Supporting Information for:

Make the Ylides Shine: Synthesis and Structure–Property Relationships of Phosphasquaraines

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Experimental Section

All experiments were performed under ambient atmosphere and atmosphere of dry argon using Schlenk techniques. Commercially available reagents were used as received without further purification. Separations were performed by gravity column chromatography on silica gel (ACROS organic silica gel, for column chromatography, 0.035-0.070 mm, 60 Å). SEC (size exclusion chromatography) purification was performed on a LC-9160 II NEXT system from the Japan Analytical Industry Co., Ltd. (JAI) equipped with coupled UV-vis 4Ch NEXT through a set of two JAIGEL-2H columns at an elution rate of chloroform of 10 $mL.min^{-1}$. ^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded on Bruker AV III 300, AV III 400, and AV III 500 MHz NMR spectrometers equipped with BBFO heads. The assignment of H and C atoms is based on ^{1}H-^{1}H COSY, ^{1}H-^{13}C edited-HSQC and HMBC experiments. ^{1}H, and ^{13}C NMR chemical shifts were reported in parts per million (ppm) using residual solvent signal as reference. High-resolution mass spectra were obtained on a Varian MAT 311 at CRMPO (Scanmat, UAR 2025). UV-Visible absorption and emission spectra were recorded at room temperature on a Specord 205 UV/Vis/NIR spectrophotometer and FL 920 Edimburgh Instrument equipped with a Hamamatsu R5509-73 photomultiplier for the NIR domain (300-1700 nm) corrected for the response of the photomultiplier. The absolute quantum yields were measured with a C9920-03 Hamamatsu. The electrochemical studies were carried out under argon using an Eco Chemie Autolab PGSTAT 30 potentiostat for cyclic voltammetry with the three-electrode conFigureuration: the working electrode was a gold disk, the reference electrode was a silver chloride electrode, and the counter electrode was a platinum wire. All potentials were internally referenced to the decamethylferrocene/decamethylferrocenium couple. For the measurements, concentrations of 10^{-3} M of the electroactive species were used in freshly distilled and degassed dichloromethane and 0.2 M tetrabutylammonium hexafluorophosphate. **1**,[1] **3**[2]**-4**[3], **7**[4] , diethyl squarate[5] and **A**(R = Me)[6] were prepared according to published procedures.

[1] L. J. Higham, P. G. Kelly, D. M. Corr, H. M. Bunz, B. J. Walker, D. G. Gilheany, *Chem. Commun*. **2004**, 684-685.

[2] C. H. Lee, H. J. Yun, M. R. Jung, J. G. Lee, S. H. Kim, J. H. Kim, *Electrochim. Acta* **2014**, *138*, 148-154.

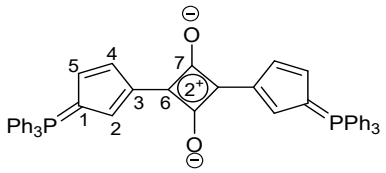
[3] G. Cicero, G. Musso, A. Lamberti, B. Camino, S. Bianco, D. Pugliese, F. Risplendi, A. Sacco, N. Shahzad, A. M. Ferrari, B. Ballarin, C. Barolo, E. Tressoad, G. Caputobc, *Phys. Chem. Chem. Phys.*, **2013**, *15*, 7198-7203

[4] S. Sreejith, J. Joseph, M. Lin, N. V. Menon, P. Borah, H. J. Ng, Y. X. Loong, Y. Kang, S. W. K. Yu, Y. Zhao, *ACS Nano* **2015**, *9*, 5695-5704.

[5] L. A. Marchetti, T. Krämer, R. B. P. Elmes, *Org. Biomol. Chem*. **2022**, *20*, 7056-7066.

[6] S. Khopkar, S. Deshpande, G. Shankarling, *ACS Sustainable Chem. Eng*. **2018**, 6, 10798−10805.

Phospha-squaraine **2**



1 (100 mg; 0.31 mmol; 2 eq.), squaric acid (17 mg; 0.15 mmol; 1 eq.), and activated molecular sieve 3Å were mixed in the mixture of dry *n*-butanol/toluene (each of 1 mL). The reaction mixture was degassed with argon. Then, the reaction mixture was stirred at 110 °C for 3 h under argon atmosphere. After, the solvent was removed via a vacuum trap. The crude product was purified via silica-gel column chromatography (EtOAc to 1/10:MeOH/EtOAc) to afford ***2*** as a purple solid. (24 mg, 22 % yield).

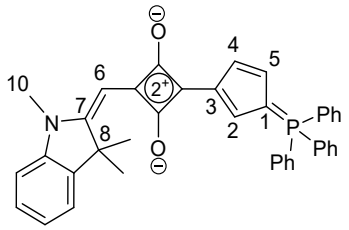
^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.76-7.54 (m, 30H, H_{Ph}), 7.33-7.27 (m, 2H, H_2), 7.10 (td, *J*(H,H) = 4 Hz, *J*(H,H) = 2 Hz, 2H, H_4), 6.33 (dt, *J*(H,H) = 5 Hz, *J*(H,H) = 2 Hz, 2H, H_5).

^{31}P NMR (121 MHz, CD_2Cl_2): δ + 14.3.

^{13}C NMR (126 MHz, CD_2Cl_2): δ 182.9 (s, C_7), 180.7 (s, C_6), 133.8 (d, *J*(C,P) = 10 Hz, C_{ortho}), 133.6 (d, *J*(C,P) = 3 Hz, C_{para}), 129.4 (d, *J*(C,P) = 13 Hz, C_{meta}), 127.2 (d, *J*(C,P) = 14 Hz, C_2), 123.5 (d, *J*(C,P) = 91 Hz, C_{ipso}), 123.1 (d, *J*(C,P) = 20 Hz, C_3), 121.0 (d, *J*(C,P) = 15 Hz, C_5), 118.4 (d, *J*(C,P) = 14 Hz, C_4), 94.7 (d, *J*(C,P) = 107 Hz, C_1).

HRMS (ESI, CH_3OH/CH_2Cl_2:50/50): $[M+Na]^+$ ($C_{50}H_{36}O_2NaP_2$), m/z Calc.: 753.2082. Found: 753.2086.

Phospha-squaraine-**5**



3 (50 mg, 0.19 mmol), **1** (61 mg, 0.19 mmol), and activated molecular sieve 3Å (50 mg) were mixed in the mixture of dry *n*-butanol/toluene (each of 1 mL). The reaction mixture was degassed with argon. Then, the reaction mixture was stirred at 110 °C for 4 h under argon atmosphere. After, the solvent was removed via vacuum trap. The crude product was purified via silica-gel column chromatography (EtOAc to 1/10:MeOH/EtOAc) to yield **5** as a dark blue solid in 43% (46 mg).

^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.78-7.69 (m, 3H, H_{PPh3}), 7.68-7.56 (m, 12H, H_{PPh3}), 7.37 (dt, *J*(H,H) = 6 Hz, *J*(H,H) = 2 Hz, 1H, H_2), 7.32 – 7.21 (m, 2H, H_{Ph}), 7.16 (td, *J*(H,H) = 5 Hz, *J*(H,H) = 2 Hz, 1H, H_4),

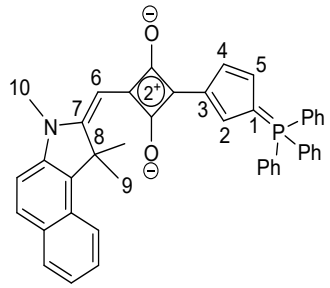
7.06 (t, *J*(H,H) = 7 Hz, 1H, H_{Ph}), 6.93 (d, *J*(H,H) = 8 Hz, 1H, H_{Ph}), 6.40 (dt, *J*(H,H) = 5 Hz, *J*(H,H) = 2 Hz, 1H, H_5), 5.76 (s, 1H, H_6), 3.44 (s, 3H, H_{10}), 1.72 (s, 6H, H_9).

^{31}P NMR (121 MHz, CD_2Cl_2): δ + 14.4.

^{13}C NMR (75 MHz, CD_2Cl_2): δ 182.5 (s, C_{CO}), 180.6 (s, C_{CO}), 179.8, 168.8, 143.4, 141.9, 133.8 (d, *J*(C,P) = 3.0 Hz, C_{HPh}), 133.8 (d, *J*(C,P) = 10 Hz, C_{HPh}), 129.6 (d, *J*(C,P) = 13 Hz, C_{HPh}), 128.6 (d, *J*(C,P) = 14 Hz, C_2), 127.6, 122.9 (d, *J*(C,P) = 20 Hz, C_3), 122.9 (d, *J*(C,P) = 91 Hz, C_{qPh}), 122.7, 122.1 (d, *J*(C,P) = 15 Hz, C_5), 121.9, 119.2 (d, *J*(C,P) = 14 Hz, C_4), 108.6, 97.7 (d, *J*(C,P) = 106 Hz, C_1), 86.6 (s, C_6), 48.6 (s, C_8), 30.2 (s, C_{10}), 27.0 (s, C_9).

HRMS (ESI, CH_3COCH_3/CH_2Cl_2:90/10): $[M+Na]^+$ ($C_{39}H_{32}NO_2NaP$), m/z Calc.: 600.2063. Found: 600.2063.

Phospha-squaraine-**6**



4 (50 mg, 0.16 mmol), **1** (51 mg, 0.16 mmol), and activated molecular sieve 3Å (50 mg) were mixed in the mixture of dry *n*-butanol/toluene (each of 1 mL). The reaction mixture was degassed with argon. Then, the reaction mixture was stirred at 110°C for 4 h under argon atmosphere. After, the solvent was removed via vacuum trap. The crude product was purified via silica-gel column chromatography (EtOAc to 1/10:MeOH/EtOAc) to yield **6** as a dark blue solid in 60% (59 mg).

^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.15 (d, *J*(H,H) = 9 Hz, 1H, H_{napht}), 7.85 (t, *J*(H,H) = 9 Hz, 2H, H_{napht}), 7.77-7.70 (m, 3H, H_{PPh3}), 7.68-7.57 (m, 12H, H_{PPh3}), 7.54-7.49 (m, 1H, H_{napht}), 7.39-7.33 (m, 2H, H_{napht} +H_2), 7.29 (d, *J*(H,H) = 9 Hz, 1H, H_{napht}), 7.17 (td, *J*(H,H) = 5 Hz, *J*(H,H) = 2 Hz, 1H, H_4), 6.41 (dt, *J*(H,H) = 5 Hz, *J*(H,H) = 2 Hz, 1H, H_5), 5.82 (s, 1H, H_6), 3.57 (s, 3H, H_{10}), 1.99 (s, 6H, H_9).

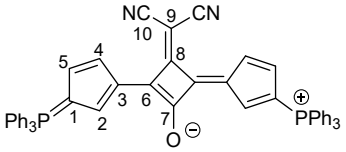
^{31}P NMR (162 MHz, CD_2Cl_2): δ + 14.4.

^{13}C NMR (101 MHz, CD_2Cl_2): δ 182.5 (s, C_{CO}), 180.1 (s, C_{CO}), 178.9, 170.7, 145.2, 140.5, 133.8 (d, *J*(C,P) = 10 Hz, C_{HPh}), 133.8 (d, *J*(C,P) = 3 Hz, C_{HPh}), 131.0, 129.6 (d, *J*(C,P) = 12 Hz, C_{HPh}), 129.4, 128.7, 128.6, 128.4 (d, *J*(C,P) = 13 Hz, C_2), 127.0, 123.7, 123.0 (d, *J*(C,P) = 91 Hz, C_{qPh}), 122.9 (d, *J*(C,P) = 20 Hz, C_3), 122.5, 122.0

(d, J(C,P) = 15 Hz, C_5), 119.1 (d, J(C,P) = 14 Hz, C_4), 110.0, 97.4 (d, J(C,P) = 106 Hz, C_1), 86.4 (s, C_6), 50.6 (s, C_8), 30.6 (s, C_{10}), 26.6 (s, C_9).

HRMS (ESI, CH_3COCH_3/CH_2Cl_2:90/10): $[M+Na]^+$ ($C_{43}H_{34}NO_2NaP$), m/z Calc.: 650.222. Found: 650.222.

Cyano-phospha-squaraine **8**



1 (112 mg, 0.34 mmol), **7** (50 mg, 0.17 mmol), activated molecular sieve 3 Å were mixed in the mixture of dry *n*-butanol/toluene (each of 1 mL). The reaction mixture was degassed with argon. Then, the reaction mixture was stirred at 110 °C for 3 h under argon atmosphere. After, the solvent was removed via vacuum trap. The crude product was purified via silica-gel column chromatography (DCM to 1/1:DCM/EtOAc) to afford **8** as a blue solid with some impurities. After, this product was further purified via SEC to yield **8** in 4% (5.4 mg).

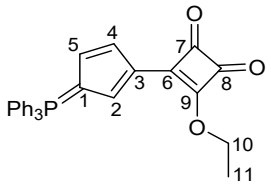
^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.77-7.53 (m, 32H, H_{PPh3} + H_2), 7.42 (td, J(H,H) = 5 Hz, J(H,H) = 2 Hz, 2H, H_4), 6.36 (br, 2H, H_5).

