{abs} plot of **3**.

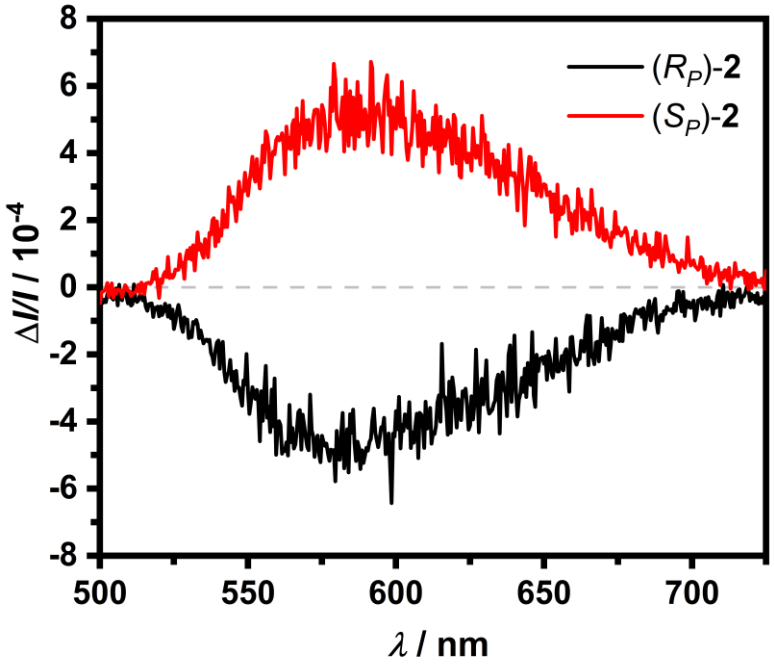


Figure S27. CPL spectra of **2**.

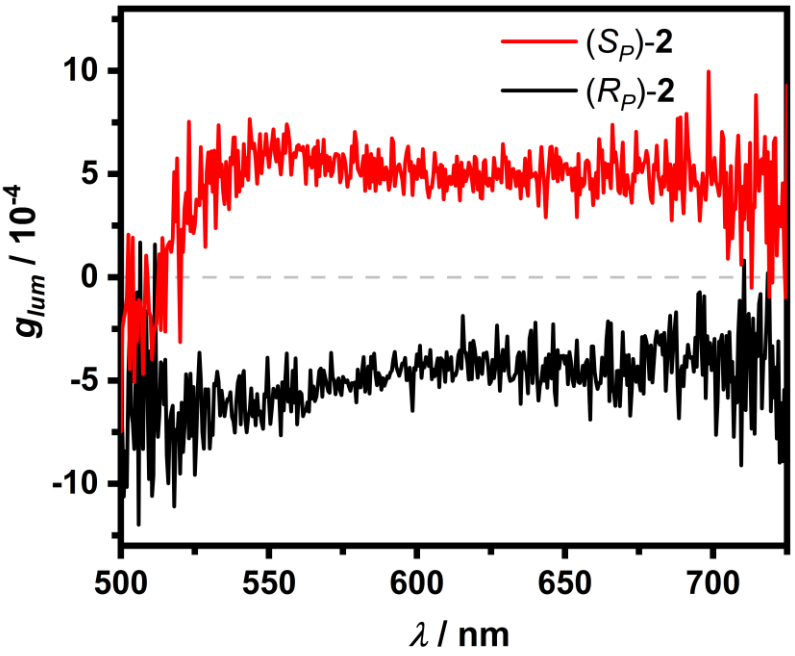


Figure S28. g_{lum} plot of **2**.

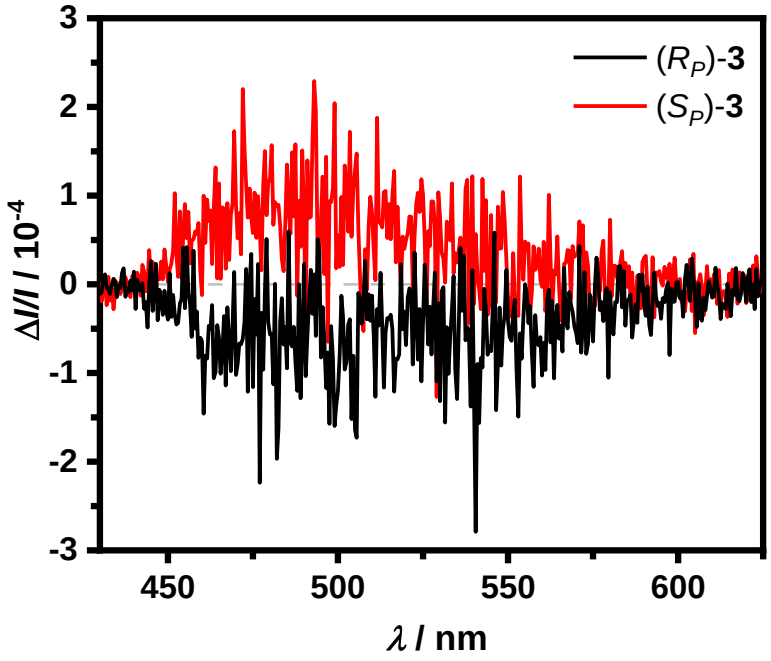


Figure S29. CPL spectra of **3**.

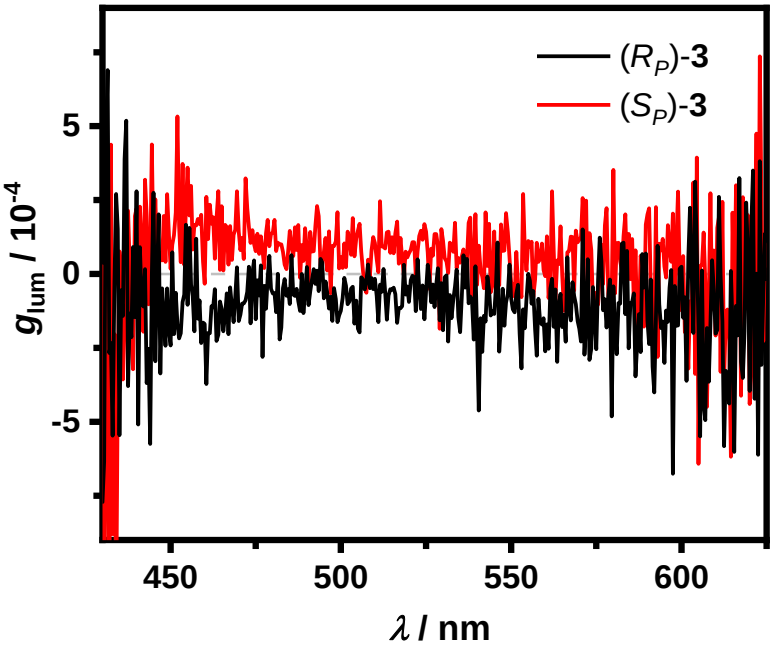


Figure S30. g_{lum} plot of **3**.

7. DFT Calculations

Calculations were performed with Gaussian 09[4] (release D.01) software. The geometries of the potential energy surface minima were optimized at D3-B3LYP/6-31g(d) level of theory. In a subsequent frequency calculation, all of the vibrational frequencies were real, confirming the character of found stationary points as minima. UltraFine integration grid was used in all calculations. CAM-B3LYP/6-31g(d) was used for time dependent calculations and to optimize the geometries of the excited states. To simulate CD spectra, first 10 transitions were calculated. Empirical vibrational broadening of 0.3 and 0.2 eV was used for **2** and **3**, respectively, and the calculated spectra were shifted by –0.2 eV for both. The velocity form of the rotatory strength was used.

Table S1. Electronic transitions and their respective energies (*E*), wavelengths (*λ*), oscillator strengths (*f*) and orbital contributions for **2**.

Transition	*E* / eV	*λ* / nm	*f*	Orbital contributions[a]
1	2.9181	424.88	0.3393	HOMO→LUMO (82%)
2	3.9212	316.19	0.0266	HOMO→LUMO+1 (44%) HOMO-1→LUMO+2 (16%)
3	3.9484	314.01	1.2119	HOMO-1→LUMO (48%) HOMO-3→LUMO (16%) HOMO-6→LUMO (12%)
4	4.2212	293.72	0.5349	HOMO-1→LUMO+1 (25%) HOMO-3→LUMO+3 (14%) HOMO→LUMO+2 (12%)
5	4.3199	287.01	0.5691	HOMO-2→LUMO+1 (18%) HOMO→LUMO+2 (13%)

[a]Only the contributions larger than 10% are listed.

Table S2. Electronic transitions and their respective energies (*E*), wavelengths (*λ*), oscillator strengths (*f*) and orbital contributions for **3**.

Transition	*E* / eV	*λ* / nm	*f*	Orbital contributions[a]
1	3.3321	372.09	0.3268	HOMO-2→LUMO (94%)
2	3.9473	314.1	0.9212	HOMO→LUMO+1 (74%) HOMO-1→LUMO+2 (16%)
3	4.079	303.96	0.3218	HOMO-1→LUMO+1 (73%)
4	4.2262	293.37	0.0012	HOMO→LUMO (86%) HOMO-1→LUMO (12%)
5	4.3545	284.73	0.3258	HOMO→LUMO+2 (45%) HOMO-3→LUMO+1 (19%)

[a]Only the contributions larger than 10% are listed.

Table S3. Calculated energies (*E*), oscillator strengths (*f*), electric (*μ*) and magnetic (*m*) transition dipole moments, and angles (θ) between them, rotatory strengths (*R*, velocity form), dipole strengths (*D*) and calculated dissymmetry factor (g_{abs}) values for ground state geometries.

Compound (Transition)	*E* / eV	*f*	$\|\boldsymbol{\mu}\|$ / 10^{-18} esu·cm	$\|\boldsymbol{m}\|$ / 10^{-20} erg·G^{-1}	θ / °	*R* / 10^{-40} esu erg cm G^{-1}	*D* / 10^{-36} esu^2 cm^2 erg^2 G^{-2}	g_{abs} / 10^{-3}
R_P-**2** (S0 – S1)	2.9181	0.3393	5.54	5.78	91.69	-95.6253	30.66	-1.25
R_P-**2** (S0 – S2)	3.9212	0.0266	1.34	9.29	126.52	-746.8473	1.80	-166.24
R_P-**2** (S0 – S3)	3.9484	1.2119	9.00	0.73	45.92	450.5324	80.94	2.23
R_P-**3** (S0 – S1)	3.3321	0.3268	5.09	3.69	90.44	-14.3600	25.87	-0.22
R_P-**3** (S0 – S2)	3.9473	0.9212	7.84	6.27	102.88	-1075.3783	61.55	-6.99
R_P-**3** (S0 – S3)	4.0790	0.3218	4.56	1.68	18.09	710.5698	20.81	13.66

Table S4. Calculated energies (*E*), oscillator strengths (*f*), electric (*μ*) and magnetic (*m*) transition dipole moments, and angles (θ) between them, rotatory strengths (*R*, velocity form), dipole strengths (*D*) and calculated dissymmetry factor (g_{lum}) values for 1st excited state geometries.

Compound (Transition)	*E* / eV	*f*	$\|\boldsymbol{\mu}\|$ / 10^{-18} esu·cm	$\|\boldsymbol{m}\|$ / 10^{-20} erg·G^{-1}	θ / °	*R* / 10^{-40} esu erg cm G^{-1}	*D* / 10^{-36} esu^2 cm^2 erg^2 G^{-2}	g_{lum} / 10^{-3}
R_P-**2** (S1 – S0)	2.0811	0.3787	6.93	4.78	91.39	-82.9015	47.98	-0.69
R_P-**3** (S1 – S0)	2.6229	0.4367	6.63	3.20	90.49	-18.3871	43.91	-0.17

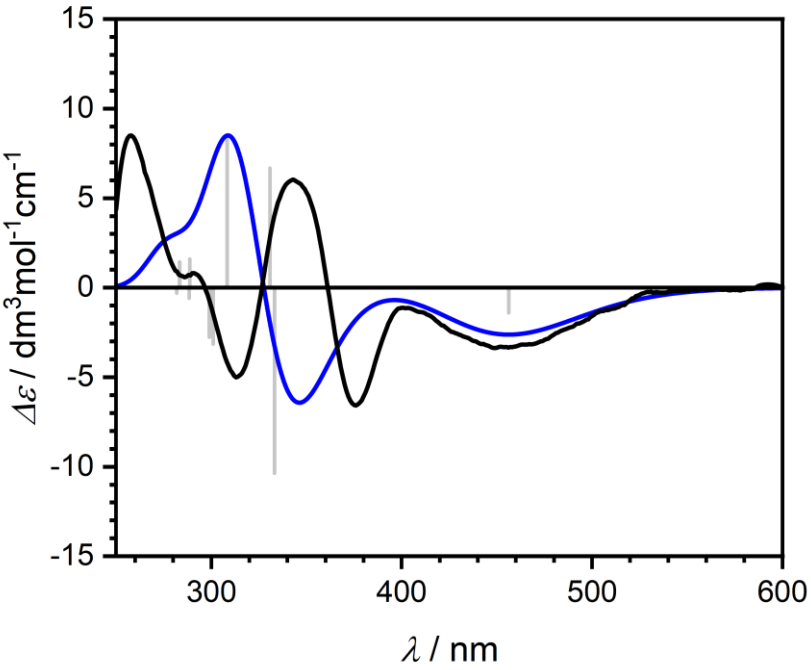


Figure S31. Experimental (black) and calculated (blue) CD spectra of (R_P)-**2** with excitation transitions (grey lines).

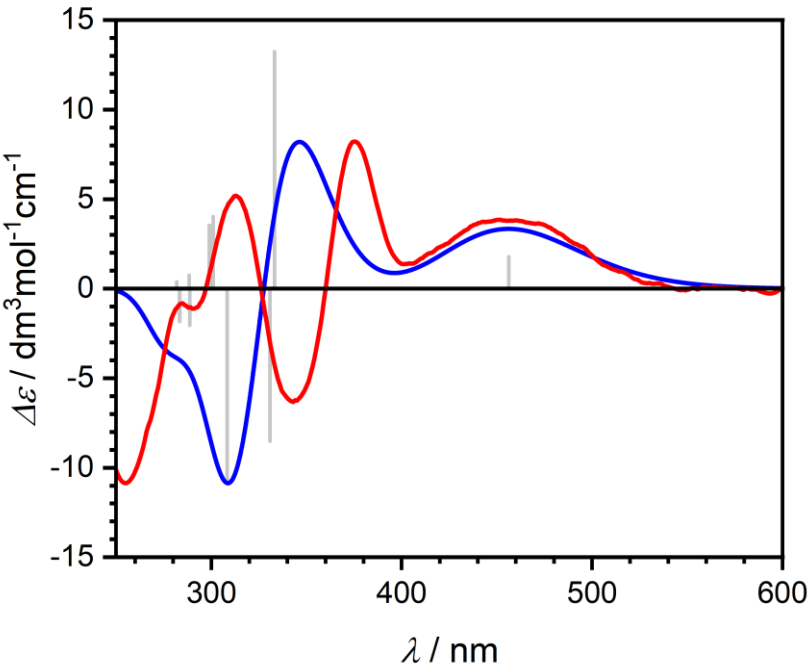


Figure S32. Experimental (red) and calculated (blue) CD spectra of (S_P)-**2** with excitation transitions (grey lines).