^{31}P NMR (162 MHz, CD_2Cl_2): δ + 14.3.

^{13}C NMR (101 MHz, CD_2Cl_2): δ 178.3 (s, C_7), 174.3, 170.2, 166.7, 166.3, 164.1, 133.8 (d, J(C,P) = 10 Hz, C_{ortho}), 133.8 (C_{para} (Overlap with C_{ortho})), 129.6 (d, J(C,P) = 13 Hz, C_{meta} (Possibly overlap with C_2)), 122.8 (d, J(C,P) = 91 Hz, C_{ipso}), 122.4 (br, C_3), 121.9 (br, C_5), 121.5 (d, J(C,P) = 13 Hz, C_4). C_1 and C_{CN} was not attribute due by overlapping

HRMS (ESI, CH_3OH/CH_2Cl_2:90/10): $[M+Na]^+$ ($C_{53}H_{36}N_2O_2NaP_2$), m/z Calc.: 801.2195. Found: 801.2193.

Hemi-phospha-squaraine **9**



1 (575 mg, 1.76 mmol) and diethyl squarate (150 mg, 0.88 mmol) were mixed in the mixture of *n*-butanol/toluene (each of 1 mL). The reaction mixture was stirred at 110 °C overnight. After, the solvent was removed via vacuum trap. The crude product was purified via silica-gel column chromatography (DCM to 1/1:DCM/EtOAc) and further purified via size exclusion chromatography ($CHCl_3$) to yield **9** as a yellow solid in 46% (185 mg).

^{1}H NMR (300 MHz, $CDCl_3$) : δ 7.77-7.40 (m, 15H, PPh_3), 7.21 (d, *J* = 5.3 Hz, 1H, H_2), 6.93 (t, *J* = 4.5 Hz, 1H, H_4), 6.35 (dt, *J* = 4.7, 2.5 Hz, 1H, H_5), 4.85 (q, *J* = 7.1 Hz, 2H, H_{10}), 1.48 (t, *J* = 7.1 Hz, 3H, H_{11}).

^{13}C NMR (75 MHz, $CDCl_3$) : δ 194.7 ($C_{7,8}$), 188.4 ($C_{7,8}$), 187.4 (C_9), 173.0 (C_6), 133.8 (d, *J*(C-P) = 10.3 Hz, C_{ortho}), 133.6 (d, *J*(C-P) = 2.9 Hz, C_{para}), 129.5 (d, *J*(C-P) = 12.5 Hz, C_{meta}), 124.4 (d, *J*(C-P) = 15.0 Hz, C_2), 123.8 (d, *J*(C-P) = 90.5 Hz, C_{ipso}), 120.1 (d, *J*(C-P) = 14.8 Hz, C_5), 117.3 (d, *J*(C-P) = 19.9 Hz, C_3), 116.4 (d, *J*(C-P) = 14.9 Hz, C_4), 91.1 (d, *J*(C-P) = 109.4 Hz, C_1), 69.2 (C_{10}), 16.0 (C_{11}).

^{31}P NMR (121 MHz, $CDCl_3$) : δ + 14.5.

HRMS (ESI, CH_3OH/CH_2Cl_2:90/10): $[M+Na]^+$ ($C_{29}H_{23}O_3NaP$), m/z Calc.: 473.1277. Found: 473.1277.

Crystallographic data and structure refinement parameters:

Suitable crystals for Single Crystal X-ray diffraction experiment were selected and mounted on the goniometer head of a D8 Venture diffractometer using Mo-*Kα* radiation (λ = 0.71073 Å, multilayer monochromator), or APEXII Kappa-CCD (Bruker-AXS) diffractometer equipped with a CCD plate detector, using Mo-*Kα* radiation (λ = 0.71073 Å, graphite monochromator). All measurements were done at T = 150(2) K. The structure was solved by dual-space algorithm using the *SHELXT* program,[7] and then refined with full-matrix least-squares methods based on F^2 (*SHELXL*).[8] All non-Hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. The contribution of the disordered solvents to the calculated structure factors was estimated following the *BYPASS* algorithm,[9] implemented as the *SQUEEZE* option in *PLATON*.[10]

Table S1: Crystallographic data

[7] G. M. Sheldrick, *Acta Cryst.*, **2015**, *A71*, 3-8
[8] Sheldrick G.M., *Acta Cryst.*, **2015**, *C71*, 3-8
[9] P. v.d. Sluis and A.L. Spek, *Acta Cryst.* **1990** *A46*, 194-201
[10] A. L. Spek, *J. Appl. Cryst.* **2003**, *36*, 7-13

Compound	**9**
CCDC	2471886
Formula	$C_{29}H_{23}O_3P$
MW ($g.mol^{-1}$)	450.44
a (Å)	13.7395(15)
b (Å)	10.4643(12)
c (Å)	16.2174(18)
α (°)	90
β (°)	98.524(4)
γ (°)	90
V ($Å^3$)	2305.9(4)
Z	4
*D*c ($g.cm^{-3}$)	1.298
Crystal system	monoclinic
Space group	$P\ 2_1/n$
T (K)	150(2)
Radiation	Mo-*Kα*
μ (mm^{-1})	0.148
F (000)	944
θ limit (°)	2.324 to 27.491°
Index ranges *hkl*	$-17 \leq h \leq 17$
	$-13 \leq k \leq 13$
	$-21 \leq l \leq 21$
Refl. collect. / unique	25239 / 5251
Reflections [$I>2\sigma(I)$]	4396
Data / restraints / parameters	5251 / 0 / 299
Goodness-of-fit on F^2	1.055
Final *R* indices [$I>2\sigma(I)$]	*R1 = 0.0433, wR2 = 0.1049*
R indices (all data)	*R1 = 0.0546, wR2 = 0.1129*
Largest diff peak and hole ($e\ Å^{-3}$)	-0.292, 0.495

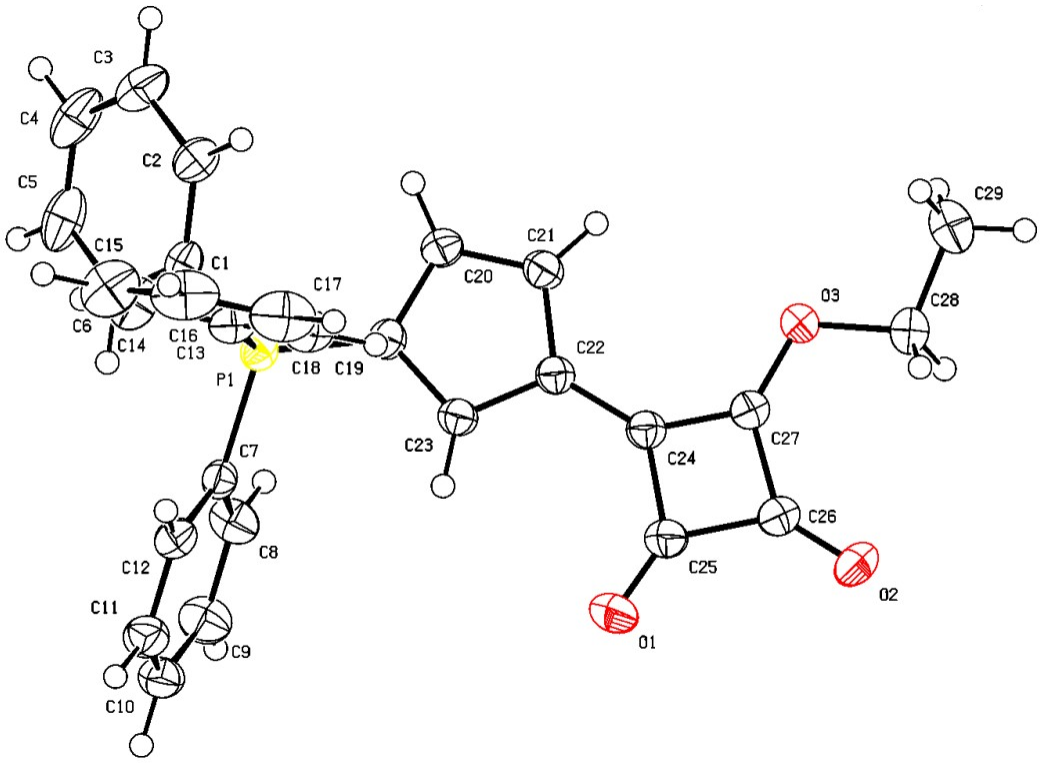


Figure S1. ORTEP representation **9** with 50% probability ellipsoids.

Optical and electrochemical properties

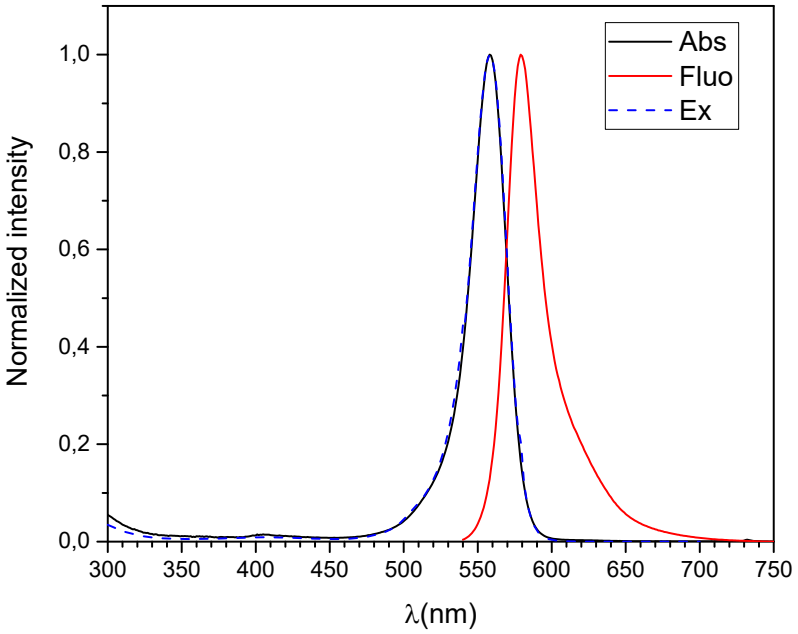


Figure S2. Absorption, emission, and excitation spectra of **2** in $CHCl_3$ solution ($c \approx 4 \times 10^{-6}$ M).

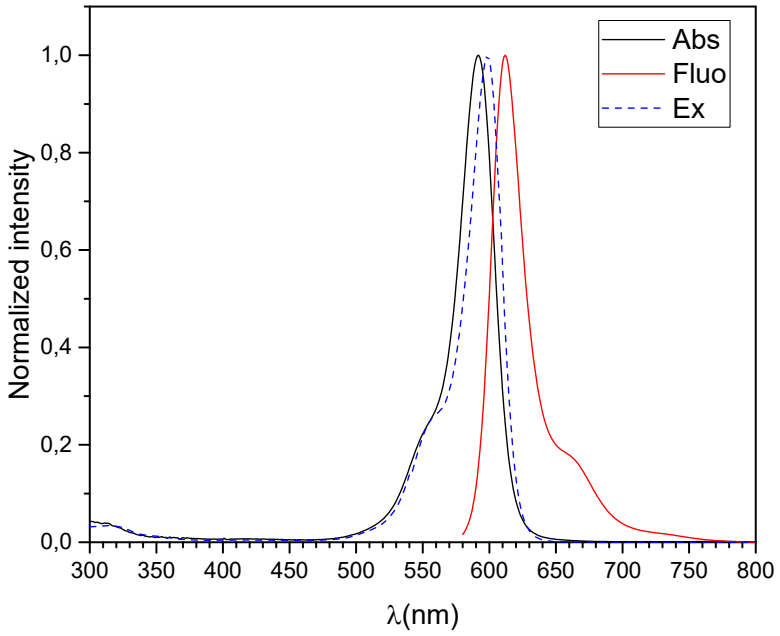


Figure S3. Absorption, emission, and excitation spectra of **5** in $CHCl_3$ solution (c $\approx$ 3 x 10^{-6} M).

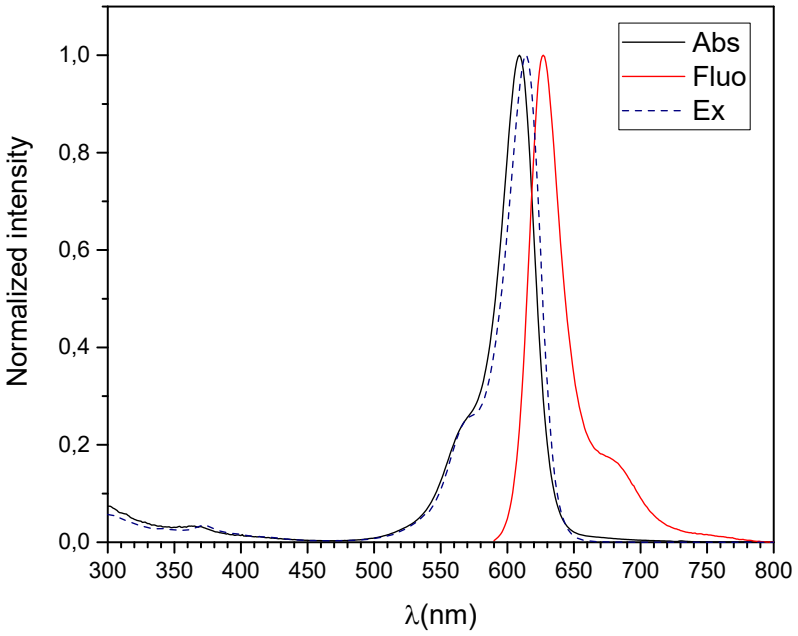


Figure S4. Absorption, emission, and excitation spectra of **6** in $CHCl_3$ solution (c ≈ 2 x 10^{-6} M).