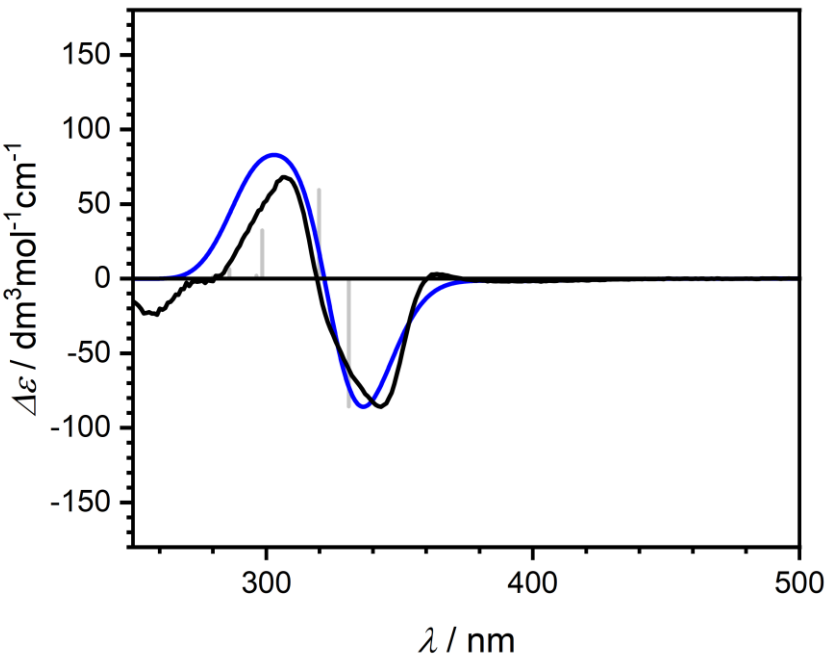


Figure S33. Experimental (black) and calculated (blue) CD spectra of (R_P)-**3** with excitation transitions (grey lines).

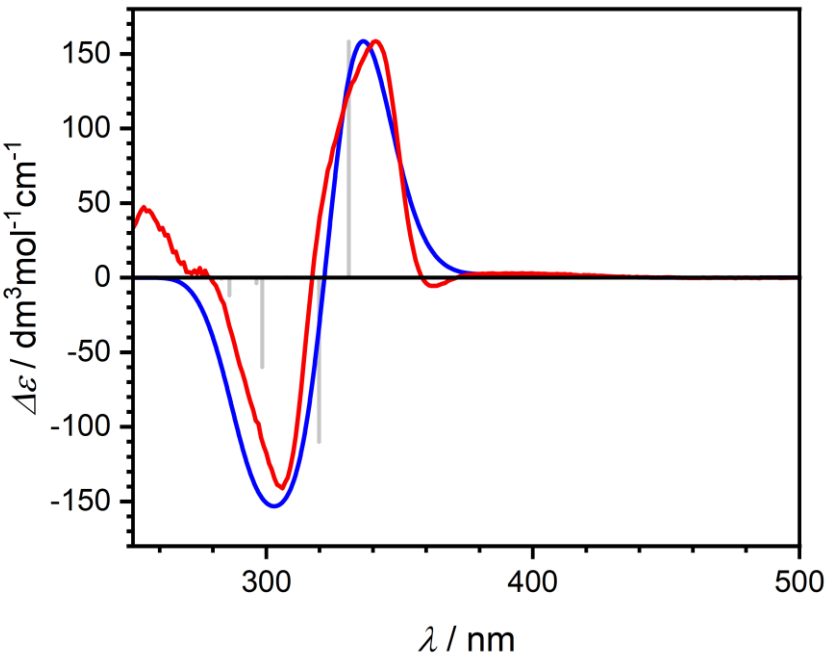


Figure S34. Experimental (red) and calculated (blue) CD spectra of (S_P)-**3** with excitation transitions (grey lines).

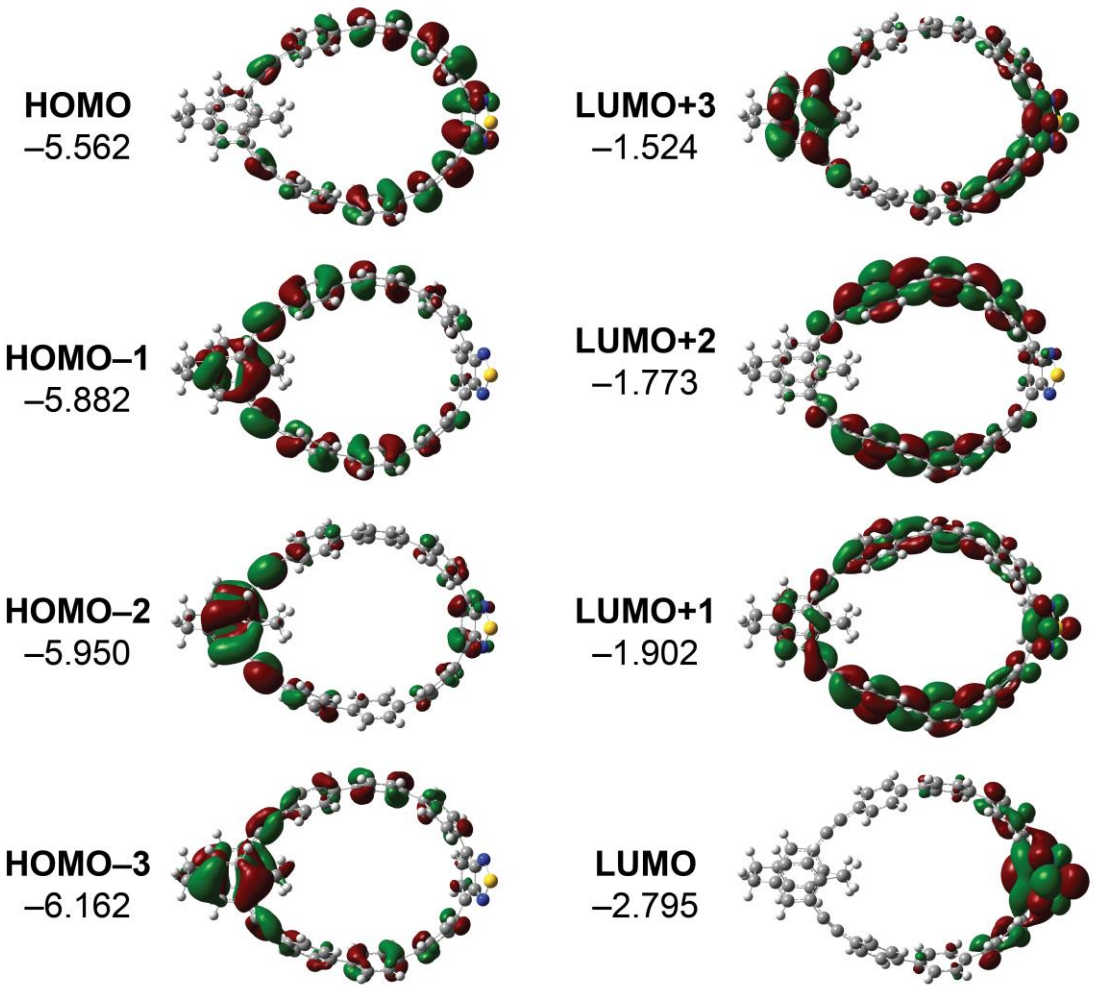


Figure S35. Frontier molecular orbitals of **2** with energies in eV.

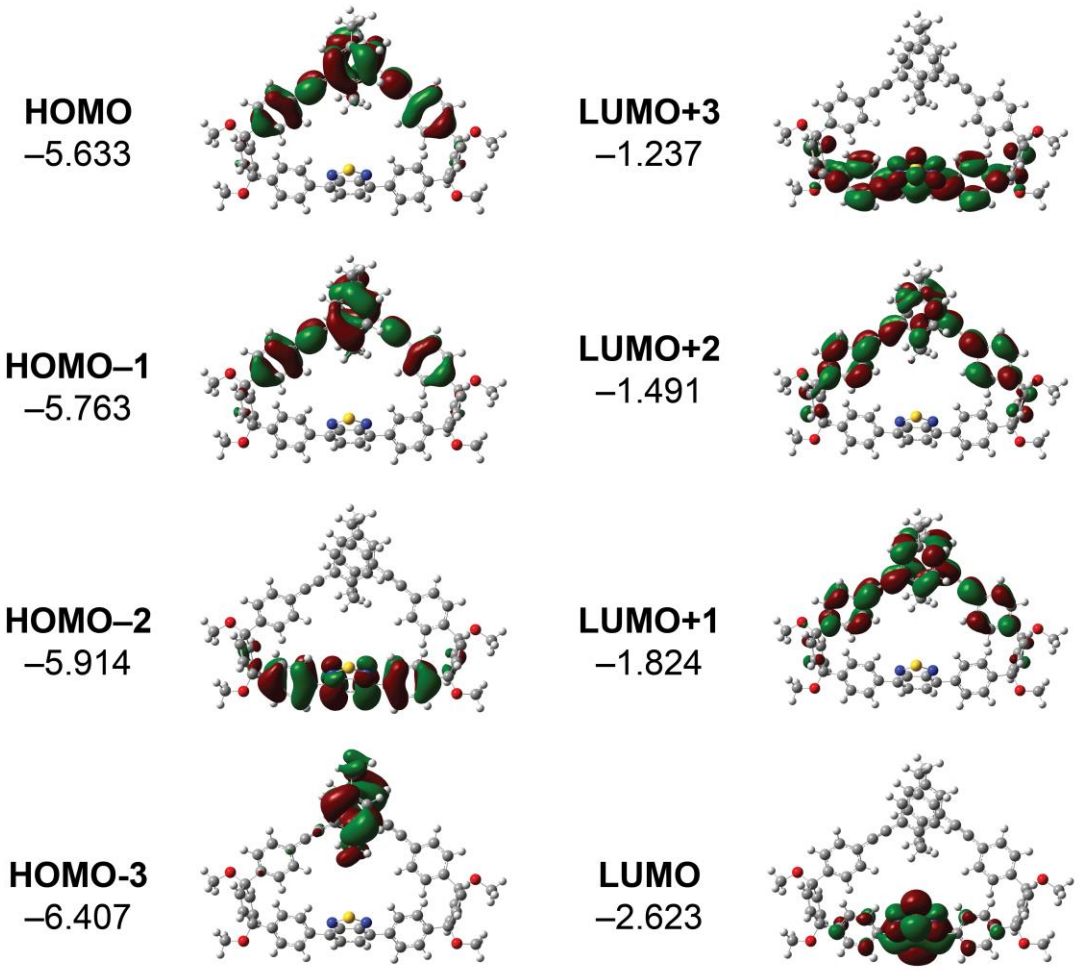


Figure S36. Frontier molecular orbitals of **3** with energies in eV.

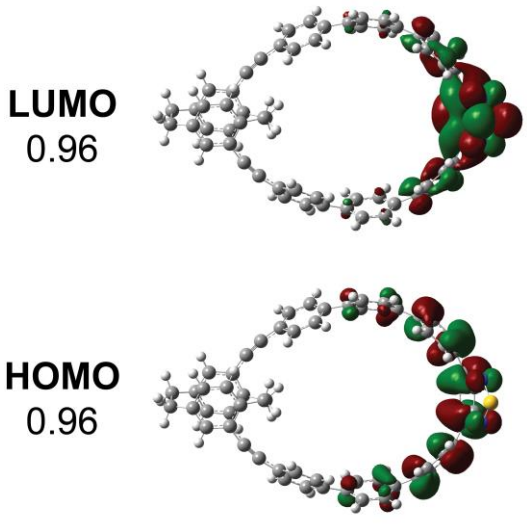


Figure S37. Natural transition orbitals and occupancies of the $S_0 \rightarrow S_1$ transition in **2**.

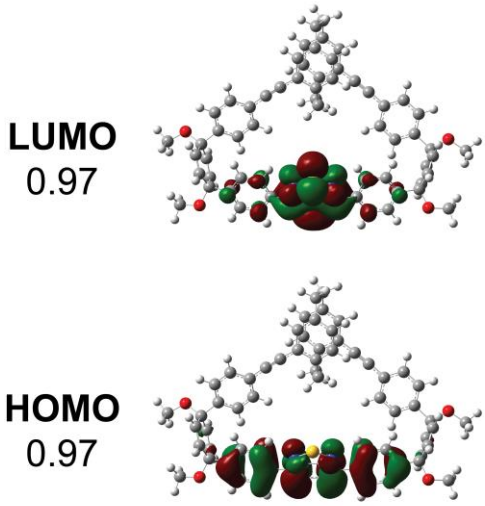


Figure S38. Natural transition orbitals and occupancies of the $S_0 \rightarrow S_1$ transition in **3**.

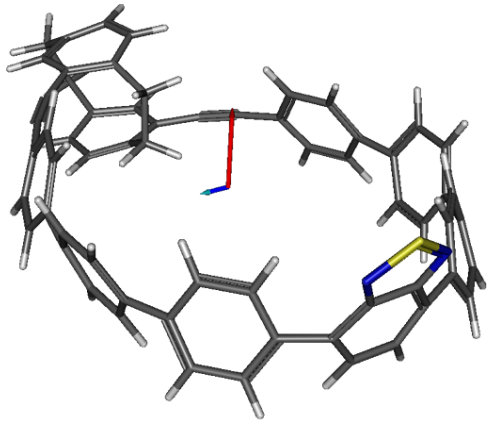


Figure S39. Electric (μ, blue) and magnetic (m, red) transition dipole moments of the $S_0 \rightarrow S_1$ transition in **2**. The vectors are scaled by a factor of 2 for visualization due to small size of μ.