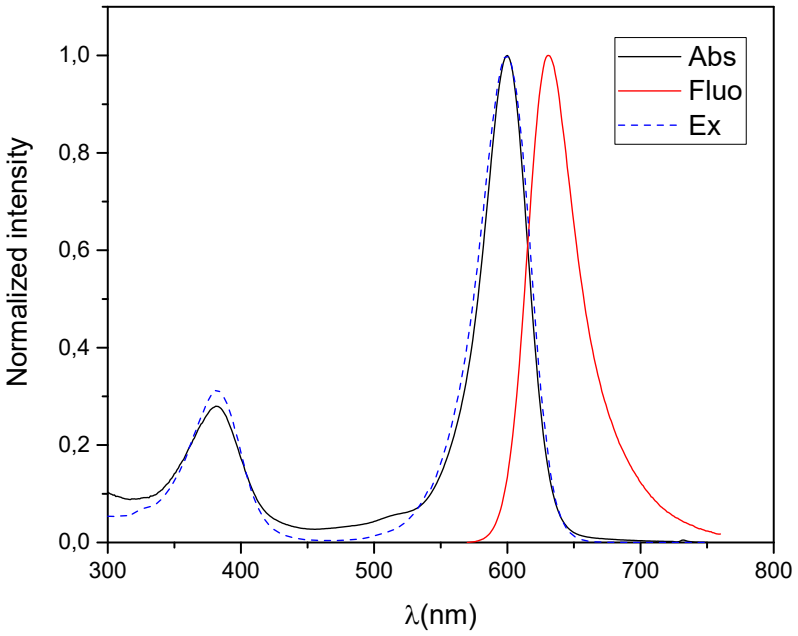


Figure S5. Absorption, emission, and excitation spectra of **8** in $CHCl_3$ solution (c ≈ 10^{-5} M).

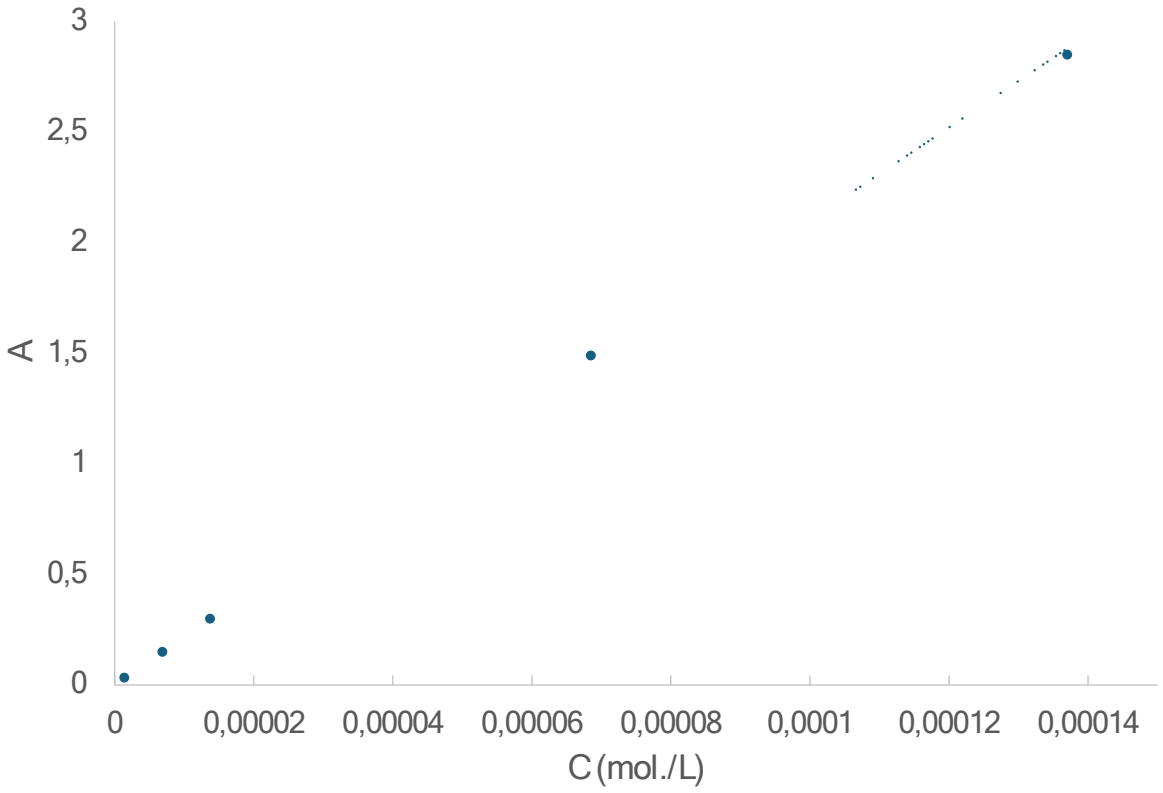


Figure S6. Concentration effect on the maximal absorption of **2** in DCM and its linear fit. (R = 0,9997)

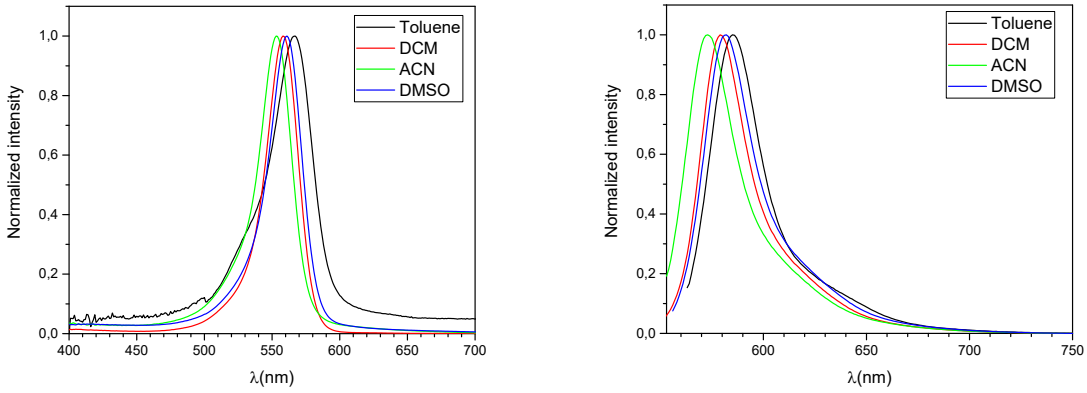


Figure S7: Solvatochromism in absorption (left) and emission (right) for compound **2** (C = 10^{-5} M)

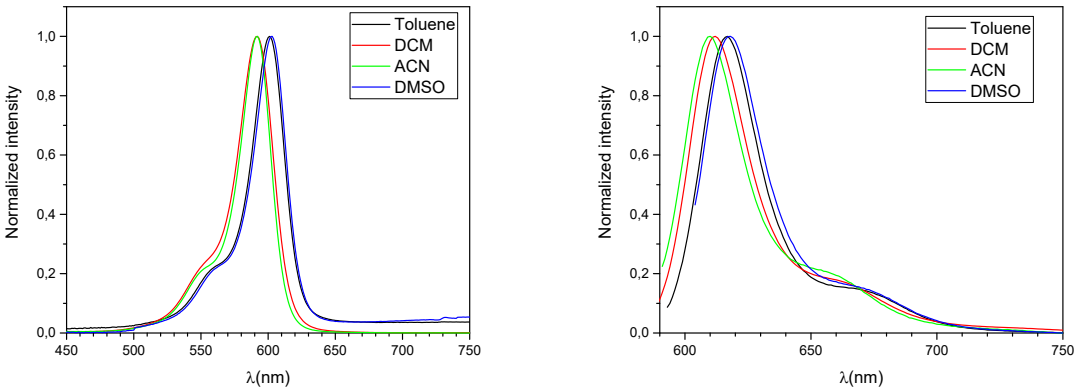


Figure S8: Solvatochromism in absorption (left) and emission (right) for compound **5** (C = 10^{-5} M)

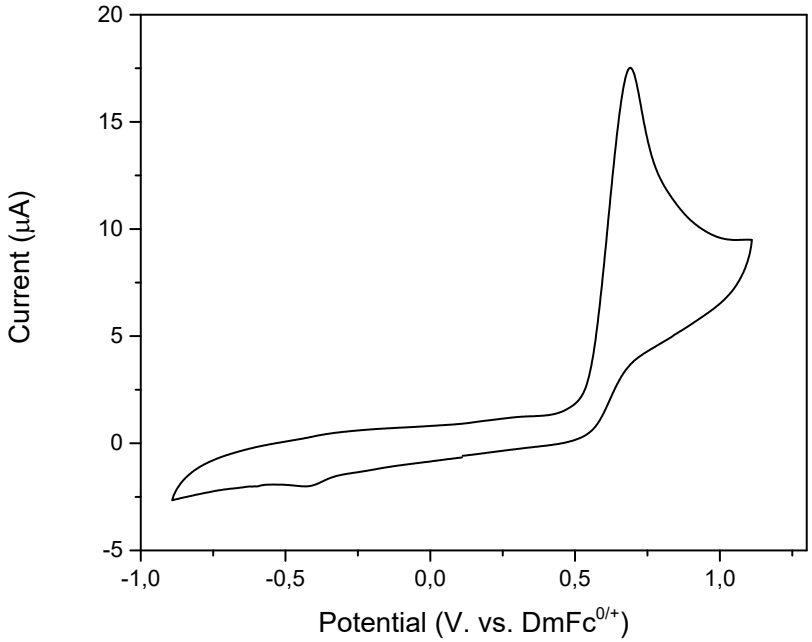


Figure S9. Cyclic voltammogram of **1** in DCM solution (c ≈ 10^{-3} M).

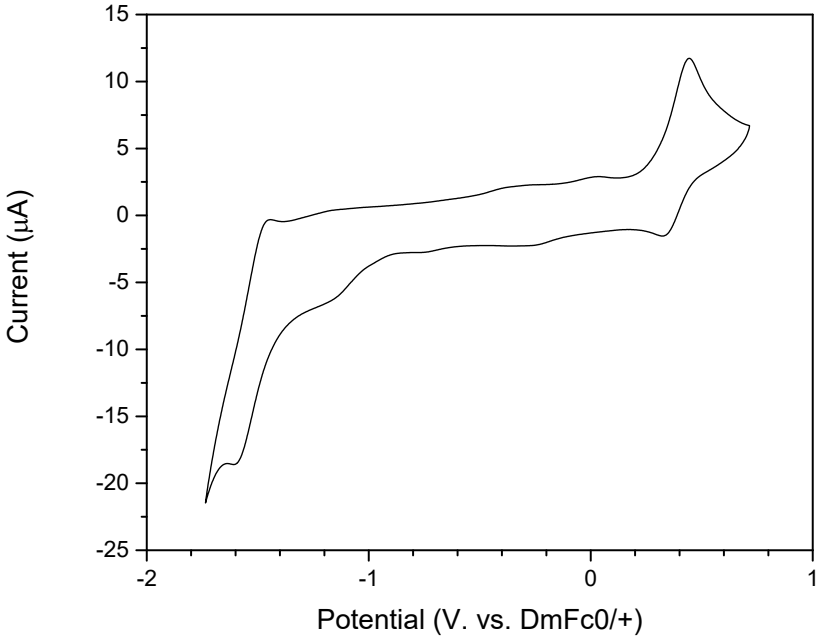


Figure S10. Cyclic voltammogram of **2** in DCM solution (c ≈ 10^{-3} M)

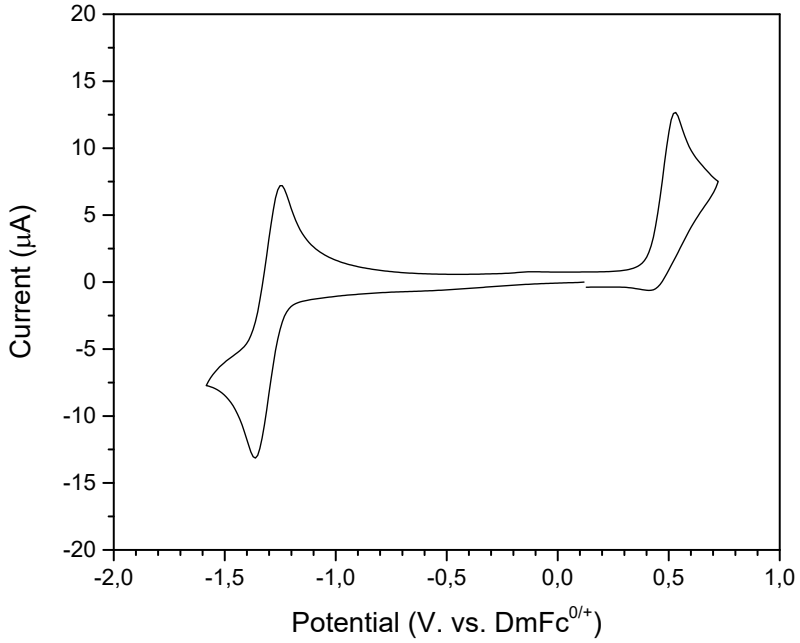


Figure S11 Cyclic voltammogram of **5** in DCM solution (c ≈ 10^{-3} M)

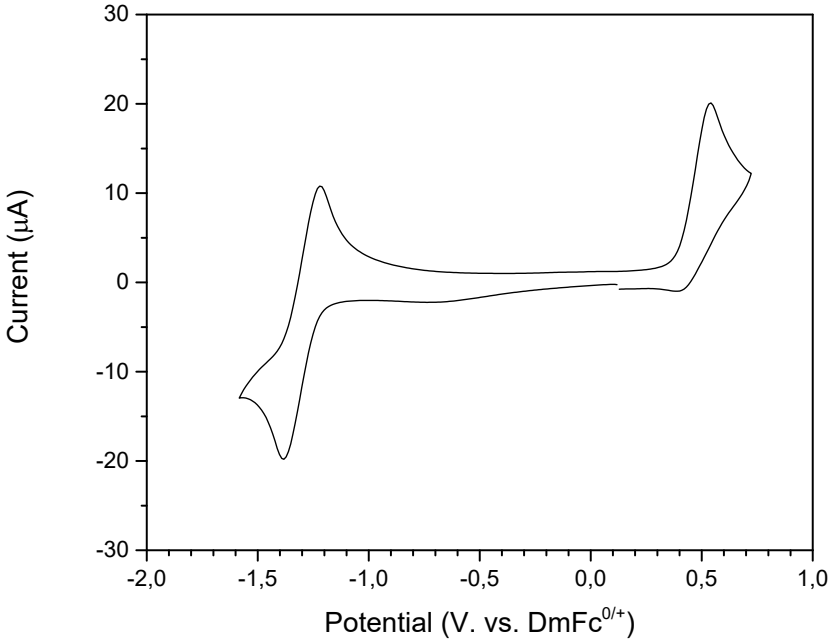


Figure S12 Cyclic voltammogram of **6** in DCM solution (c ≈ 10^{-3} M)

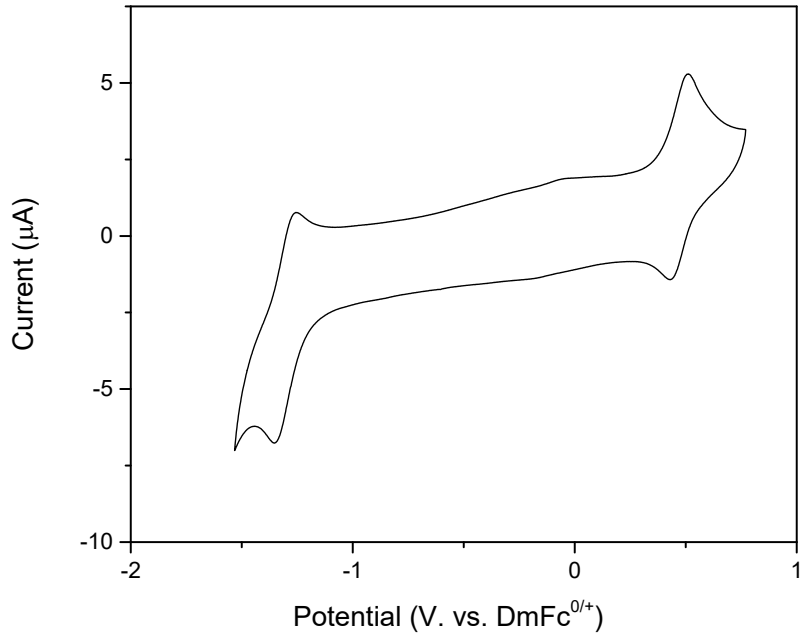


Figure S13 Cyclic voltammogram of **8** in DCM solution (c ≈ 10^{-3} M)

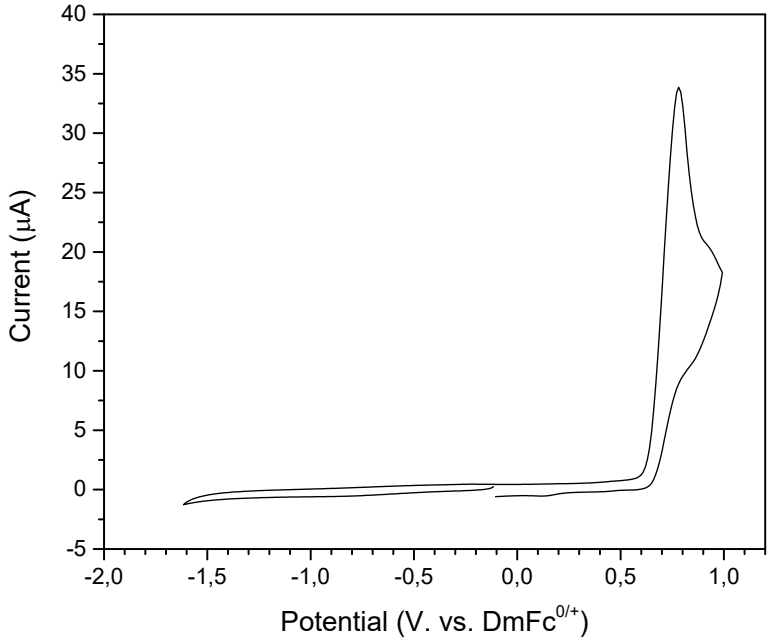


Figure S14 Cyclic voltammogram of **9** in DCM solution (c ≈ 10^{-3} M)

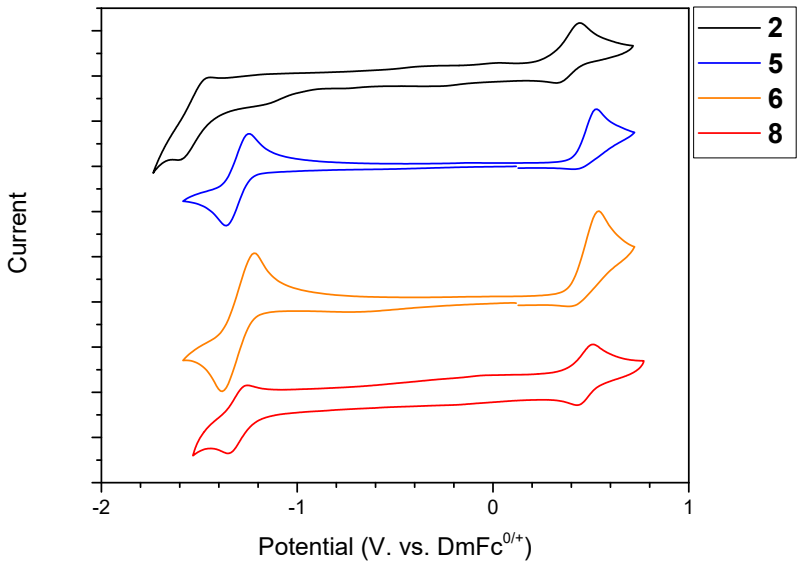


Figure S15: Cyclic voltammograms of **2, 5-6, 8** (c = 10^{-3} M) in DCM (Bu_4NPF_6 (0.2 M), 200 mVs^{-1}, potentials *vs* $DmFc^+$/DmFc).

Table S2: spectroscopic and redox data

	λ_{abs}[a] (nm)	ε_{max}[a] ($M^{-1}.cm^{-1}$)	λ_{em}[a] (nm)	$\lambda_{0\text{-}0}$[a] (nm)	σ[a] (cm^{-1})	Φ[b]	E^{ox}[c] (V *vs* DmFc)	E^{red}[c] (V *vs* DmFc)
A (R = ^{i}Pr)[8]	637	250000	646	-	219	0.24	0.01 V *vs* Fc	-1.72 V *vs* Fc
2	558	217000	579	570	650	0.15	+0.39	-1.54
5	592	166000	612	602	552	0.09	+0.48	-1.30
6	609	173000	627	623	471	0.21	+0.46	-1.29
8	600	70200	631	617	820	0.35	+0.48	-1.30

[a] In CH_2Cl_2 (2.10^{-6}M). [b] absolute quantum yields measured in integrated sphere [c]. (c = 10^{-3} M) recorded in CH_2Cl_2 with $Bu_4N^+PF_6^-$(0.2 M) at a scan rate of 200 mVs^{-1}. Note that E^{ox} (DmFc) = -0.52 V *vs* Fc.[11]

[11] I. Noviandri, K. N. Brown, D. S. Fleming, P. T. Gulyas, P. A. Lay, A. F. Masters, L. Phillips, *J. Phys. Chem. B* **1999**, 103, 6713-6722.

Photostability

General considerations. Photostability of compounds **2**, **5** and **A** was assessed by continuously irradiating the compounds at their maximum of absorption thanks to a homemade setup under air. Briefly, Time-profiles were obtained on a homemade photokinetic setup, by monitoring the change of the absorption spectrum overtime, while the sample is continuously irradiated at the maximum of absorption, under continuous stirring (400 rpm) at T=20°C. The temperature and stirring were controlled thanks to Peltier device. The irradiation wavelength (source Xe lamp Zolix instruments, model Sirius 300P) was selected by passing through a monochromator (Zolix instruments, model Omni-l200i, halfwidth of ±10 nm). Absorption spectra were acquired with a Flame spectrophotometer (Ocean Insights) combined to a DHBAL-2000 D/Hal lamp. Light intensity was measured using a Thorlabs (PM100USB) power-meter. Experimental data are a matrix of full spectra over the full time of acquisition; useful photokinetic profiles were extracted at the maximum of absorbance.

Quantum yields of degradation were obtained from eq. S1

$$\phi_{deg} = \frac{-a^{mol}}{\varepsilon^{mol}(obs) * I_0\left(1 - 10^{-(A_0)}\right) * l} \; with\; l = 1cm \qquad \text{(eq. S1)}$$

where a^{mol} represents the slope of the kinetic curve at the beginning of the process and is obtained from eq. S2; $\varepsilon^{mol}(obs)$ is the extinction coefficient of the molecule at the observation wavelength; I_0 is the incident irradiation light intensity given by eq. S4; A_0 is the initial absorption at the irradiation wavelength and l the light pathway (l=1 cm).

The photodegradation process quantum yields were determined by recording the absorption time-profiles upon irradiation at the maximum of absorption. The time-profiles were fitted with a monoexponential decay function of the kind

$$y = y_0 + A_1.e^{-\frac{t}{t_1}} \qquad \text{(eq. S2)}$$

Therefore, the slope of the kinetic profile at the beginning of the process is given by eq. S3:

$$a^{mol} = -\frac{A_1}{t_1} \qquad \text{(eq. S3)}$$

Eventually, I_0 is given by eq. S4:

$$I_0 = \frac{8.36\ 10^{-9} \times I \times \lambda_{irr}}{V} \qquad \text{(eq. S4)}$$

Where I_0 is expressed in Einstein s^{-1}, λ_{irr} (in nm) defines the irradiation wavelength, I stands for the light intensity (in mW) and V for the total volume of the solution (in mL).

*Compound **A** (R = Me).* Photodegradation monitoring of compound A at 20°C, under irradiation at 630 nm ($I = 0.44\ mW$). An isobestic point located at 530 nm is indicated by the black circle.

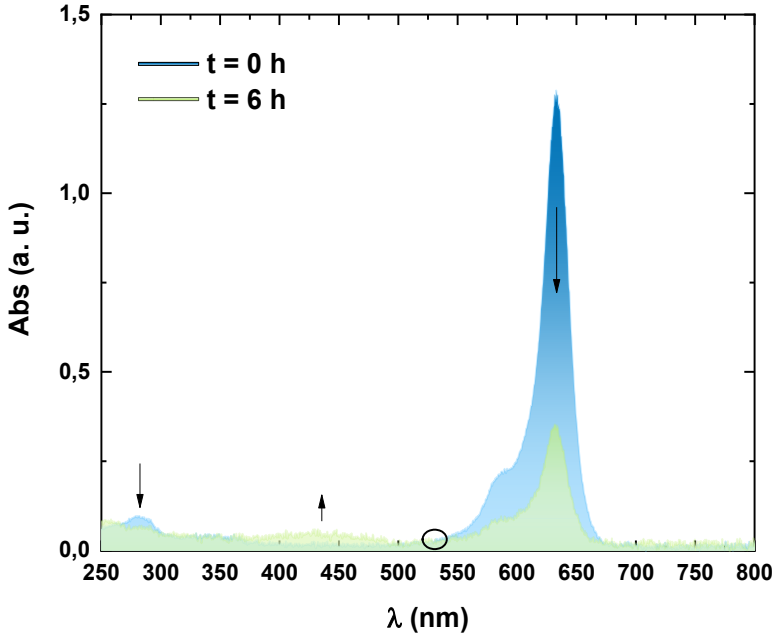


Figure S16. Photodegradation of compound **A** (R=Me)

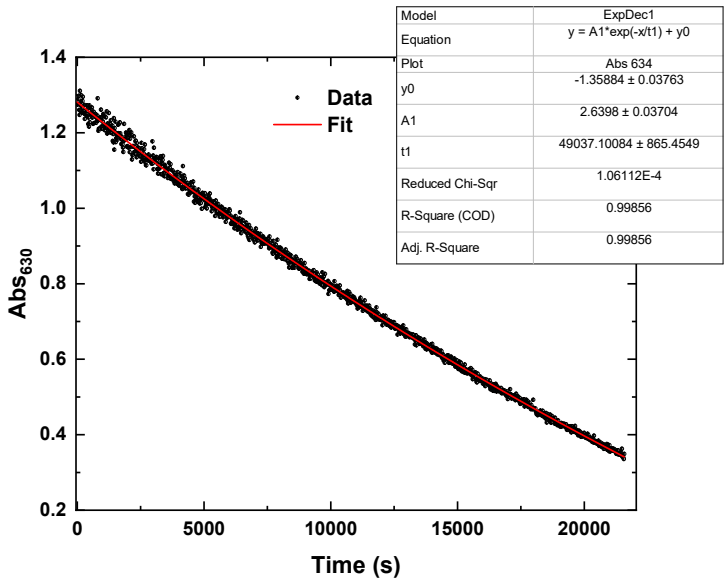


Figure S17. Time profile evolution of the absorbance at 630 nm together with the corresponding monexponential fitting parameters. ($I = 0.44\ mW$, V = 3mL, A_0 = 1.29)

Photodegradation monitoring of compound **2** at 20°C, under irradiation at 560 nm ($I = 0.44\ mW$). Isobestic points located at 507 nm and 588 nm are indicated by the black circles.