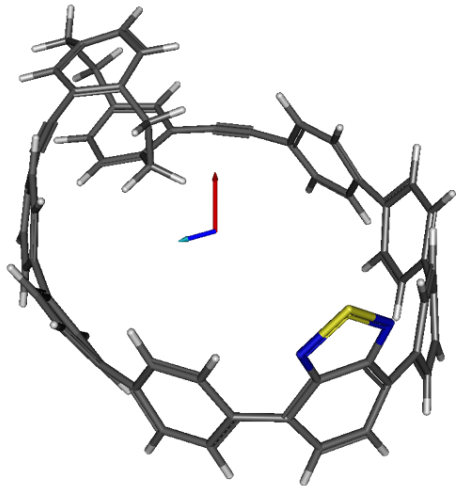


Figure S40. Electric (μ, blue) and magnetic (m, red) transition dipole moments of the $S_1 \rightarrow S_0$ transition in **2**. The vectors are scaled by a factor of 2 for visualization due to small size of μ.

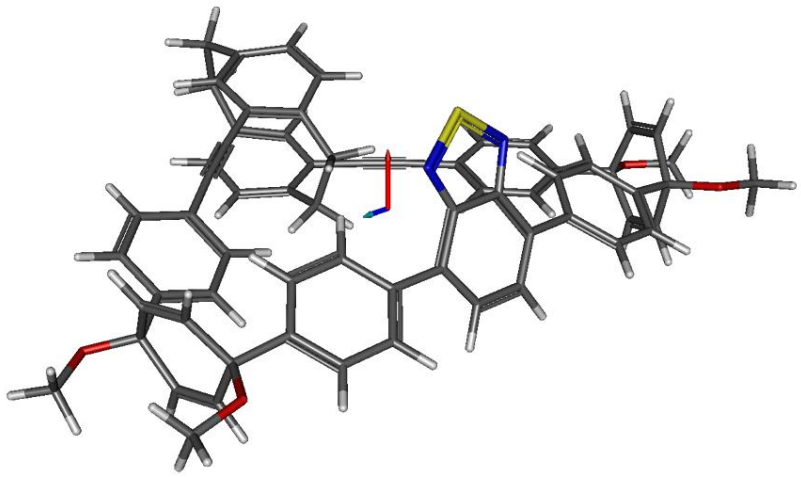


Figure S41. Electric (μ, blue) and magnetic (m, red) transition dipole moments of the $S_0 \rightarrow S_1$ transition in **3**. The vectors are scaled by a factor of 2 for visualization due to small size of μ.

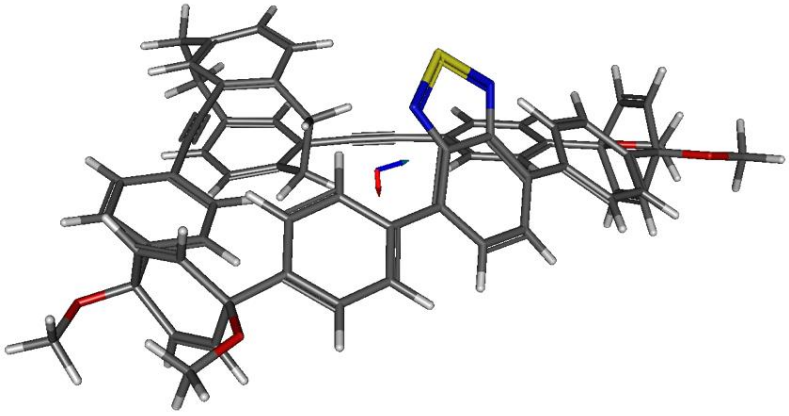


Figure S42. Electric (μ, blue) and magnetic (m, red) transition dipole moments of the $S_1 \rightarrow S_0$ transition in **3**. The vectors are scaled by a factor of 2 for visualization due to small size of μ.

The structure of **2** was modified with methoxy groups and the resulting structure **2'** was optimized at D3-B3LYP/6-31g(d) level of theory with the coordinates of all atoms frozen except of the cyclohexadiene moieties and added methoxy groups (Figure S43).

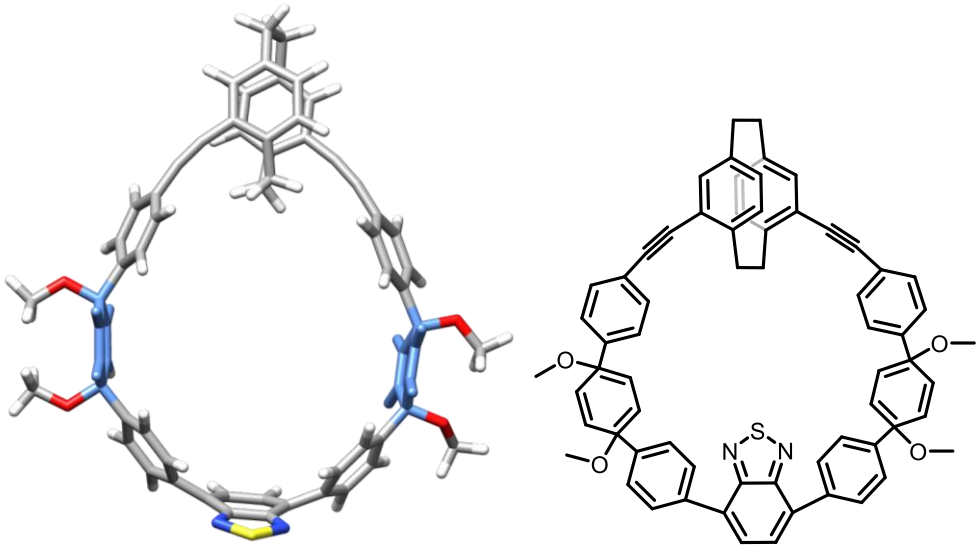


Figure S43. The optimized structure of **2**' with the optimized atoms marked in blue.

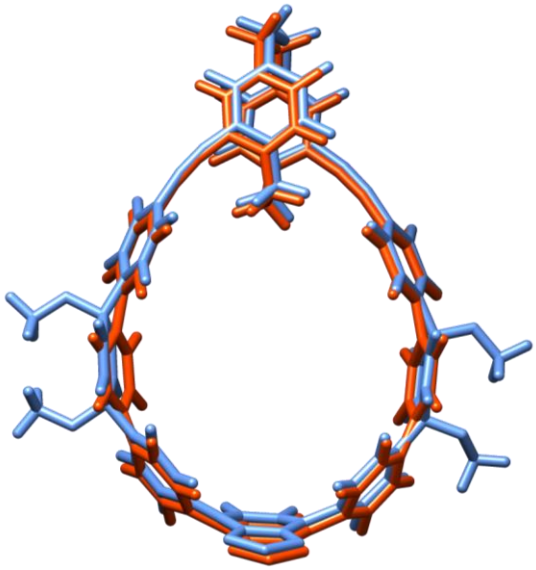


Figure S44. Overlay of the structures of **2** (orange) and **2'** (blue).

Table S5. Electronic transitions and their respective energies (*E*), wavelengths (*λ*), oscillator strengths (*f*) and orbital contributions for **2'**.

Transition	*E* / eV	*λ* / nm	*f*	Orbital contributions[a]
1	3.0812	402.39	0.3680	HOMO→LUMO (95%)
2	4.2666	290.59	0.0990	HOMO-2→LUMO+1 (54%)
3	4.325	286.67	0.2172	HOMO-1→LUMO+1 (54%)
4	4.5014	275.44	0.3558	HOMO-15→LUMO (22%) HOMO→LUMO+2 (21%)
5	4.5058	275.16	0.4364	HOMO→LUMO+2 (32%)

[a]Only the contributions larger than 10% are listed.

Table S6. Calculated energies (*E*), oscillator strengths (*f*), electric (*μ*) and magnetic (*m*) transition dipole moments, and angles (θ) between them, rotatory strengths (*R*, velocity form), dipole strengths (*D*) and calculated dissymmetry factor (g_{abs}) values for ground state geometry of **2'**.

Transition	*E* / eV	*f*	$\lvert\boldsymbol{\mu}\rvert$ / 10^{-18} esu·cm	$\lvert\boldsymbol{m}\rvert$ / 10^{-20} erg·G^{-1}	θ / °	*R* / 10^{-40} esu erg cm G^{-1}	*D* / 10^{-36} esu^2 cm^2 erg^2 G^{-2}	g_{abs} / 10^{-3}
S0 – S1	3.0812	0.3680	5.61	4.47	90.49	-21.6343	31.50	-0.27
S0 – S2	4.2666	0.0990	2.47	1.85	62.63	202.8829	6.12	13.27
S0 – S3	4.325	0.2172	3.64	7.40	105.19	-693.0067	13.25	-20.92

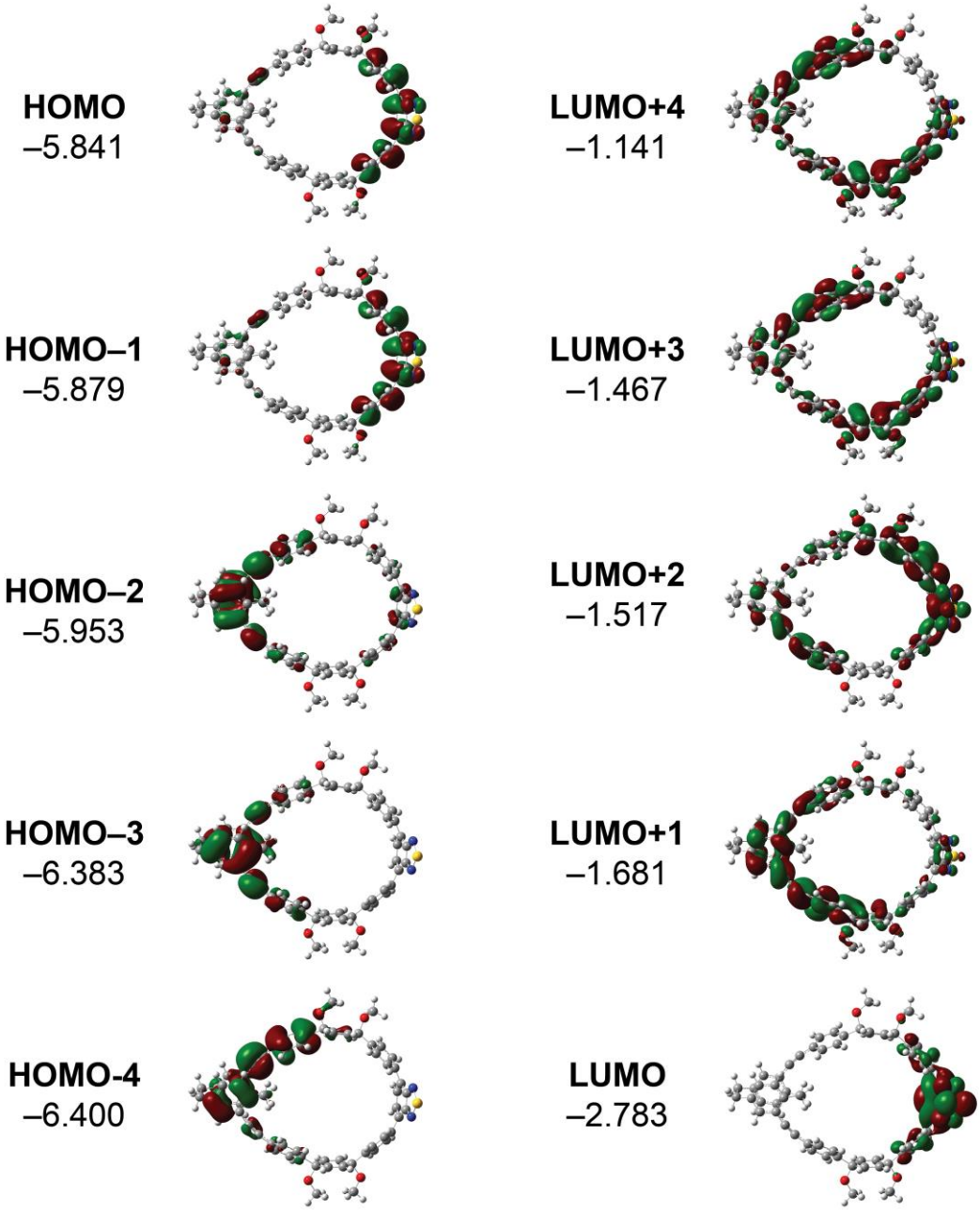


Figure S45. Frontier molecular orbitals of **2'** with energies in eV.

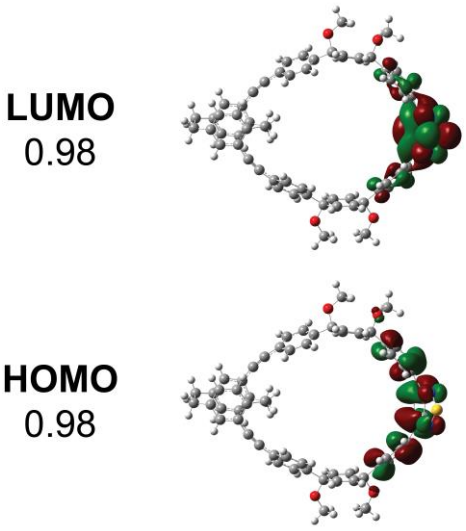


Figure S46. Natural transition orbitals and occupancies of the $S_0 \rightarrow S_1$ transition in **2'**.

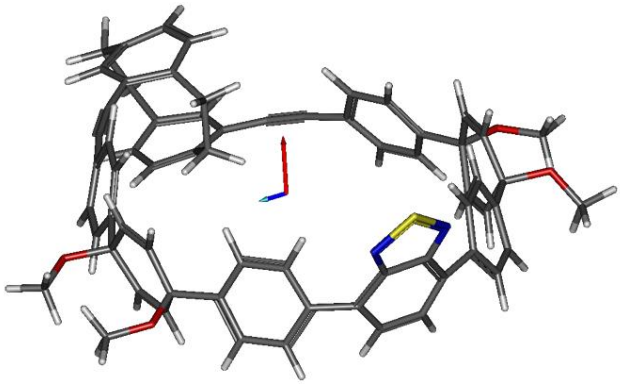


Figure S47. Electric (μ, blue) and magnetic (m, red) transition dipole moments of the $S_0 \rightarrow S_1$ transition in **2'**. The vectors are scaled by a factor of 2 for visualization due to small size of μ.

Geometry of **1** was taken from ref.[1] and optimized at D3-B3LYP/6-31g(d) level of theory. **1'** is a *pseudopara*-isomer of **1** and was optimized at the same level of theory.

Table S7. Electronic transitions and their respective energies (E), wavelengths (λ), oscillator strengths (f) and orbital contributions for **1**.