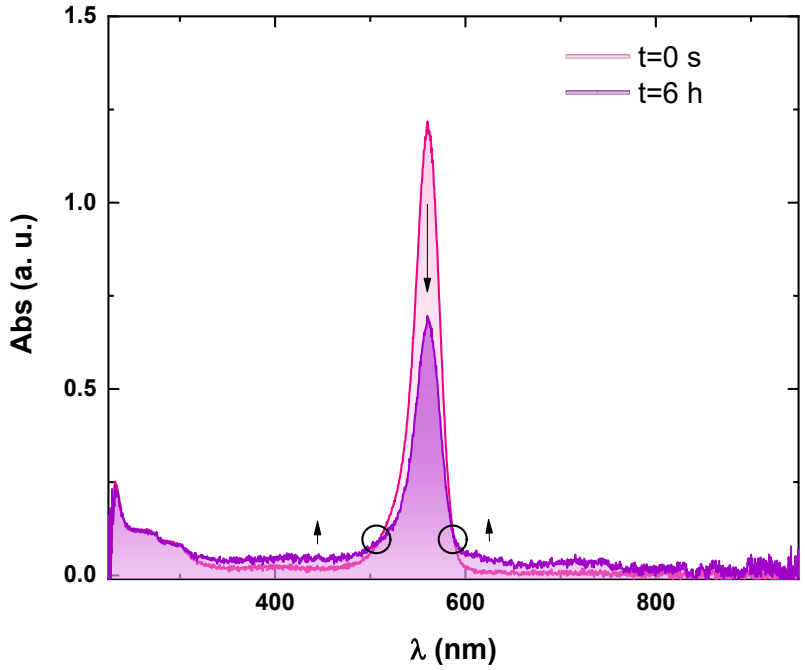


Figure S18. Photodegradation of compound **2**

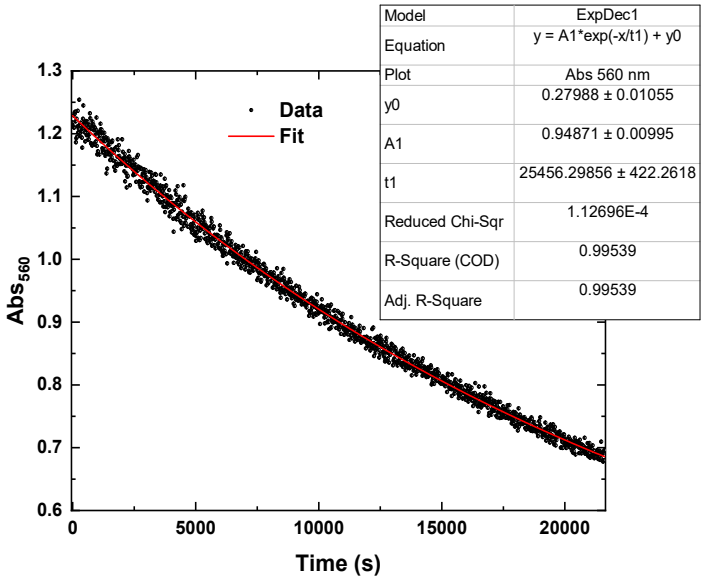


Figure S19. Time profile evolution of the absorbance at 560 nm together with the corresponding monexponential fitting parameters. ($I = 0.44\ mW$, V = 3mL, A_0 = 1.21)

Photodegradation monitoring of compound **5** at 20°C, under irradiation at 590 nm ($I = 0.43\ mW$). Isobestic points located at 532 nm and 630 nm are indicated by the black circles.

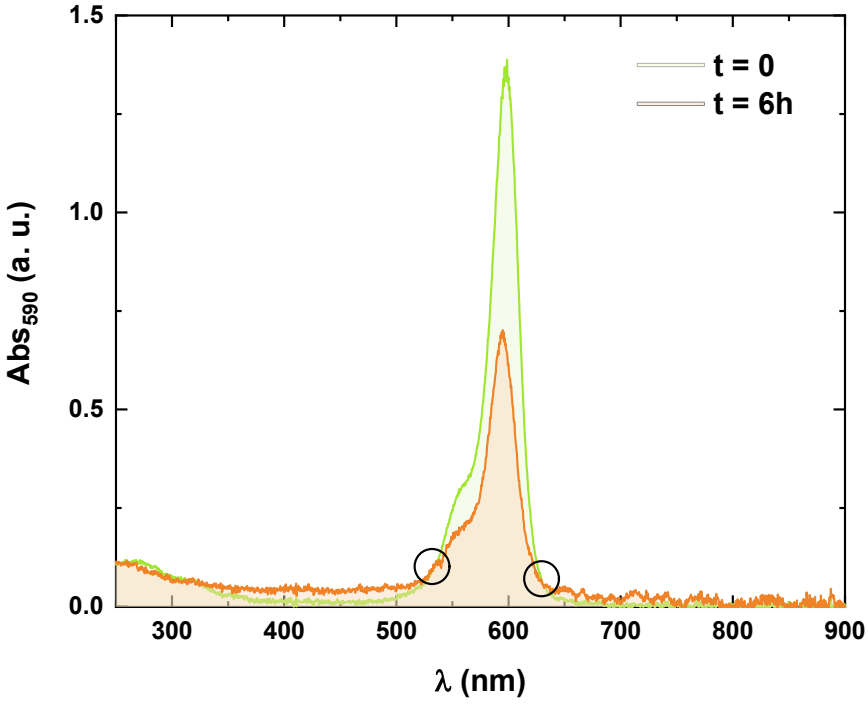


Figure S20. Photodegradation of compound **5**

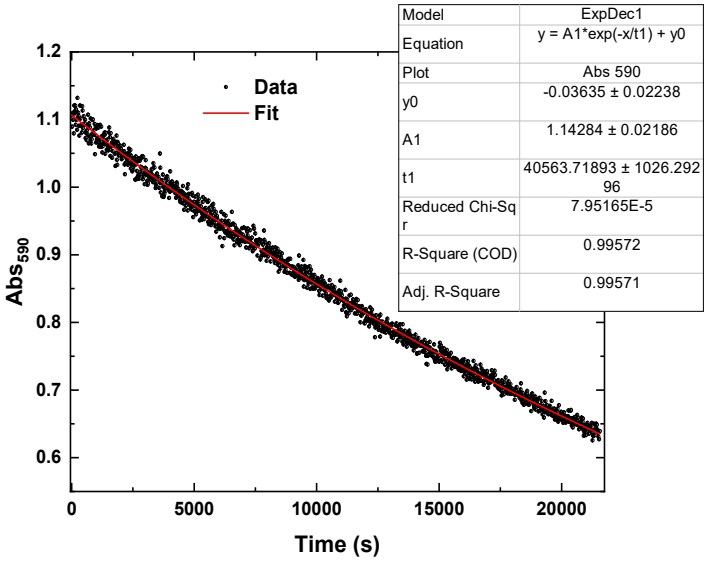


Figure S21. Time profile evolution of the absorbance at 590 nm together with the corresponding monexponential fitting parameters. ($I = 0.43\ mW$, V = 3.1 mL, A_0 = 1.11)

Table S3

Compounds	I_0 (einstein s^{-1})	A_0 (a. u.)	ε^{mol}(L mol^{-1} cm^{-1})	ϕ_{deg}
A (R = Me)	7.72464 10^{-7}	1.28	252000	2.9 10^{-4}
2	6.86635 10^{-7}	1.21	231000	2.5 10^{-4}
5	6.84172 10^{-7}	1.11[a]	165000[a]	2.7 10^{-4}

[a] taken at 590 nm.

NMR Spectra

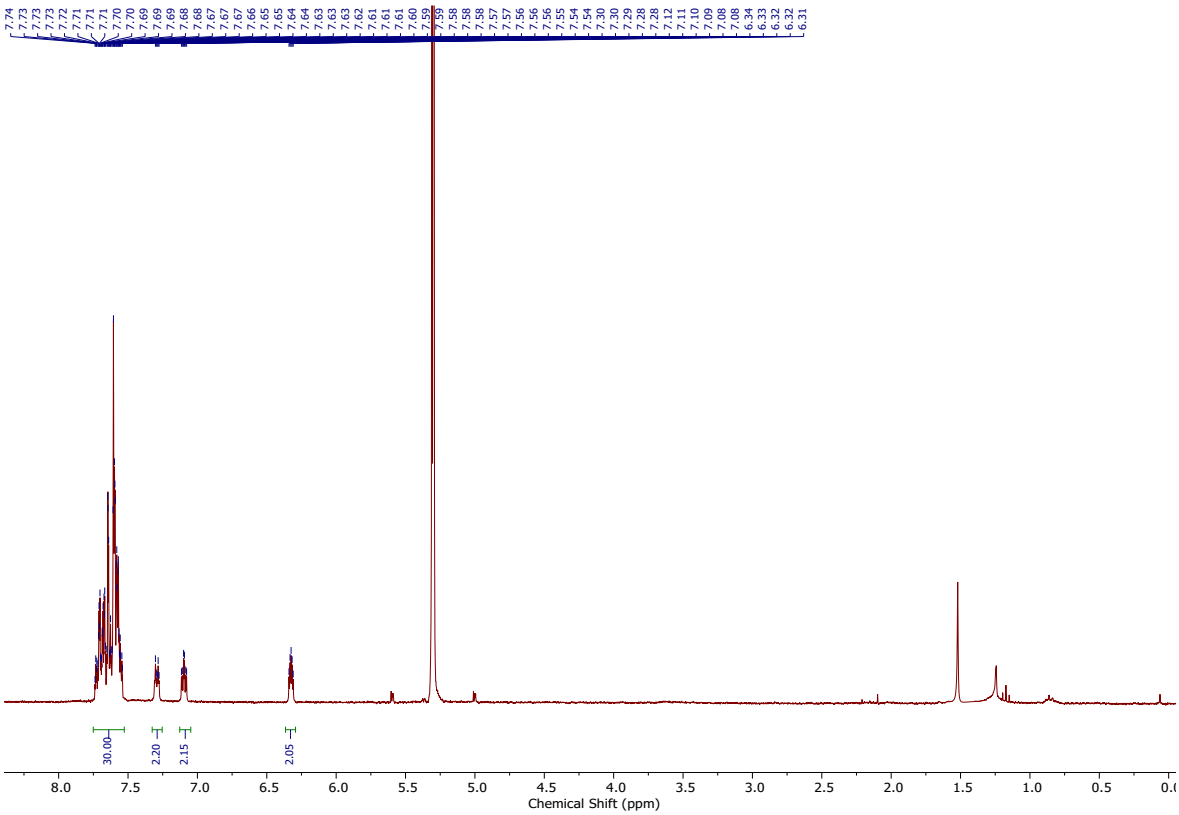


Figure S22: ^{1}H NMR (300 MHz) spectrum of **2** in CD_2Cl_2

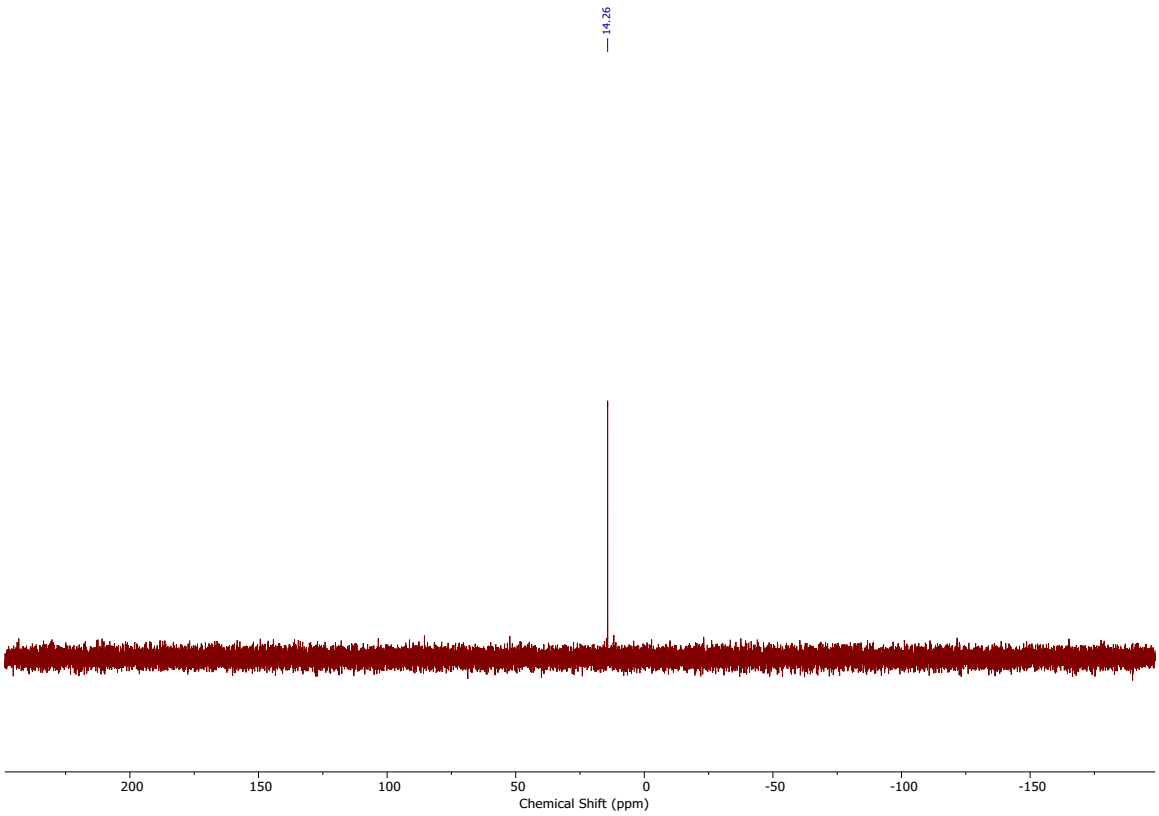


Figure S23: $^{31}P\{^{1}H\}$ NMR (121 MHz) spectrum of **2** in CD_2Cl_2

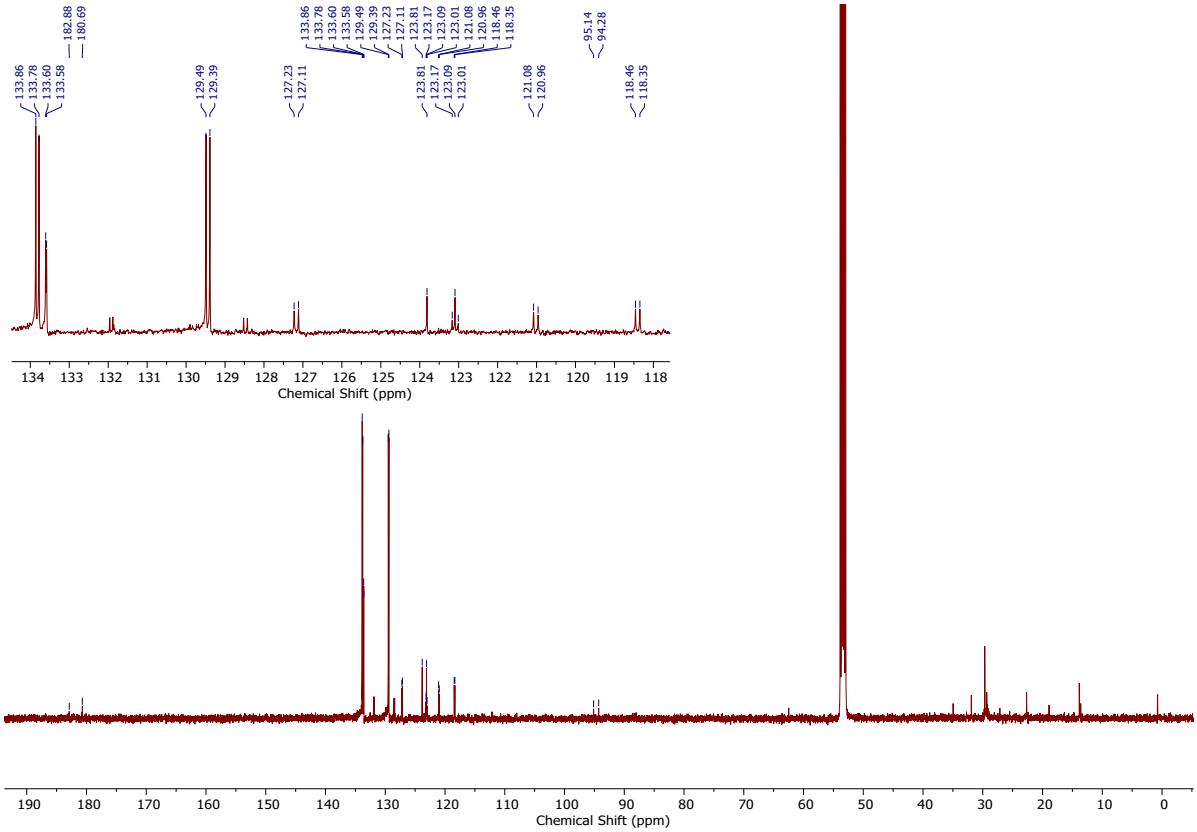


Figure S24: ^{13}C NMR (75 MHz) spectrum of **2** in CD_2Cl_2

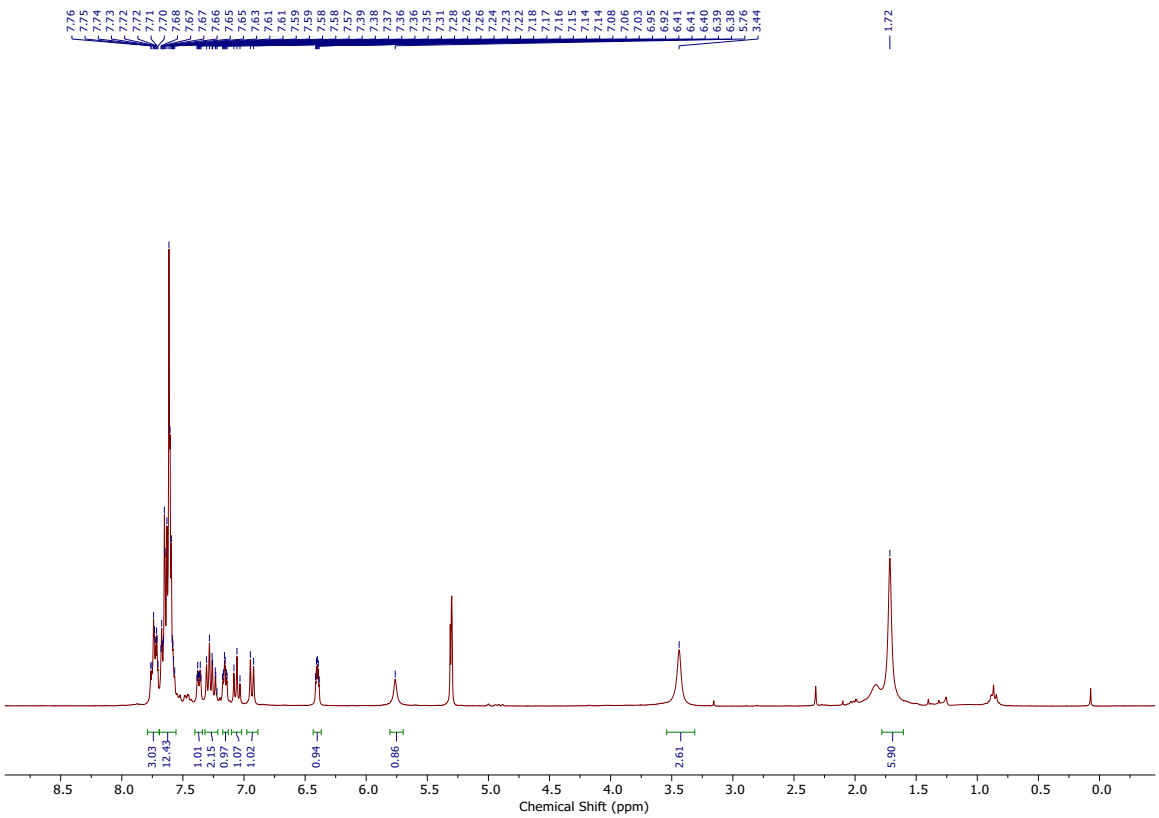


Figure S25: ^{1}H NMR (300 MHz) spectrum of **5** in CD_2Cl_2

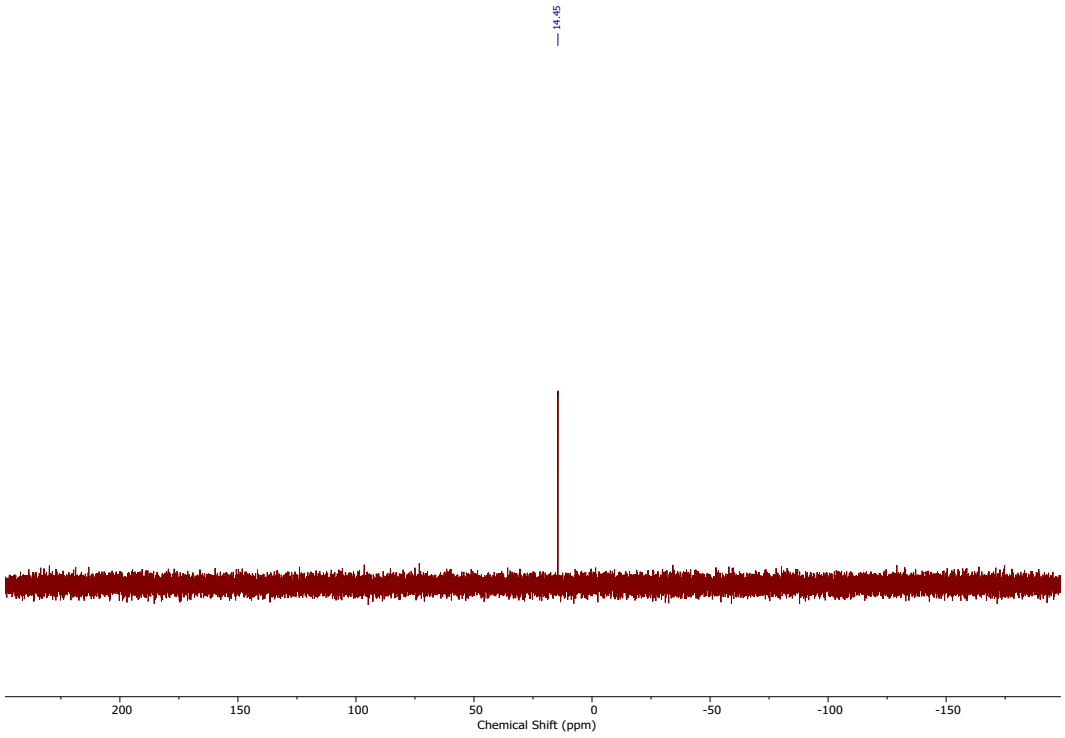


Figure S26: $^{31}P\{^{1}H\}$ NMR (121 MHz) spectrum of **5** in CD_2Cl_2