Transition	E / eV	λ / nm	f	Orbital contributions[a]
1	3.6809	336.83	0.2045	HOMO→LUMO (65%) HOMO-1→LUMO+1 (17%)
2	4.0777	304.05	1.8086	HOMO-1→LUMO (34%) HOMO→LUMO+1 (32%)
3	4.2874	289.18	0.8578	HOMO-2→LUMO (16%) HOMO-1→LUMO+1 (13%) HOMO→LUMO+2 (12%)
4	4.3417	285.56	0.6623	HOMO-3→LUMO+2 (12%) HOMO-1→LUMO+1 (13%)
5	4.5616	271.8	0.0872	HOMO-1→LUMO+2 (12%)

[a]Only the contributions larger than 10% are listed.

Table S8. Electronic transitions and their respective energies (*E*), wavelengths (*λ*), oscillator strengths (*f*) and orbital contributions for **1'**.

Transition	*E* / eV	*λ* / nm	*f*	Orbital contributions[a]
1	3.5654	347.74	0.0256	HOMO→LUMO+1 (44%) HOMO-1→LUMO (23%)
2	3.7988	326.38	1.3062	HOMO-1→LUMO (27%) HOMO→LUMO+1 (27%) HOMO-2→LUMO (10%) HOMO→LUMO (15%)
3	4.1326	300.02	1.7061	HOMO→LUMO+2 (17%) HOMO-2→LUMO (16%) HOMO-2→LUMO+1 (15%) HOMO-1→LUMO+1 (15%)
4	4.2554	291.35	0.2673	HOMO-3→LUMO (15%) HOMO-3→LUMO+1 (15%) HOMO-3→LUMO+3 (10%) HOMO-1→LUMO (10%)
5	4.3375	285.84	0.2219	HOMO-3→LUMO (14%) HOMO→LUMO (12%) HOMO-1→LUMO (11%)

[a]Only the contributions larger than 10% are listed.

Table S9. Calculated energies (*E*), oscillator strengths (*f*), electric (*μ*) and magnetic (*m*) transition dipole moments, and angles (θ) between them, rotatory strengths (*R*, velocity form), dipole strengths (*D*) and calculated dissymmetry factor (g_{abs}) values for ground state geometry of **1** and **1'**.

Compound (Transition)	*E* / eV	*f*	$\lvert\mu\rvert$ / 10^{-18} esu·cm	$\lvert m\rvert$ / 10^{-20} erg·G^{-1}	θ / °	*R* / 10^{-40} esu erg cm G^{-1}	*D* / 10^{-36} esu^2 cm^2 erg^2 G^{-2}	g_{abs} / 10^{-3}
R_P-**1** (S0 – S1)	3.6809	0.2045	3.83	11.18	99.96	-735.8439	14.66	-20.08
R_P-**1** (S0 – S2)	4.0777	1.8086	10.81	1.89	54.44	1171.318	116.96	4.01
R_P-**1** (S0 – S3)	4.2874	0.8578	7.26	1.09	116.09	-343.6208	52.76	-2.61
R_P-**1'** (S0 – S1)	3.5654	0.0256	1.38	11.54	110.57	-544.6392	1.90	-114.40
R_P-**1'** (S0 – S2)	3.7988	1.3062	9.52	2.48	77.98	486.448	90.68	2.15
R_P-**1'** (S0 – S3)	4.1326	1.7061	10.43	1.88	82.34	258.3594	108.87	0.95

Table S10. Calculated energies (*E*), oscillator strengths (*f*), electric (*μ*) and magnetic (*m*) transition dipole moments, and angles (θ) between them, rotatory strengths (*R*, velocity form), dipole strengths (*D*) and calculated dissymmetry factor (g_{lum}) values for 1st excited state geometry of **1** and **1'**.

Compound (Transition)	*E* / eV	*f*	$\lvert\boldsymbol{\mu}\rvert$ / 10^{-18} esu·cm	$\lvert\boldsymbol{m}\rvert$ / 10^{-20} erg·G^{-1}	θ / °	*R* / 10^{-40} esu erg cm G^{-1}	*D* / 10^{-36} esu^2 cm^2 erg^2 G^{-2}	g_{lum} / 10^{-3}
R_P-**1** (S1 – S0)	2.835	0.6127	7.55	9.17	92.72	-329	57.00	-2.31
R_P-**1'** (S1 – S0)	2.834	0.5308	7.03	9.04	90.6	-66	49.39	-0.53

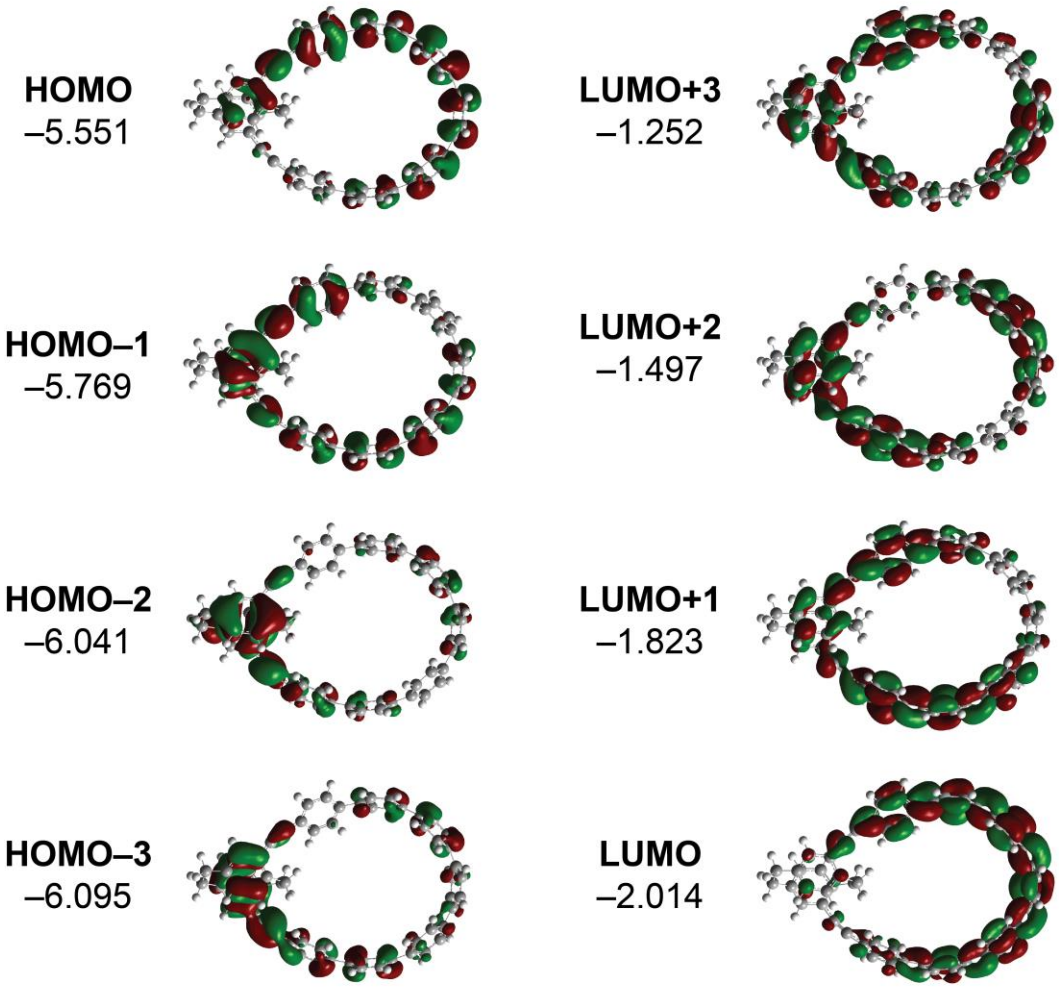


Figure S48. Frontier molecular orbitals of **1** with energies in eV.

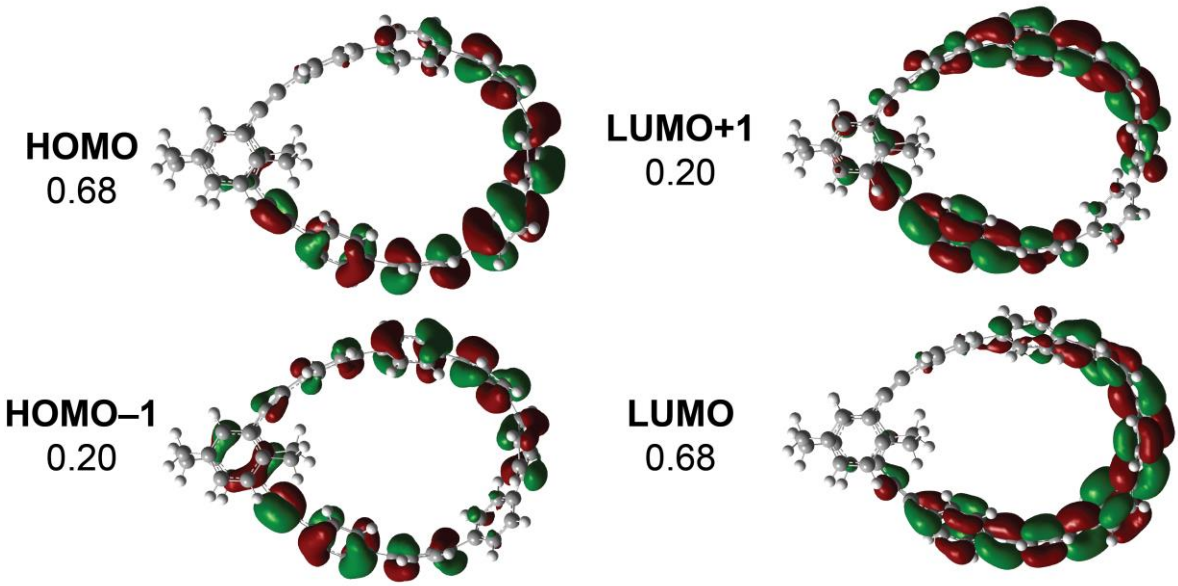


Figure S49. Natural transition orbitals and occupancies of the $S_0 \rightarrow S_1$ transition in **1**.

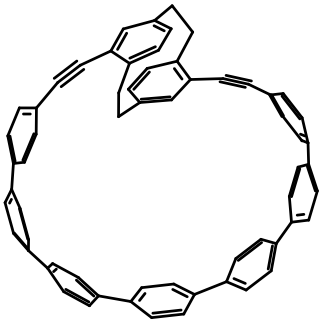


Figure S50. Structure of **1'**

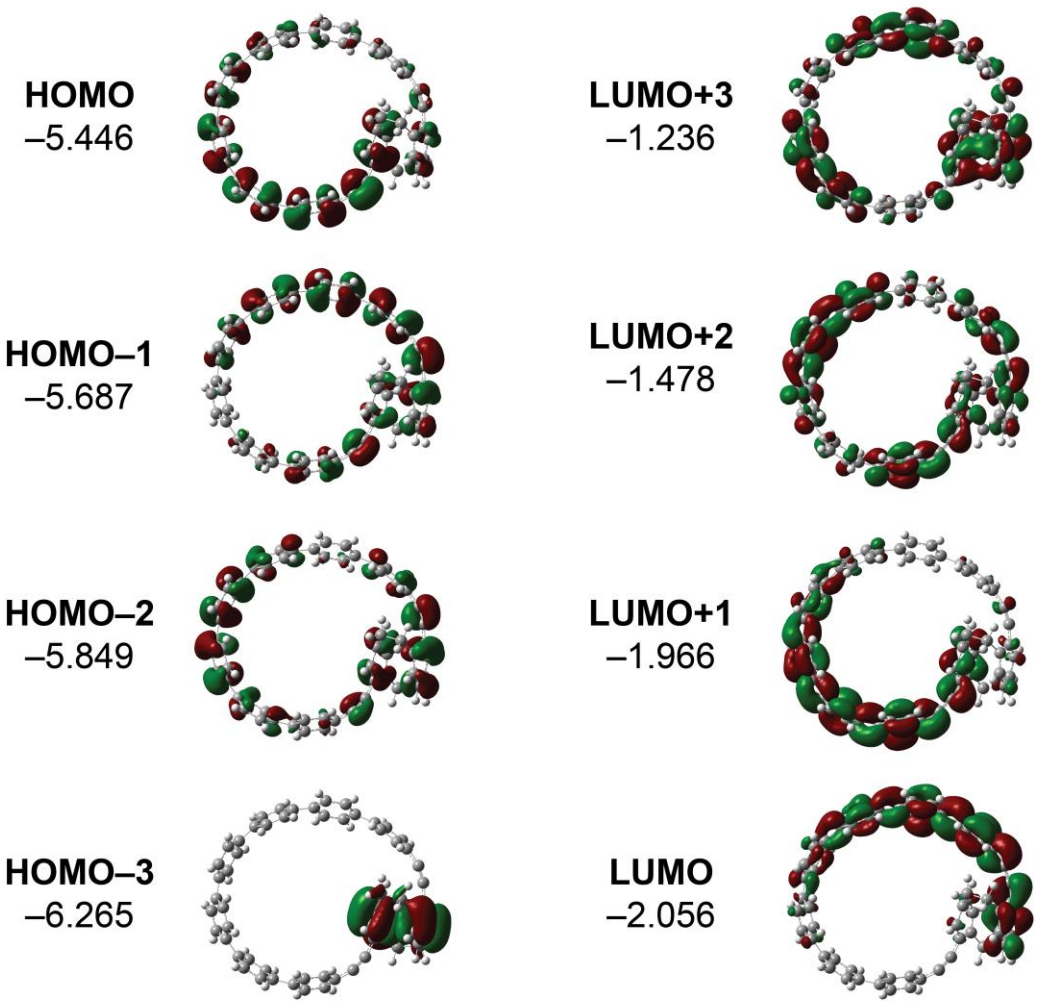


Figure S51. Frontier molecular orbitals of **1'** with energies in eV.