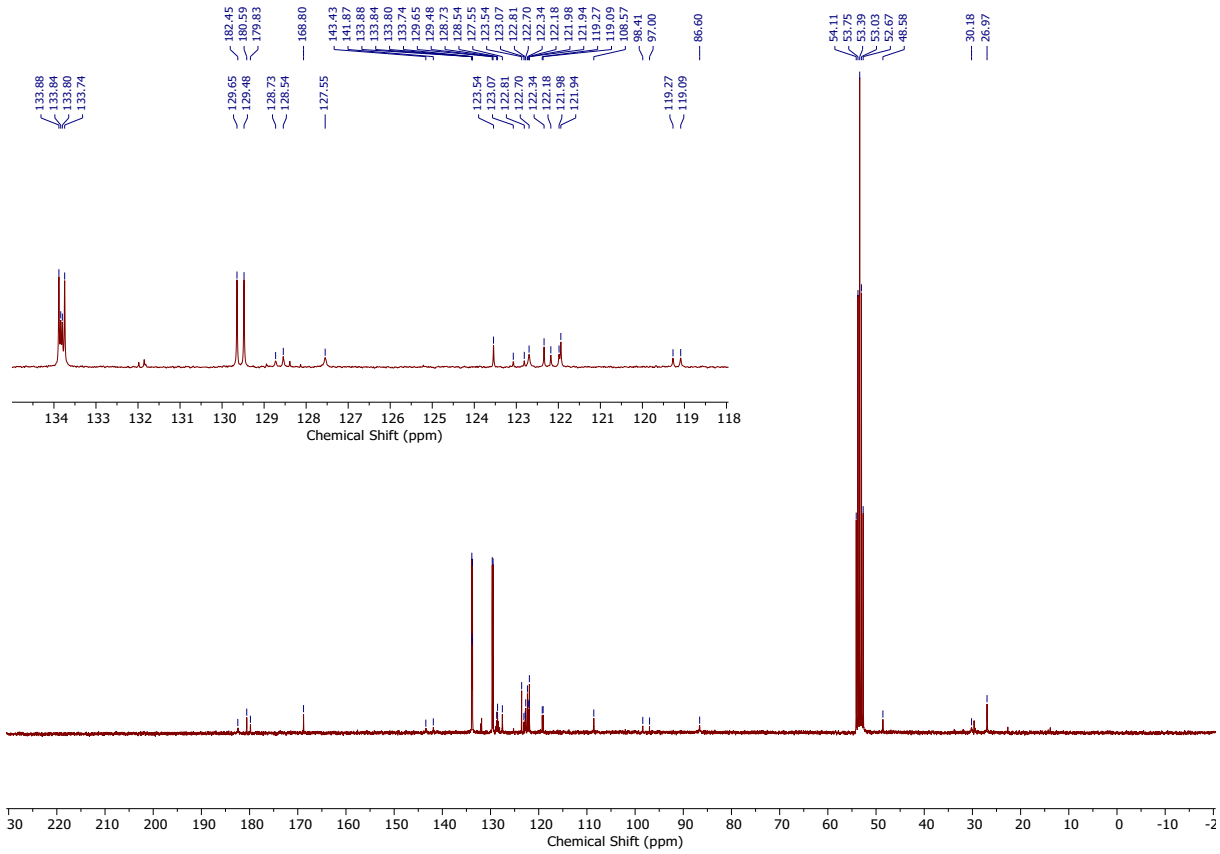


Figure S27: ^{13}C NMR (75 MHz) spectrum of **5** in CD_2Cl_2

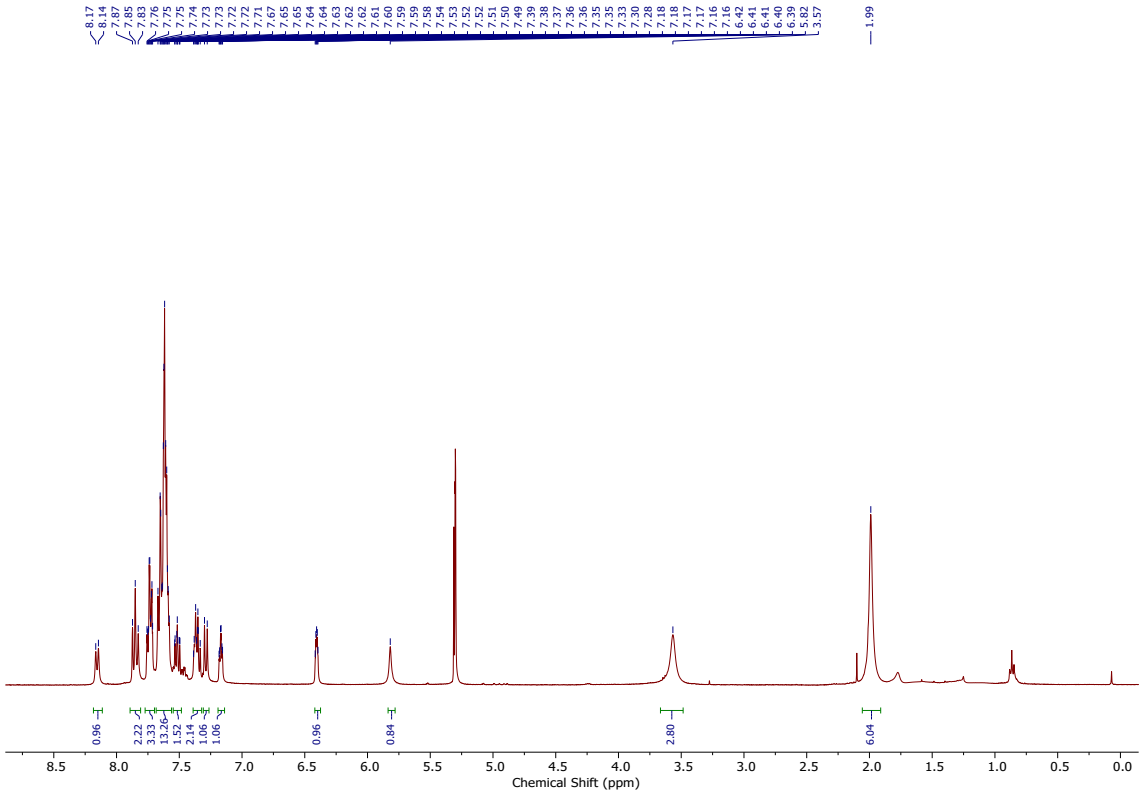


Figure S28: ^{1}H NMR (400 MHz) spectrum of **6** in CD_2Cl_2

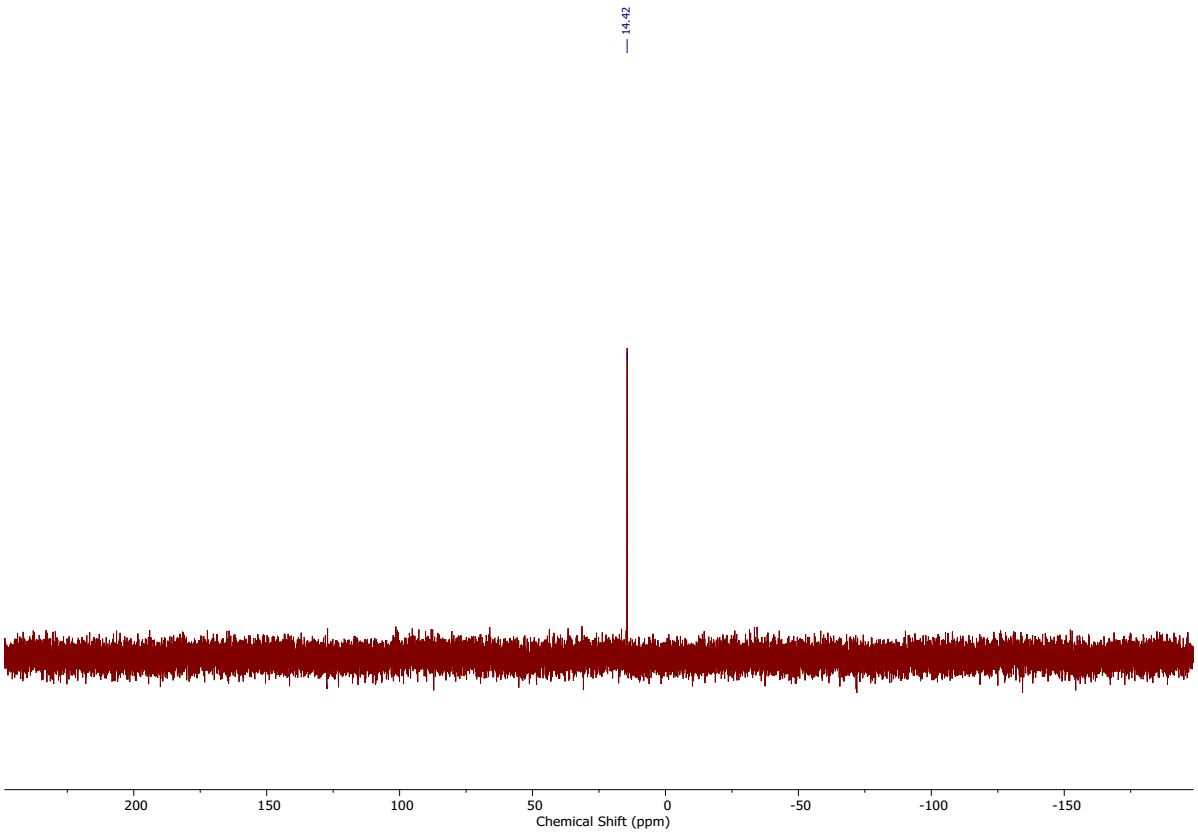


Figure S29: $^{31}P\{^{1}H\}$ NMR (162 MHz) spectrum of **6** in CD_2Cl_2

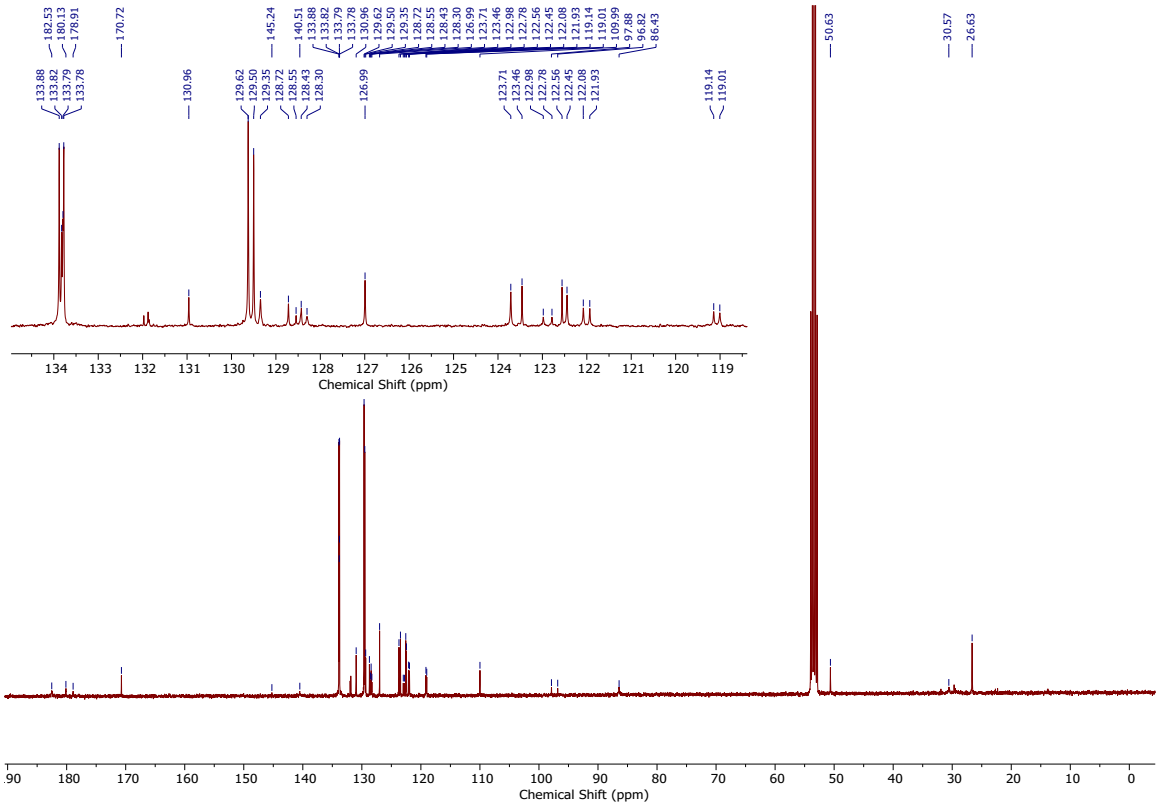


Figure S30: ^{13}C NMR (101 MHz) spectrum of **6** in CD_2Cl_2

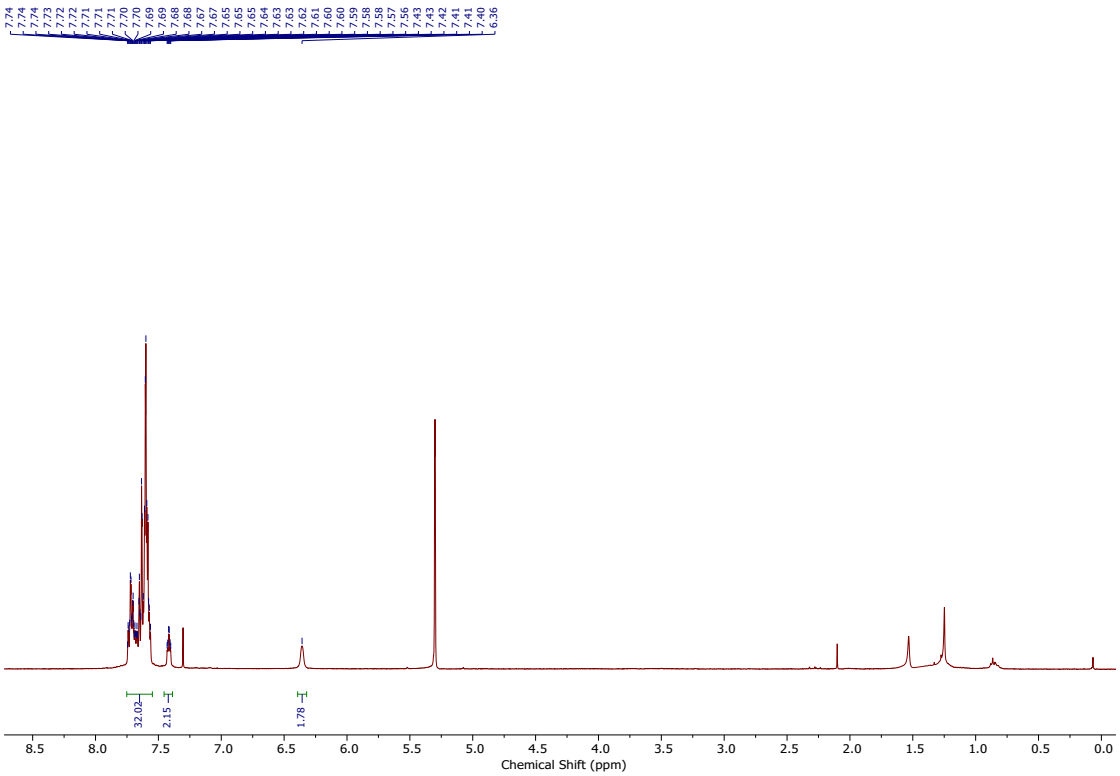