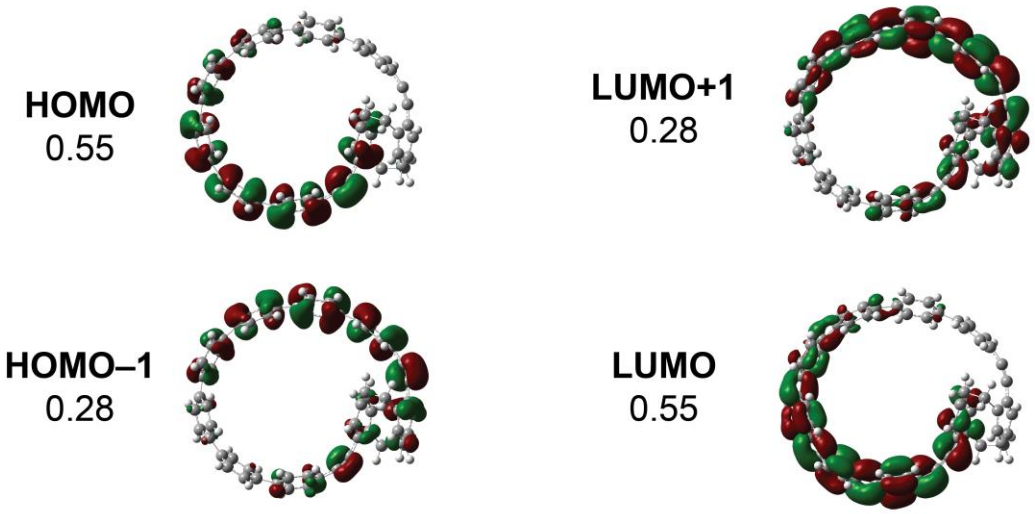


Figure S52. Natural transition orbitals and occupancies of the $S_0 \rightarrow S_1$ transition in **1'**.

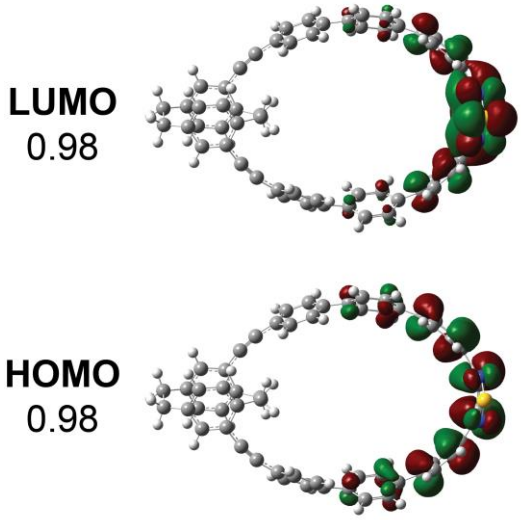


Figure S53. Natural transition orbitals and occupancies of the $S_1 \rightarrow S_0$ transition in **2**.

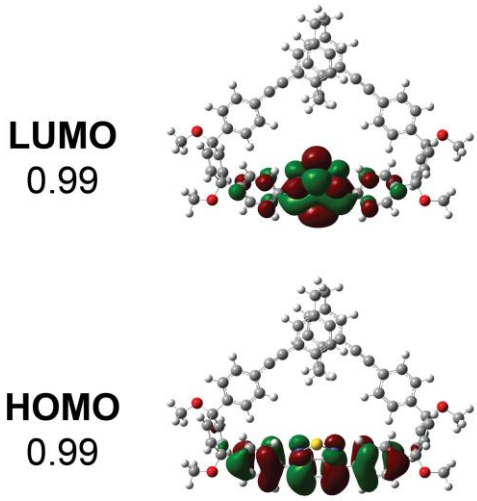


Figure S54. Natural transition orbitals and occupancies of the $S_1 \rightarrow S_0$ transition in **3**.

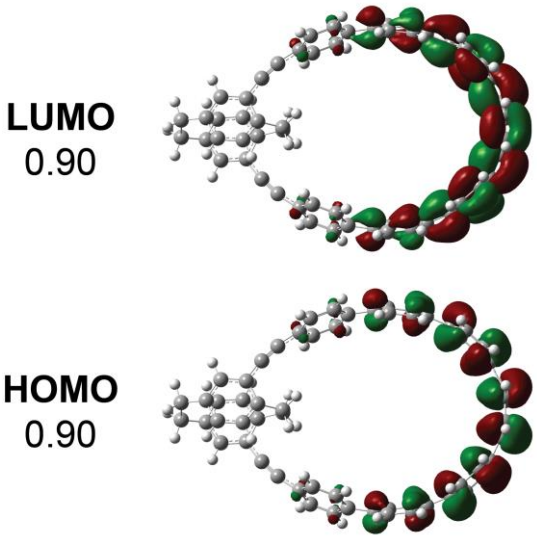


Figure S55. Natural transition orbitals and occupancies of the $S_1 \rightarrow S_0$ transition in **1**.

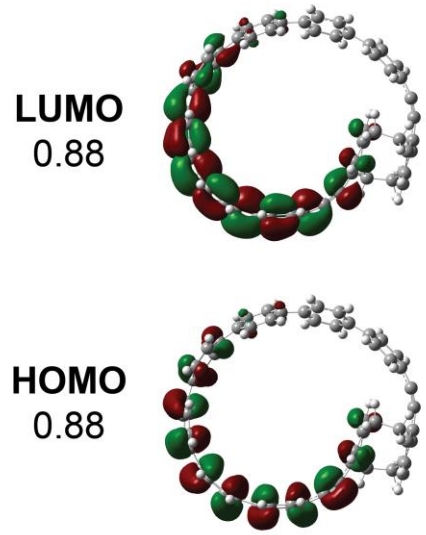


Figure S56. Natural transition orbitals and occupancies of the $S_1 \rightarrow S_0$ transition in **1'**.

Figure S57. The solid state fluorescence of **2** (left) and **3** (right).

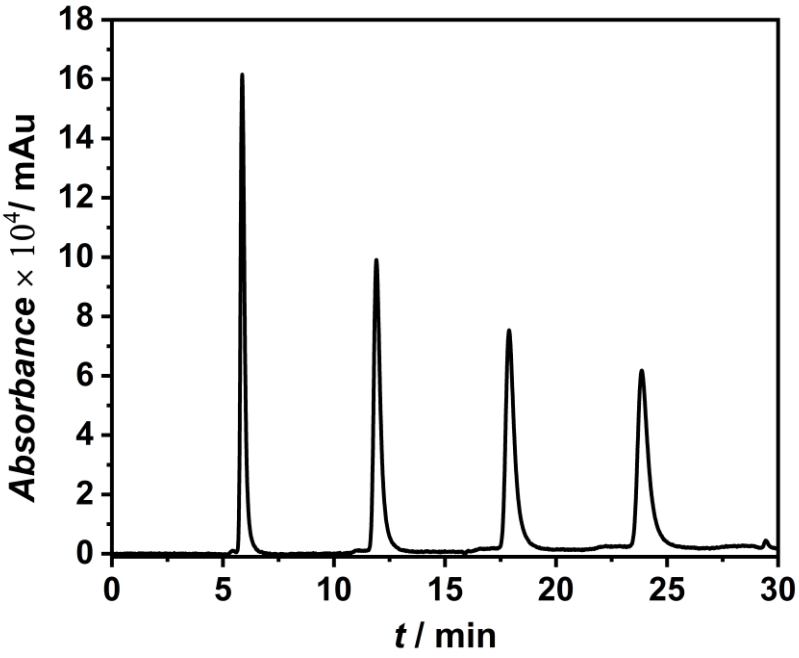


Figure S58. Analytical HPLC chromatogram of enantiomer 1 reinjection for **3** on Phenomenex IC column (flow rate: 3 ml/min, 100% Chloroform) which corresponds to (R_P)-enantiomer.

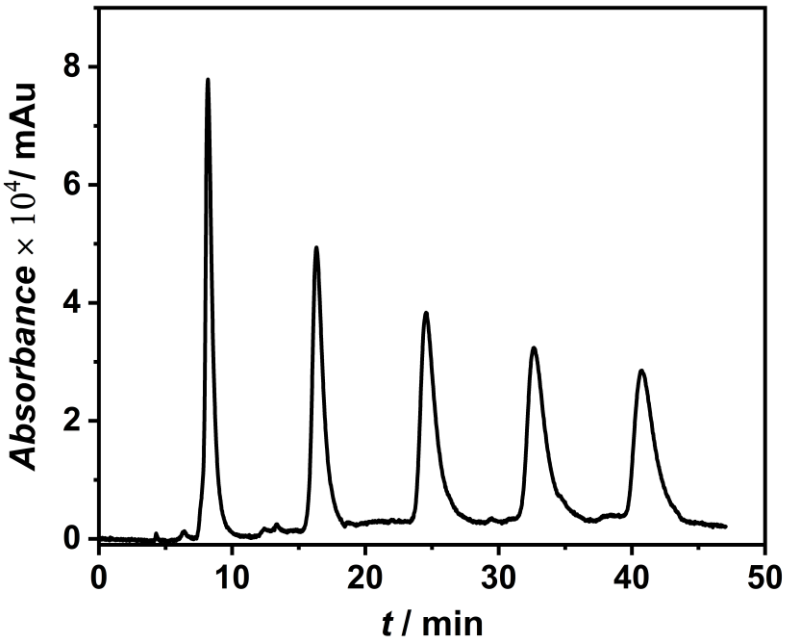


Figure S59. Analytical HPLC chromatogram of enantiomer 2 reinjection for **3** on Phenomenex IC column (flow rate: 3 ml/min, 100% Chloroform) which corresponds to (S_P)-enantiomer.

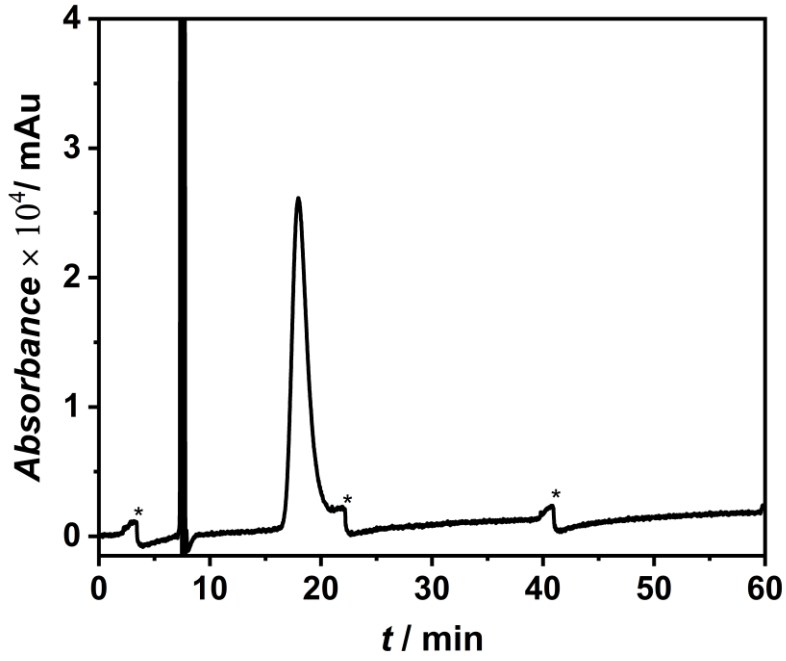


Figure S60. Analytical HPLC chromatogram of enantiomer 1 reinjection for **3** on the Chiralpak IG column (4.6x250mm, Flow rate: 1 ml/ min, toluene/TBME/*n*-heptane, v/v, 1:7:2) which corresponds to (R_P)-enantiomer. *= sudden change in the baseline signal.

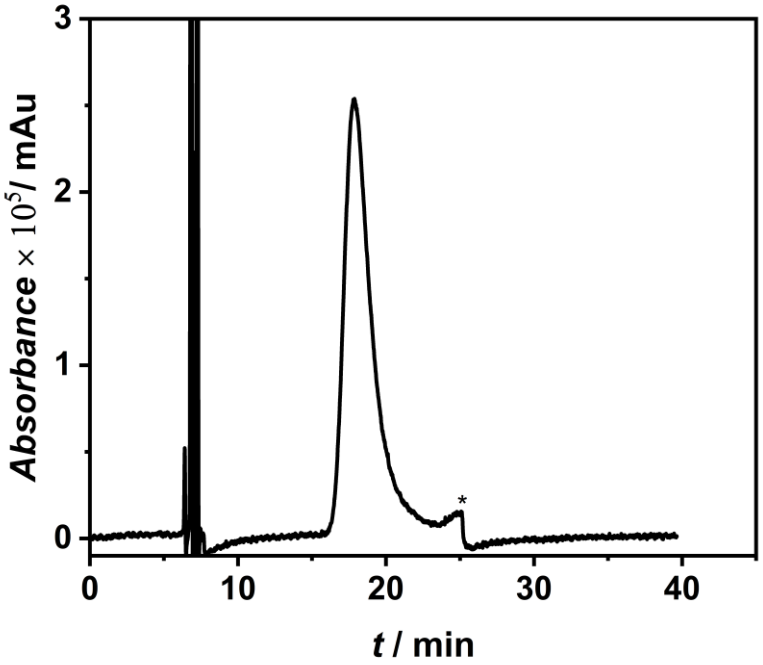


Figure S61. Analytical HPLC chromatogram of enantiomer 2 reinjection for **3** on the Chiralpak IG column (4.6x250mm, Flow rate: 1 ml/ min, toluene/TBME/*n*-heptane, v/v, 1:7:2) which corresponds to (S_P)-enantiomer. *= sudden change in the baseline signal.

8. Cartesian Coordinates

2

Ground state

E = -2894.34837854

C	-7.87952	1.67161	-1.07414
C	-6.47867	1.57311	-1.02401
C	-5.86573	0.30007	-1.16022
C	-6.65515	-0.73643	-1.66505
C	-8.04331	-0.62012	-1.73558
C	-8.67943	0.54255	-1.28343
C	-8.23733	0.71717	1.89462
C	-6.84782	0.78239	1.99438
C	-6.04059	-0.27966	1.57731
C	-6.67775	-1.52649	1.34494
C	-8.07757	-1.57414	1.22881
C	-8.85605	-0.41890	1.35772
C	-10.09186	0.48876	-0.73747
C	-10.19059	-0.31042	0.64827
C	-4.53391	-0.00924	-0.50754
C	-4.63157	-0.01369	1.08694
C	-5.65097	2.68357	-0.67765
C	-5.85243	-2.64761	1.03179
C	-4.77630	3.49331	-0.42858
C	-4.97596	-3.44694	0.75610
C	1.18761	5.36104	-1.25969
C	2.56962	5.21698	-1.26806
C	3.31960	5.28772	-0.07997
C	2.63346	5.66867	1.08894
C	1.24793	5.80110	1.10010
C	0.48679	5.57480	-0.06071
C	4.68089	4.69908	-0.05380
C	-0.97491	5.33022	-0.02607
C	-1.52109	4.56025	1.01736
C	-2.80558	4.03785	0.93064
C	-3.59721	4.26775	-0.21163
C	-3.10080	5.13844	-1.20204
C	-1.81397	5.65651	-1.10688
C	5.49162	4.62108	-1.20357
C	6.49845	3.66798	-1.30752
C	6.74695	2.75939	-0.26054
C	6.10352	3.00272	0.96748
C	5.08579	3.94416	1.06109
C	0.78421	-4.93205	-1.52749
C	2.16074	-4.81820	-1.68656
C	3.04828	-5.22603	-0.67451
C	2.49814	-5.89876	0.43213
C	1.12060	-6.00957	0.59289
C	0.23124	-5.45800	-0.34770
C	4.43298	-4.69650	-0.67944
C	-1.19908	-5.22120	-0.03823
C	-1.56087	-4.81252	1.25907
C	-2.82621	-4.31136	1.53035
C	-3.78952	-4.19900	0.50742
C	-3.46748	-4.70214	-0.76813
C	-2.19548	-5.20170	-1.03115
C	5.13438	-4.41276	-1.86720
C	6.18854	-3.50673	-1.87697
C	6.58545	-2.83898	-0.70031
C	6.03667	-3.29977	0.51166
C	4.97996	-4.20237	0.51693
C	7.02867	0.76116	-1.69159
C	6.98423	-0.65355	-1.80273
C	7.23451	-1.50989	-0.74386
C	7.82972	-0.87586	0.40575
C	7.86683	0.58018	0.52327
C	7.32175	1.42014	-0.51050
N	8.34361	-1.50270	1.46779
S	8.83626	-0.33576	2.51858
N	8.40317	1.00602	1.67020
H	-8.34011	2.61748	-0.80119
H	-6.19766	-1.70688	-1.83960
H	-8.63759	-1.49735	-1.98205
H	-8.82511	1.61424	2.07673
H	-6.38129	1.73458	2.23475
H	-8.53483	-2.49832	0.88518
H	-10.78202	0.01338	-1.44469
H	-10.45573	1.50929	-0.57578
H	-10.94027	0.19343	1.26991
H	-10.57291	-1.31604	0.44192
H	-3.76031	0.71271	-0.78768
H	-4.20123	-0.99851	-0.83373
H	-3.91705	-0.75614	1.45758
H	-4.31247	0.96701	1.45237
H	0.63505	5.18107	-2.17725
H	3.05491	4.92026	-2.19266
H	3.18477	5.81037	2.01443
H	0.74310	6.04054	2.03236
H	-0.89605	4.28941	1.86334
H	-3.18130	3.38500	1.71308
H	-3.71243	5.35431	-2.07270
H	-1.43553	6.29041	-1.90420
H	5.28390	5.26475	-2.05391
H	7.04968	3.57696	-2.23984
H	6.30963	2.36272	1.81730
H	4.51004	3.99066	1.98033
H	0.13049	-4.49582	-2.27724
H	2.54537	-4.29040	-2.55413
H	3.15623	-6.29427	1.20114
H	0.72615	-6.49263	1.48285
H	-0.81165	-4.80606	2.04508
H	-3.06535	-3.94069	2.52235
H	-4.20770	-4.65278	-1.56118
H	-1.95926	-5.55253	-2.03205
H	4.80690	-4.85638	-2.80368
H	6.66234	-3.25956	-2.82315
H	6.35589	-2.85823	1.44763
H	4.48801	-4.41809	1.46067
H	6.60405	1.32679	-2.51503
H	6.52716	-1.05105	-2.70305

2

Excited state 1

E = -2892.75367097

C	-8.04362	1.71278	-0.82471
C	-6.64984	1.62501	-0.90223
C	-6.04840	0.37157	-1.14354
C	-6.86781	-0.63979	-1.63641
C	-8.25169	-0.53278	-1.58637
C	-8.84933	0.59030	-1.01699
C	-8.16884	0.53205	2.08660
C	-6.78289	0.61981	2.08084
C	-5.99849	-0.39943	1.54808
C	-6.62677	-1.64154	1.31832
C	-8.02380	-1.71069	1.30100
C	-8.80515	-0.57973	1.53665
C	-10.20526	0.48402	-0.35344
C	-10.18600	-0.45145	0.93100
C	-4.67169	0.03269	-0.61755
C	-4.64101	-0.07525	0.96523
C	-5.78889	2.72877	-0.59324
C	-5.79575	-2.74278	0.93107
C	-4.89559	3.52279	-0.40022
C	-4.92263	-3.52356	0.62455
C	1.13609	5.00471	-1.42498
C	2.50887	4.84065	-1.43582
C	3.27598	5.02073	-0.27505
C	2.60732	5.50855	0.85986
C	1.23133	5.66727	0.87107
C	0.45628	5.35530	-0.25343
C	4.64745	4.48940	-0.22498
C	-1.01356	5.18859	-0.19521
C	-1.60195	4.60575	0.93326
C	-2.91038	4.15128	0.90503
C	-3.67761	4.26401	-0.26078
C	-3.13386	4.95700	-1.35060
C	-1.82567	5.41055	-1.31413
C	5.39135	4.23907	-1.39542
C	6.45285	3.36550	-1.39401
C	6.84925	2.68173	-0.21286
C	6.26591	3.14396	0.99460
C	5.18727	4.00147	0.97769
C	0.87752	-4.58406	-1.67849
C	2.24317	-4.42004	-1.82465
C	3.14430	-4.91168	-0.86846
C	2.61105	-5.69804	0.16548
C	1.24352	-5.85978	0.31164
C	0.34210	-5.24813	-0.56977
C	4.52726	-4.40904	-0.85367
C	-1.09949	-5.10807	-0.26309
C	-1.50144	-4.87937	1.05839
C	-2.78440	-4.45238	1.35295
C	-3.71782	-4.23969	0.32989
C	-3.35676	-4.57767	-0.98048
C	-2.06898	-5.00339	-1.26785
C	5.14124	-3.88523	-2.00800
C	6.22708	-3.04632	-1.92083
C	6.77380	-2.66766	-0.66422
C	6.30735	-3.39726	0.45937
C	5.20925	-4.22447	0.36140
C	7.76556	0.77453	-1.53269
C	7.74466	-0.58846	-1.65013
C	7.52179	-1.44470	-0.52396
C	7.80834	-0.84005	0.75162
C	7.81714	0.60740	0.87625
C	7.55858	1.42950	-0.27612
N	7.96359	-1.47180	1.90526
S	8.14709	-0.31238	3.08146
N	7.97490	1.03199	2.12122
H	-8.48469	2.64123	-0.47333
H	-6.42134	-1.59197	-1.90878
H	-8.85951	-1.39896	-1.83590

H	-8.75383	1.40475	2.36612
H	-6.31294	1.56404	2.34160
H	-8.49169	-2.62912	0.95809
H	-10.96518	0.09454	-1.03952
H	-10.53477	1.48386	-0.05456
H	-10.90981	-0.04989	1.64838
H	-10.54407	-1.44567	0.64659
H	-3.92330	0.77187	-0.91531
H	-4.36697	-0.93016	-1.03501
H	-3.88744	-0.82093	1.23309
H	-4.31064	0.88490	1.37008
H	0.57027	4.75021	-2.31497
H	2.97559	4.45631	-2.33541
H	3.16743	5.73264	1.76170
H	0.74427	6.00664	1.78025
H	-0.99764	4.42064	1.81536
H	-3.32437	3.63606	1.76542
H	-3.72908	5.08294	-2.24861
H	-1.41231	5.90780	-2.18606
H	5.09211	4.69707	-2.33229
H	6.94490	3.15648	-2.33629
H	6.60648	2.72501	1.93131
H	4.68434	4.20987	1.91569
H	0.21161	-4.09333	-2.38063
H	2.60645	-3.79979	-2.63619
H	3.27513	-6.16050	0.88844
H	0.86505	-6.44165	1.14652
H	-0.77182	-4.94869	1.85844
H	-3.05672	-4.21030	2.37453
H	-4.07862	-4.45189	-1.78062
H	-1.80009	-5.22170	-2.29670
H	4.71902	-4.09683	-2.98492
H	6.60753	-2.60846	-2.83543
H	6.75730	-3.21113	1.42454
H	4.80467	-4.65081	1.27307
H	7.82911	1.36397	-2.43916
H	7.80298	-1.01785	-2.64314

3

Ground state

E = -3354.82818420

C	1.61405	6.35837	-0.76867
C	1.52074	5.00510	-1.14462
C	0.24278	4.42645	-1.34912
C	-0.84210	5.29996	-1.47033
C	-0.73474	6.64196	-1.10404
C	0.47257	7.14571	-0.60102
C	1.11835	5.68362	2.23401
C	1.14177	4.33585	1.87388
C	0.01021	3.70688	1.34609
C	-1.22849	4.38349	1.47929
C	-1.23741	5.74444	1.83806
C	-0.04958	6.44122	2.07186
C	0.49483	8.32094	0.35350
C	0.01142	7.93588	1.83761
C	0.00921	2.94648	-1.12805
C	0.16137	2.52735	0.40810
C	2.67585	4.17606	-1.11785
C	-2.42799	3.74932	1.05298
C	3.62768	3.41812	-1.08756
C	-3.41743	3.16246	0.65559
C	7.59370	-1.64233	-1.95293
C	7.24436	-2.85788	-1.53368
C	7.09750	-3.24068	-0.07176
C	7.68238	-2.18214	0.83524
C	8.02764	-0.96442	0.41746
C	7.89188	-0.49169	-1.01824
C	5.60189	-3.45188	0.20256
C	6.77262	0.55959	-1.07522
C	5.43831	0.16741	-1.25050
C	4.41308	1.10415	-1.24880
C	4.69214	2.47431	-1.07296
C	6.03367	2.86515	-0.89386
C	7.05580	1.91985	-0.89394
C	4.96831	-4.62339	-0.23371
C	3.59121	-4.77702	-0.09732
C	2.80361	-3.76997	0.48719
C	3.45043	-2.61553	0.95536
C	4.82476	-2.45896	0.80881
C	-7.49390	-1.11875	-2.11776
C	-7.25433	-2.41265	-1.90612
C	-7.29818	-3.06853	-0.53598
C	-7.98211	-2.17567	0.47441
C	-8.22600	-0.88266	0.26195
C	-7.85067	-0.14852	-1.01439
C	-5.84632	-3.36572	-0.13307
C	-6.67619	0.78380	-0.67970
C	-5.35118	0.38431	-0.89511
C	-4.28939	1.17118	-0.46627
C	-4.52161	2.39713	0.18713
C	-5.85526	2.81477	0.37074
C	-6.91279	2.01646	-0.05394
C	-5.18679	-4.49436	-0.63859
C	-3.82837	-4.68608	-0.40035
C	-3.07962	-3.75560	0.34379
C	-3.76042	-2.65332	0.88618
C	-5.11818	-2.46653	0.65247
C	0.59528	-4.36837	-0.52364
C	-0.82687	-4.36238	-0.55659
C	-1.61166	-3.87743	0.47203
C	-0.89284	-3.42701	1.63478
C	0.56353	-3.42268	1.66338
C	1.33048	-3.87950	0.53729
N	-1.44355	-2.98960	2.77405
S	-0.20576	-2.60506	3.78165
N	1.07115	-2.97991	2.82028
H	2.58348	6.73874	-0.45784
H	-1.82549	4.88982	-1.68478
H	-1.63321	7.25359	-1.05993
H	2.05143	6.18115	2.48917
H	2.09610	3.81698	1.83766
H	-2.17790	6.28536	1.77527
H	-0.14458	9.13584	-0.00499
H	1.51294	8.72003	0.41709
H	0.69135	8.42172	2.54689
H	-0.98071	8.37119	1.99899
H	0.70683	2.33312	-1.70827
H	-1.00453	2.69721	-1.45503
H	-0.57934	1.74690	0.61280
H	1.15376	2.08927	0.54947
H	7.64916	-1.40052	-3.01191
H	7.00362	-3.65111	-2.23832
H	5.19743	-0.88008	-1.39076
H	3.38474	0.78496	-1.39021
H	6.26552	3.91761	-0.76067
H	8.08566	2.23386	-0.76832
H	5.56467	-5.41688	-0.67153
H	3.11848	-5.69618	-0.43324
H	2.87153	-1.82607	1.42035
H	5.29078	-1.54160	1.15062
H	-5.14497	-0.56308	-1.37922
H	-3.26806	0.83609	-0.62128
H	-6.05086	3.76352	0.86132
H	-7.93555	2.34512	0.09544
H	-5.74737	-5.22242	-1.21500
H	-3.34132	-5.57557	-0.79081
H	-3.22157	-1.92290	1.47687
H	-5.60489	-1.58931	1.06201
H	1.12238	-4.70775	-1.41083
H	-1.31008	-4.69072	-1.47204
O	9.09167	0.18497	-1.43194
O	7.72105	-4.51468	0.17421
H	7.76786	-2.46713	1.88156
H	8.41172	-0.21625	1.10775
C	9.11374	-4.56616	-0.10096
H	9.43245	-5.58306	0.14127
H	9.68134	-3.85420	0.51466
H	9.33596	-4.36040	-1.15765
C	10.27375	-0.60123	-1.39080
H	11.08046	0.04806	-1.73994
H	10.20674	-1.47908	-2.04852
H	10.50488	-0.94950	-0.37437
H	-6.96267	-3.07531	-2.71826
H	-7.40621	-0.67948	-3.10899
O	-7.95828	-4.34317	-0.61222
O	-8.92690	0.70995	-1.43138
H	-8.22704	-2.65142	1.42138
H	-8.68156	-0.25896	1.02819
C	-10.15306	0.04725	-1.70601
H	-10.85539	0.82586	-2.01388
H	-10.55218	-0.46977	-0.82200
H	-10.05076	-0.68755	-2.51693
C	-9.30611	-4.29579	-1.05805
H	-9.66210	-5.32902	-1.05716
H	-9.39272	-3.88515	-2.07404
H	-9.93940	-3.69558	-0.38970

3

Excited state 1

E = -3353.02175348

C	1.61879	6.51721	-0.79024
C	1.53706	5.14762	-1.07237
C	0.27390	4.56268	-1.29281
C	-0.78850	5.42561	-1.55052
C	-0.69129	6.78637	-1.28853
C	0.47919	7.31651	-0.74584
C	0.80952	6.11817	2.20816
C	0.86530	4.75197	1.96400
C	-0.21897	4.07148	1.41491
C	-1.46233	4.73470	1.41902
C	-1.50295	6.11559	1.65055
C	-0.34087	6.84256	1.89541
C	0.44363	8.55488	0.12165
C	-0.26174	8.30724	1.52752
C	0.00179	3.11169	-0.96871

C	0.01514	2.82433	0.59361
C	2.69338	4.31453	-0.96900
C	-2.63568	4.03309	1.00372
C	3.63616	3.55754	-0.91718
C	-3.58713	3.37560	0.64749
C	7.43289	-1.52700	-1.97185
C	7.10040	-2.76535	-1.62637
C	7.04778	-3.26505	-0.19743
C	7.65938	-2.26272	0.74992
C	7.97937	-1.02026	0.40583
C	7.79742	-0.44732	-0.98264
C	5.58613	-3.54901	0.14955
C	6.70735	0.63037	-0.95493
C	5.36062	0.26668	-0.98981
C	4.36456	1.22674	-0.96277
C	4.68658	2.58902	-0.89991
C	6.03731	2.95172	-0.85001
C	7.03288	1.98380	-0.87719
C	4.94926	-4.67542	-0.38935
C	3.60182	-4.88989	-0.18544
C	2.82293	-4.00527	0.59927
C	3.49496	-2.91271	1.18874
C	4.83707	-2.68559	0.94916
C	-7.26261	-1.19584	-2.11709
C	-6.98487	-2.48484	-1.95816
C	-7.09529	-3.22160	-0.63835
C	-7.82790	-2.38985	0.38520
C	-8.10294	-1.10020	0.22570
C	-7.72938	-0.29462	-1.00086
C	-5.67620	-3.55816	-0.18033
C	-6.63701	0.70964	-0.61681
C	-5.29100	0.34719	-0.66354
C	-4.30386	1.22518	-0.25080
C	-4.63380	2.50349	0.21699
C	-5.98401	2.87229	0.24975
C	-6.97020	1.98495	-0.15940
C	-4.98488	-4.62782	-0.76611
C	-3.65741	-4.85693	-0.47003
C	-2.94824	-4.03953	0.44648
C	-3.68471	-3.01485	1.08361
C	-5.00715	-2.77759	0.76280
C	0.64923	-4.84870	-0.28368
C	-0.71960	-4.85614	-0.31921
C	-1.52280	-4.18124	0.65189
C	-0.82018	-3.58817	1.75448
C	0.62625	-3.57058	1.78444
C	1.38871	-4.15853	0.72357
N	-1.38417	-3.01663	2.81453
S	-0.14872	-2.48085	3.79825
N	1.13653	-2.98346	2.86355
H	2.57329	6.91815	-0.46160
H	-1.75819	5.00491	-1.80091
H	-1.58334	7.40411	-1.35576
H	1.71820	6.64370	2.49104
H	1.81957	4.23963	2.04693
H	-2.44188	6.63666	1.48702
H	-0.07895	9.37926	-0.37499
H	1.46825	8.89460	0.30082
H	0.28387	8.88330	2.28233
H	-1.27405	8.72073	1.48733
H	0.73211	2.44604	-1.43759
H	-0.98304	2.84671	-1.36212
H	-0.73355	2.05428	0.79994
H	0.99066	2.41067	0.86171
H	7.42905	-1.21571	-3.01359
H	6.81702	-3.49664	-2.37963
H	5.08407	-0.77937	-1.05326
H	3.32210	0.92906	-1.00295
H	6.30352	4.00241	-0.80268
H	8.07509	2.27657	-0.85878
H	5.53030	-5.38522	-0.96716
H	3.14436	-5.77623	-0.61090
H	2.93933	-2.23484	1.82039
H	5.30628	-1.81133	1.38503
H	-5.00687	-0.63439	-1.02344
H	-3.26188	0.92498	-0.28441
H	-6.25621	3.86123	0.60321
H	-8.01135	2.28296	-0.13661
H	-5.50770	-5.27876	-1.45729
H	-3.16253	-5.70013	-0.93783
H	-3.19114	-2.39527	1.81788
H	-5.52230	-1.95477	1.24404
H	1.18814	-5.30460	-1.10502
H	-1.20510	-5.31817	-1.16909
O	8.98965	0.21943	-1.39491
O	7.70468	-4.52992	-0.09145
H	7.79926	-2.61329	1.76984
H	8.39197	-0.32726	1.13538
C	9.07610	-4.53552	-0.42995
H	9.41724	-5.56400	-0.29951
H	9.66162	-3.87845	0.22498
H	9.24533	-4.23013	-1.47009
C	10.14818	-0.58328	-1.47134
H	10.95391	0.07583	-1.79934
H	10.03464	-1.39814	-2.19707
H	10.41367	-1.01774	-0.49956
H	-6.62279	-3.08526	-2.78945
H	-7.13542	-0.71008	-3.08153
O	-7.74088	-4.48112	-0.82547
O	-8.84099	0.49081	-1.43002
H	-8.09586	-2.91037	1.30160
H	-8.60584	-0.53552	1.00737
C	-9.99884	-0.23205	-1.79060
H	-10.74071	0.51051	-2.08962
H	-10.39633	-0.81886	-0.95310
H	-9.81237	-0.91061	-2.63235
C	-9.06200	-4.41997	-1.32190
H	-9.40319	-5.45308	-1.40771
H	-9.10957	-3.94276	-2.30873
H	-9.72960	-3.87761	-0.64107

2'

Ground state

E = -3352.92778226

C	-8.11290	1.91835	-1.09924
C	-6.71612	1.77813	-1.03629
C	-6.14207	0.48358	-1.13371
C	-6.95998	-0.54143	-1.61616
C	-8.34338	-0.38436	-1.69988
C	-8.94605	0.80920	-1.28385
C	-8.51921	1.05633	1.89147
C	-7.12902	1.08139	1.99954
C	-6.35243	-0.01596	1.61710
C	-7.02642	-1.24841	1.41378
C	-8.42627	-1.25605	1.28880
C	-9.16938	-0.07430	1.38088
C	-10.36296	0.81380	-0.74692
C	-10.49532	0.05595	0.65909
C	-4.82471	0.15122	-0.46327
C	-4.93271	0.19307	1.13000
C	-5.85665	2.87155	-0.71396
C	-6.23425	-2.40252	1.13695
C	-4.95892	3.66042	-0.48044
C	-5.38122	-3.23566	0.88926
C	1.14484	5.61102	-1.29122
C	2.47511	5.46075	-1.28757
C	3.34751	5.59117	-0.04557
C	2.45695	5.52413	1.18846
C	1.13221	5.70643	1.17670
C	0.32202	5.99113	-0.07146
C	4.52818	4.58397	-0.06954
C	-1.10480	5.38957	-0.09995
C	-1.68157	4.66529	0.95977
C	-2.98107	4.18072	0.87792
C	-3.75781	4.40377	-0.27587
C	-3.22830	5.23156	-1.28572
C	-1.92672	5.71218	-1.19515
C	5.34378	4.44979	-1.21087
C	6.32127	3.46373	-1.28177
C	6.53473	2.57665	-0.20893
C	5.89127	2.87295	1.00738
C	4.90270	3.84754	1.06820
C	0.39974	-5.53262	-1.40014
C	1.73601	-5.47178	-1.55093
C	2.77780	-5.80604	-0.48632
C	2.03016	-6.03990	0.82276
C	0.69209	-6.08796	0.97660
C	-0.34068	-5.95845	-0.13640
C	3.99314	-4.81305	-0.44363
C	-1.65572	-5.14623	0.17041
C	-2.01348	-4.69165	1.45362
C	-3.26433	-4.14460	1.70213
C	-4.21708	-4.03039	0.66956
C	-3.90261	-4.57769	-0.58959
C	-2.64508	-5.12318	-0.82976
C	4.71105	-4.58340	-1.63348
C	5.79279	-3.71088	-1.66001
C	6.20261	-3.02396	-0.49891
C	5.63204	-3.43457	0.72101
C	4.54788	-4.30363	0.74286
C	6.76357	0.53258	-1.58356
C	6.67602	-0.88259	-1.65687
C	6.89282	-1.71717	-0.57353
C	7.49999	-1.07080	0.56289
C	7.58146	0.38606	0.64141
C	7.06933	1.21404	-0.41854
N	7.98736	-1.68412	1.64513
S	8.50917	-0.50481	2.66766
N	8.12335	0.82615	1.78032
H	-8.54569	2.88502	-0.85522
H	-6.53167	-1.52989	-1.76118
H	-8.96297	-1.24923	-1.92695
H	-9.08006	1.97570	2.04507
H	-6.63475	2.02493	2.21756
H	-8.90973	-2.17469	0.96687
H	-11.06296	0.34088	-1.44608
H	-10.69605	1.84907	-0.61543
H	-11.23301	0.59935	1.26146

H	-10.90729	-0.94264	0.47712
H	-4.02732	0.84112	-0.75712
H	-4.52076	-0.85632	-0.76026
H	-4.24395	-0.56071	1.52569
H	-4.58573	1.17303	1.47119
H	0.60522	5.51377	-2.22979
H	2.97057	5.22237	-2.22459
H	2.97369	5.48372	2.14254
H	0.60296	5.79677	2.12180
H	-1.07070	4.39856	1.81737
H	-3.38185	3.56120	1.67490
H	-3.82732	5.44244	-2.16632
H	-1.52362	6.31215	-2.00656
H	5.16161	5.07630	-2.07972
H	6.87538	3.33047	-2.20728
H	6.07196	2.25020	1.87560
H	4.32267	3.93662	1.98163
H	-0.22385	-5.29739	-2.25968
H	2.12903	-5.18924	-2.52496
H	2.65768	-6.26721	1.68206
H	0.29243	-6.35553	1.95268
H	-1.26941	-4.68695	2.24462
H	-3.49823	-3.73991	2.68201
H	-4.63581	-4.52706	-1.38905
H	-2.41335	-5.50809	-1.81916
H	4.37594	-5.04194	-2.56006
H	6.28008	-3.50418	-2.60904
H	5.95875	-2.97781	1.64704
H	4.04339	-4.47847	1.68852
H	6.36200	1.08846	-2.42500
H	6.21265	-1.29011	-2.54945
O	-1.01856	-7.24542	-0.32682
O	3.56049	-6.98742	-0.84866
O	0.00598	7.41830	-0.11198
O	3.88475	6.94472	0.10674
C	1.08361	8.34273	-0.20639
H	0.61601	9.32967	-0.14901
H	1.62280	8.25200	-1.15849
H	1.80920	8.22730	0.60504
C	4.63993	7.51331	-0.94765
H	5.63959	7.06708	-1.03604
H	4.75275	8.57084	-0.69216
H	4.12629	7.44297	-1.91742
C	-0.29673	-8.40725	-0.67445
H	-1.04761	-9.19927	-0.75021
H	0.43452	-8.68754	0.09234
H	0.21127	-8.30801	-1.64026
C	2.93856	-8.22272	-1.13241
H	3.75214	-8.89391	-1.42299
H	2.22706	-8.14983	-1.96325
H	2.43138	-8.64401	-0.25724

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Ground state

E = -2387.87321923

C	2.72033	4.06808	0.82232
C	-6.82133	3.88745	-0.76624
C	-7.66356	-0.38847	-1.11766
C	-7.40172	-2.53471	0.09943
C	-8.19676	0.95735	1.24781
C	-7.56243	0.99692	-1.06549
C	-7.00879	2.99137	0.30281
C	-3.46423	5.36473	0.14289
C	-3.46277	-5.08602	-1.45847
C	-5.15823	4.08834	1.44562
C	-8.29969	-0.42968	1.19510
C	-4.13457	-5.25019	-0.23264
C	-7.70542	1.68926	0.15003
C	-7.91258	-1.14169	0.04341
C	-1.29857	5.87136	1.14177
C	-6.66231	-2.91915	1.23221
C	1.90762	-3.63436	-0.88008
C	-3.38187	-5.75337	0.84442
C	3.89900	-0.06130	0.53081
C	4.12462	-0.00914	-1.04944
C	-2.80625	5.20224	-1.08930
C	-6.21801	3.18930	1.44902
C	1.44511	4.60395	0.95373
C	-5.75977	4.78801	-0.76931
C	4.59329	3.39606	-0.61624
C	9.39267	-0.83415	1.16580
C	-1.99853	-5.88070	0.75831
C	-1.42316	5.29848	-1.18696
C	-2.08371	-5.23100	-1.54969
C	-7.30736	-3.36387	-1.03441
C	2.85908	4.96721	-1.41730
C	8.37123	0.20063	-0.98431
C	-2.68436	5.78146	1.23766
C	5.45683	2.56415	-0.82812
C	-4.84092	4.83272	0.29635
C	9.63760	0.00976	-0.17410
C	0.82581	5.28547	-0.11038
C	7.63989	1.38977	-0.88877
C	-5.71386	-3.93141	1.16226
C	1.05029	-5.91937	0.45776
C	-1.30788	-5.53059	-0.41594
C	5.57873	0.20158	-1.41889
C	3.42798	4.18935	-0.38978
C	6.36509	-0.88963	-1.79916
C	7.10746	-1.91782	1.30747
C	-6.35821	-4.38038	-1.10336
C	1.58459	5.50473	-1.27462
C	2.77664	-4.25596	0.03936
C	5.15991	-0.45099	1.27456
C	-5.46094	-4.61104	-0.04269
C	0.62479	-4.11834	-1.08090
C	-0.63057	5.55844	-0.05591
C	7.32828	0.34942	2.03414
C	7.74400	-0.89338	-1.59338
C	5.71968	-1.75082	1.15532
C	5.95679	0.53473	1.86160
C	6.25220	1.41165	-1.11055
C	7.94129	-0.83330	1.60243
C	4.86761	-2.80939	0.72179
C	2.34102	-5.43918	0.66719
C	3.97827	-3.57564	0.39661
C	0.14640	-5.24418	-0.38229
H	-4.00772	-4.72652	-2.32610
H	3.15235	3.48797	1.63248
H	-7.46675	3.82522	-1.63859
H	-7.37878	-0.89530	-2.03477
H	-8.41379	1.47015	2.18131
H	-7.20337	1.52468	-1.94395
H	-4.48314	4.09980	2.29607
H	-8.59514	-0.97323	2.08877
H	-0.72131	6.14816	2.02004
H	-6.71062	-2.31632	2.13381
H	2.22982	-2.72792	-1.38341
H	-3.87143	-5.96359	1.79133
H	3.07493	-0.75509	0.72496
H	3.58278	0.93133	0.86370
H	3.47742	0.77783	-1.44960
H	3.79445	-0.96107	-1.47561
H	-3.36943	4.87321	-1.95734
H	-6.33331	2.52481	2.29992
H	0.88426	4.41362	1.86405
H	-5.60013	5.41586	-1.64197
H	10.05008	-0.42308	1.94131
H	9.71571	-1.86603	0.98991
H	-1.43889	-6.15194	1.64915
H	-0.94539	5.04876	-2.12980
H	-1.59297	-5.02821	-2.49753
H	-7.92666	-3.15809	-1.90369
H	3.40563	5.09975	-2.34602
H	-3.16415	5.98739	2.19075
H	10.04106	0.99011	0.10192
H	10.41597	-0.50318	-0.75162
H	8.11163	2.28331	-0.48837
H	-5.05827	-4.08299	2.01394
H	0.72754	-6.81556	0.98087
H	5.87434	-1.81256	-2.09814
H	7.54266	-2.87904	1.04676
H	-6.26160	-4.95058	-2.02352
H	1.15282	6.07138	-2.09501
H	-0.04874	-3.56199	-1.72507
H	7.94253	1.19146	2.34556
H	8.30152	-1.81411	-1.75085
H	5.53466	1.52305	2.02506
H	3.00516	-5.94982	1.35791

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Excited state 1

E = -2386.32904654

C	-2.42636	4.13197	-0.96548
C	6.95515	3.50021	0.90298
C	8.08279	-0.56666	1.26415
C	7.26599	-2.70136	0.23871
C	8.08284	0.56980	-1.26417
C	8.08846	0.79298	1.13901
C	7.26305	2.70369	-0.23912
C	3.79625	5.17427	-0.20430
C	3.04474	-5.48689	1.35583
C	5.63137	4.03863	-1.46740
C	8.09015	-0.78984	-1.13907
C	3.80023	-5.17311	0.20436
C	7.89035	1.42099	-0.13054
C	7.89195	-1.41812	0.13039
C	1.66951	5.63582	-1.30101
C	6.95777	-3.49740	-0.90376
C	-2.42285	-4.13193	0.96583
C	3.10457	-5.20019	-1.02228
C	-4.05027	-0.06791	-0.79005
C	-4.05066	0.06740	0.79099
C	3.10075	5.20024	1.02236
C	6.65550	3.12574	-1.45660
C	-1.13641	4.61322	-1.10029

C	5.93487	4.41520	0.88316
C	-4.32146	3.54677	0.47927
C	-9.59252	-0.47441	-0.64009
C	1.73424	-5.35109	-1.07315
C	1.73037	5.35099	1.07340
C	1.67347	-5.63399	1.30149
C	6.65981	-3.12499	1.45641
C	-2.54094	5.07455	1.24454
C	-8.22444	0.59379	1.27211
C	3.04083	5.48885	-1.35550
C	-5.19707	2.74940	0.73319
C	5.14244	4.62194	-0.27427
C	-9.59319	0.46925	0.63879
C	-0.49363	5.28192	-0.04758
C	-7.43300	1.72038	1.04928
C	5.93797	-4.41282	-0.88388
C	-1.24726	-5.55551	-1.10136
C	0.96797	-5.49142	0.09432
C	-5.41940	0.40081	1.34038
C	-3.13041	4.30093	0.23449
C	-6.21926	-0.61224	1.86169
C	-7.43111	-1.72369	-1.04980
C	5.63614	-4.03833	1.46727
C	-1.25112	5.55581	1.10176
C	-3.12694	-4.30121	-0.23410
C	-5.41851	-0.40242	-1.34001
C	5.14622	-4.62067	0.27396
C	-1.13278	-4.61276	1.10064
C	0.96415	5.49225	-0.09393
C	-7.60434	0.51508	-1.83986
C	-7.60466	-0.51849	1.83942
C	-6.03476	-1.64776	-1.09500
C	-6.21901	0.61000	-1.86156
C	-6.03661	1.64561	1.09501
C	-8.22340	-0.59775	-1.27287
C	-5.19446	-2.75092	-0.73303
C	-2.53722	-5.07471	-1.24411
C	-4.31834	-3.54766	-0.47885
C	-0.48977	-5.28134	0.04795
H	3.53821	-5.57723	2.31748
H	-2.87564	3.55457	-1.76681
H	7.49115	3.34227	1.83211
H	8.15004	-0.99762	2.25678
H	8.15043	1.00095	-2.25671
H	8.13838	1.39508	2.03894
H	5.11640	4.21830	-2.40426
H	8.14174	-1.39187	-2.03896
H	1.12470	5.83455	-2.21892
H	7.49300	-3.33859	-1.83317
H	-2.87231	-3.55463	1.76714
H	3.62925	-4.97739	-1.94384
H	-3.30289	-0.81854	-1.06035
H	-3.72770	0.88511	-1.21721
H	-3.30401	0.81863	1.06160
H	-3.72750	-0.88536	1.21830
H	3.62562	4.97669	1.94365
H	6.90811	2.62934	-2.38574
H	-0.58293	4.38254	-2.00423
H	5.70404	4.95527	1.79523
H	-10.33326	-0.08228	-1.34539
H	-9.93811	-1.46916	-0.34235
H	1.23527	-5.24426	-2.03048
H	1.23137	5.24327	2.03062
H	1.12877	-5.83207	2.21960
H	6.91330	-2.62972	2.38591
H	-3.08653	5.24681	2.16622
H	3.53441	5.57991	-2.31704
H	-9.93953	1.46369	0.34089
H	-10.33387	0.07647	1.34378
H	-7.88948	2.63997	0.69432
H	5.70693	-4.95242	-1.79617
H	-0.80341	-6.12241	-1.91343
H	-5.75892	-1.55740	2.13575
H	-7.88694	-2.64370	-0.69510
H	5.12240	-4.21931	2.40455
H	-0.80737	6.12274	1.91385
H	-0.57937	-4.38186	2.00457
H	-8.19928	1.38365	-2.11120
H	-8.19897	-1.38754	2.11058
H	-5.75935	1.55557	-2.13536
H	-3.08280	-5.24725	-2.16575

1'

Ground state

E = -2387.85757088

C	7.20258	-1.31244	-0.58340
C	6.87408	-0.48522	0.51022
C	6.22870	-1.04957	1.64012
C	6.19698	-2.44529	1.73032
C	6.51024	-3.24974	0.63682
C	6.88055	-2.67195	-0.58610
H	7.54071	-0.83757	-1.50059
H	5.76094	-2.90575	2.61382
H	6.31013	-4.31753	0.68820
C	4.36028	-1.11467	-1.70407
C	4.06652	-0.19654	-0.69573
C	3.66645	-0.64626	0.57110
C	3.23350	-1.96878	0.66536
C	3.46509	-2.89361	-0.37264
C	4.22176	-2.48983	-1.50319
H	4.84696	-0.76172	-2.61082
H	4.30515	0.85198	-0.84290
C	6.62533	-3.39930	-1.89157
H	7.00657	-4.42636	-1.85638
H	7.15912	-2.88944	-2.70084
C	5.06753	-3.47340	-2.28125
H	4.70668	-4.48890	-2.09152
H	4.98939	-3.30067	-3.36094
C	5.32175	-0.22004	2.52440
H	5.08793	-0.79637	3.42570
H	5.80988	0.70528	2.84819
C	3.94319	0.17993	1.80844
H	3.14213	0.06521	2.54798
H	3.98640	1.23854	1.53919
C	0.75068	-5.69534	0.02907
C	0.03895	-5.50388	1.23152
C	0.06081	-6.25531	-1.06529
C	-1.33861	-5.66641	1.26814
H	0.56174	-5.10945	2.09752
C	-1.31927	-6.42276	-1.01512
H	0.59981	-6.46421	-1.98445
C	-2.06185	-6.03671	0.11773
H	-1.87401	-5.37454	2.16652
H	-1.83879	-6.78391	-1.89857
C	-3.50689	-5.70712	0.04903
C	-4.00728	-5.11101	-1.12232
C	-4.33614	-5.67397	1.18664
C	-5.16575	-4.34396	-1.10050
H	-3.40682	-5.11787	-2.02682
C	-5.49651	-4.90519	1.20846
H	-4.03089	-6.19728	2.08899
C	-5.87913	-4.13581	0.09339
H	-5.43003	-3.77740	-1.98822
H	-6.07266	-4.84140	2.12792
C	5.71061	3.27711	0.17029
C	5.01497	3.73219	1.31018
C	5.38354	3.84987	-1.07575
C	3.92837	4.58716	1.18080
H	5.27763	3.33139	2.28458
C	4.30392	4.71836	-1.19118
H	5.93798	3.55049	-1.96004
C	3.50062	5.04334	-0.08054
H	3.34157	4.82177	2.06359
H	4.04558	5.10852	-2.17148
C	2.14787	5.63226	-0.23078
C	1.37284	5.30529	-1.35777
C	1.50634	6.33281	0.80814
C	0.00253	5.53501	-1.38239
H	1.82271	4.75582	-2.17900
C	0.13230	6.55555	0.78719
H	2.08330	6.67058	1.66477
C	-0.66239	6.09567	-0.27808
H	-0.57784	5.16096	-2.22065
H	-0.33944	7.05385	1.63010
C	-7.39381	-0.15950	0.14373
C	-6.92995	-0.76921	1.32265
C	-7.72436	-1.00932	-0.92872
C	-6.60445	-2.12037	1.35234
H	-6.67264	-0.15280	2.17885
C	-7.39970	-2.36255	-0.89847
H	-8.16886	-0.59042	-1.82781
C	-6.72863	-2.92352	0.20476
H	-6.10272	-2.51503	2.23076
H	-7.59726	-2.97474	-1.77456
H	2.78823	-2.33243	1.58777
H	-4.86046	5.44908	-2.16920
C	-4.25500	5.44000	-1.26683
C	-2.97834	5.99312	-1.30111
H	-2.60796	6.42120	-2.22900
C	-2.13411	5.94135	-0.17717
C	-2.68989	5.47002	1.02437
H	-2.07022	5.41739	1.91497
C	-3.96189	4.90915	1.05586
H	-4.29746	4.42956	1.97042
C	-4.73944	4.79927	-0.11082
C	-5.83747	3.80134	-0.15393
C	-5.96462	2.98251	-1.28979
H	-5.41704	3.23006	-2.19407
C	-6.62724	1.76262	-1.22738
H	-6.57423	1.09705	-2.08365
C	-7.19218	1.30142	-0.02513
C	-7.23819	2.20889	1.04968
H	-7.73790	1.92346	1.97177
C	-6.57623	3.43214	0.98611
H	-6.57600	4.07979	1.85889
C	2.85058	-4.17569	-0.25222
C	2.01944	-5.05965	-0.11615
C	6.51136	2.10243	0.27022

C	6.83948	0.93076	0.35678

1’

Excited state 1

E = -2386.31186332

C	6.71713	-1.84359	-1.13401
C	6.81748	-1.17199	0.09619
C	6.48005	-1.85006	1.28242
C	6.32426	-3.23394	1.20609
C	6.20157	-3.87976	-0.01547
C	6.25456	-3.15285	-1.20725
H	6.82837	-1.26076	-2.04367
H	6.13574	-3.79252	2.11900
H	5.91737	-4.92862	-0.03605
C	3.73143	-1.28390	-1.24692
C	3.83755	-0.56234	-0.06266
C	3.76555	-1.21831	1.17003
C	3.21368	-2.49236	1.17494
C	3.00959	-3.20332	-0.02492
C	3.49218	-2.65020	-1.24157
H	3.98324	-0.79429	-2.18430
H	4.13692	0.47928	-0.09943
C	5.55336	-3.65408	-2.45084
H	5.79162	-4.70576	-2.63864
H	5.91067	-3.09070	-3.31790
C	3.96193	-3.51935	-2.38219
H	3.52781	-4.51675	-2.27863
H	3.62087	-3.12149	-3.34334
C	5.98524	-1.11624	2.50597
H	6.06357	-1.78128	3.37080
H	6.60228	-0.23919	2.71753
C	4.46915	-0.63829	2.37461
H	3.94809	-0.90921	3.29826
H	4.45580	0.45307	2.30774
C	0.00181	-5.71249	0.07398
C	-0.70544	-5.78273	1.30237
C	-0.73195	-5.96882	-1.11342
C	-2.07223	-5.86381	1.32195
H	-0.15409	-5.67909	2.23092
C	-2.09956	-6.04409	-1.08882
H	-0.20197	-6.01714	-2.05890
C	-2.83960	-5.85704	0.11822
H	-2.57369	-5.82250	2.28117
H	-2.62427	-6.17013	-2.02849
C	-4.20743	-5.42767	0.11245
C	-4.87462	-5.05593	-1.09457
C	-4.90373	-5.08950	1.31435
C	-5.91384	-4.16707	-1.09364
H	-4.49374	-5.39636	-2.05009
C	-5.94116	-4.20052	1.31414
H	-4.57042	-5.49298	2.26370
C	-6.38403	-3.56838	0.11285
H	-6.30645	-3.83715	-2.04838
H	-6.39288	-3.93218	2.26268
C	6.06675	2.73234	0.08062
C	5.43089	3.19072	1.24342
C	5.83028	3.42319	-1.11625
C	4.46685	4.18168	1.17397
H	5.63226	2.69614	2.18789
C	4.87431	4.42443	-1.17268
H	6.34908	3.11679	-2.01842
C	4.11010	4.76557	-0.04828
H	3.90687	4.42911	2.06943
H	4.67395	4.90686	-2.12407
C	2.82852	5.50156	-0.16148
C	2.04374	5.33131	-1.30746
C	2.24422	6.17477	0.91951
C	0.70273	5.67445	-1.31756
H	2.45360	4.81046	-2.16611
C	0.89958	6.51389	0.91173
H	2.83806	6.39351	1.80183
C	0.07936	6.19873	-0.17959
H	0.10217	5.41327	-2.18244
H	0.46757	6.98686	1.78855
C	-7.26344	0.56927	0.01402
C	-7.19125	-0.12338	1.24489
C	-7.47940	-0.23324	-1.13325
C	-7.07992	-1.49090	1.29724
H	-7.09379	0.43403	2.16971
C	-7.36711	-1.59975	-1.08748
H	-7.68869	0.23953	-2.08723
C	-7.01632	-2.27843	0.11455
H	-6.90808	-1.95212	2.26232
H	-7.48827	-2.15925	-2.00821
H	2.99082	-2.99193	2.11332
H	-4.12474	5.88134	-2.10059
C	-3.53076	5.81420	-1.19451
C	-2.22443	6.27234	-1.21279
H	-1.82063	6.68400	-2.13301
C	-1.39694	6.15017	-0.08768
C	-1.99487	5.71197	1.09980
H	-1.39050	5.60756	1.99501
C	-3.29960	5.25059	1.11816
H	-3.67665	4.79606	2.02784
C	-4.07201	5.20308	-0.05145
C	-5.24812	4.31698	-0.10956
C	-5.52039	3.60042	-1.28611
H	-5.00201	3.86004	-2.20282
C	-6.30513	2.46565	-1.27398
H	-6.37156	1.87942	-2.18310
C	-6.86100	1.96743	-0.07801
C	-6.75676	2.80725	1.05285
H	-7.25796	2.53401	1.97545
C	-5.97225	3.94262	1.03679
H	-5.87554	4.52670	1.94691
C	2.24336	-4.39238	-0.00451
C	1.28901	-5.15859	0.03039
C	6.71107	1.45488	0.09138
C	6.89582	0.25637	0.09300

9. References

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