Figure S31: ^{1}H NMR (400 MHz) spectrum of **8** in CD_2Cl_2

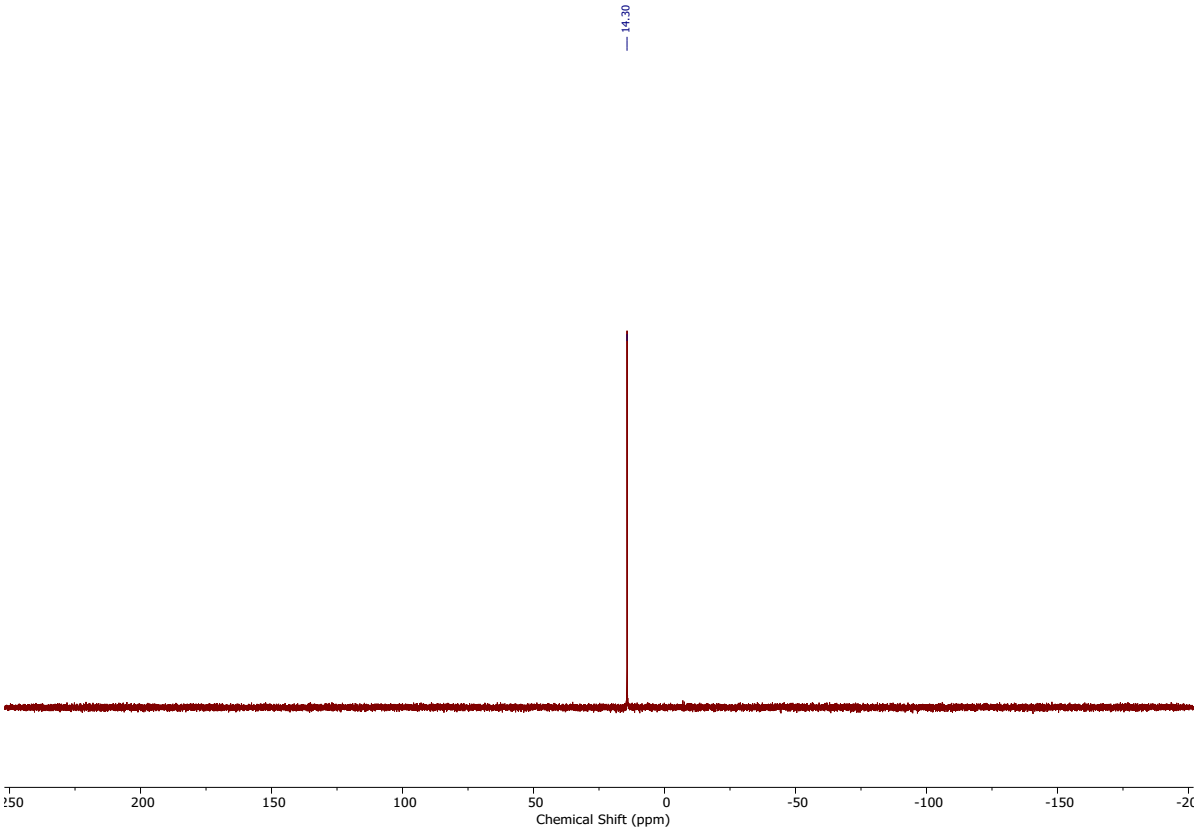


Figure S32: ^{31}P{^{1}H} NMR (162 MHz) spectrum of **8** in CD_2Cl_2

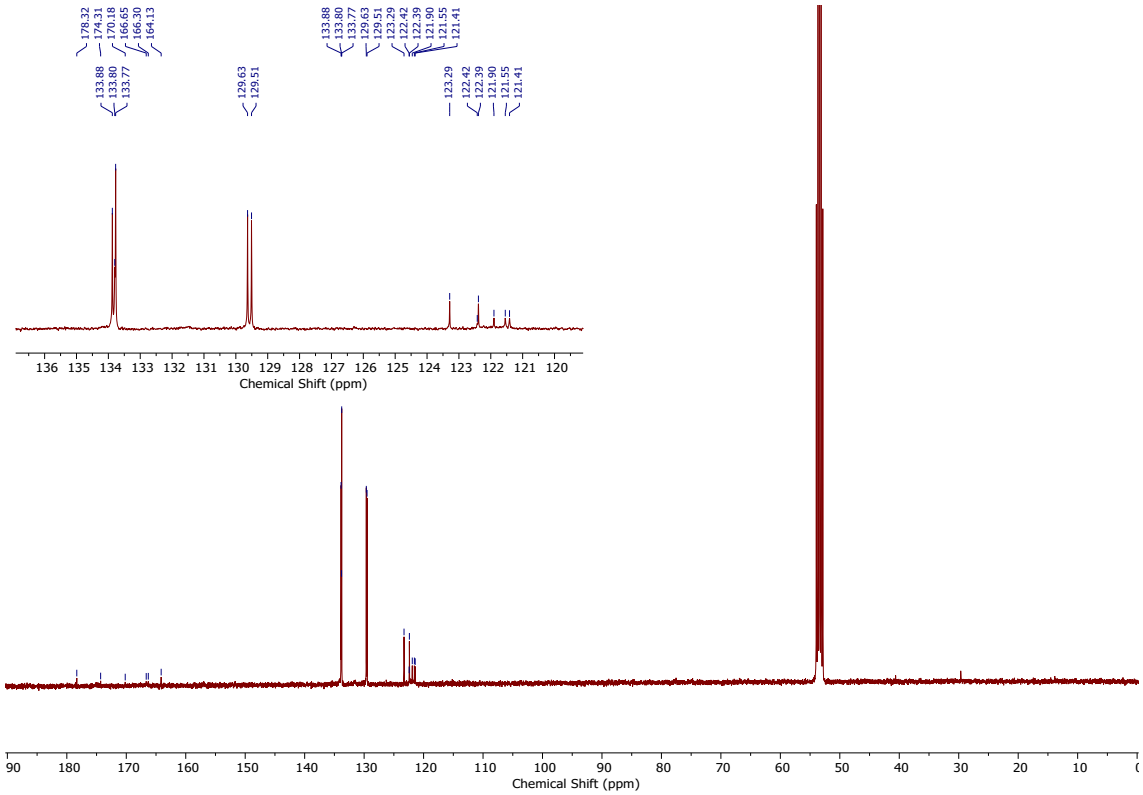


Figure S33: ^{13}C NMR (101 MHz) spectrum of **8** in CD_2Cl_2

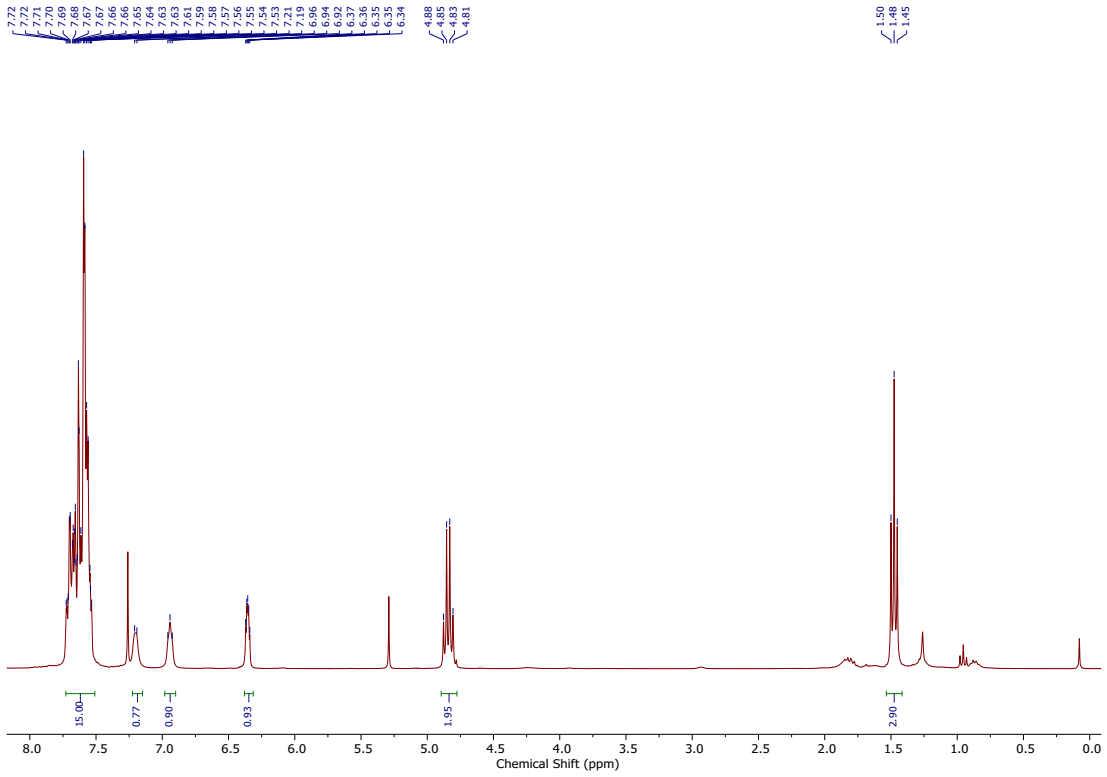


Figure S34: ^{1}H NMR (300 MHz) spectrum of **9** in $CDCl_3$

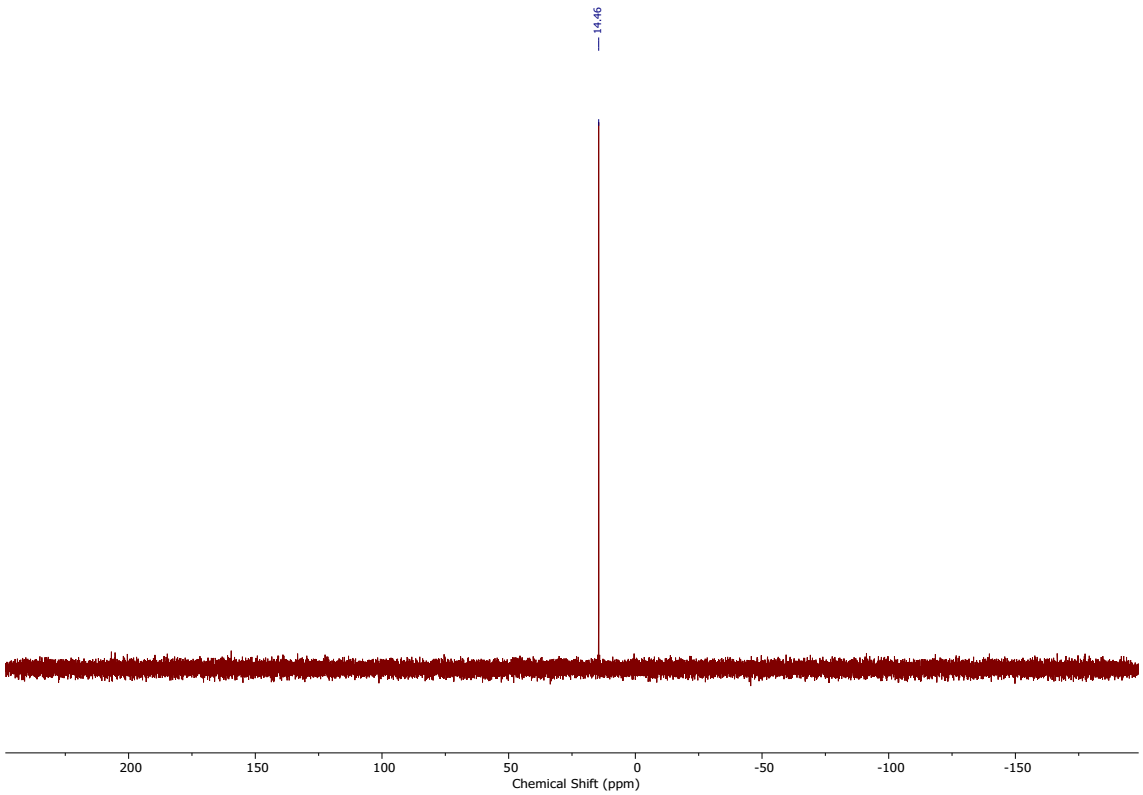


Figure S35: $^{31}P\{^{1}H\}$ NMR (121 MHz) spectrum of **9** in $CDCl_3$

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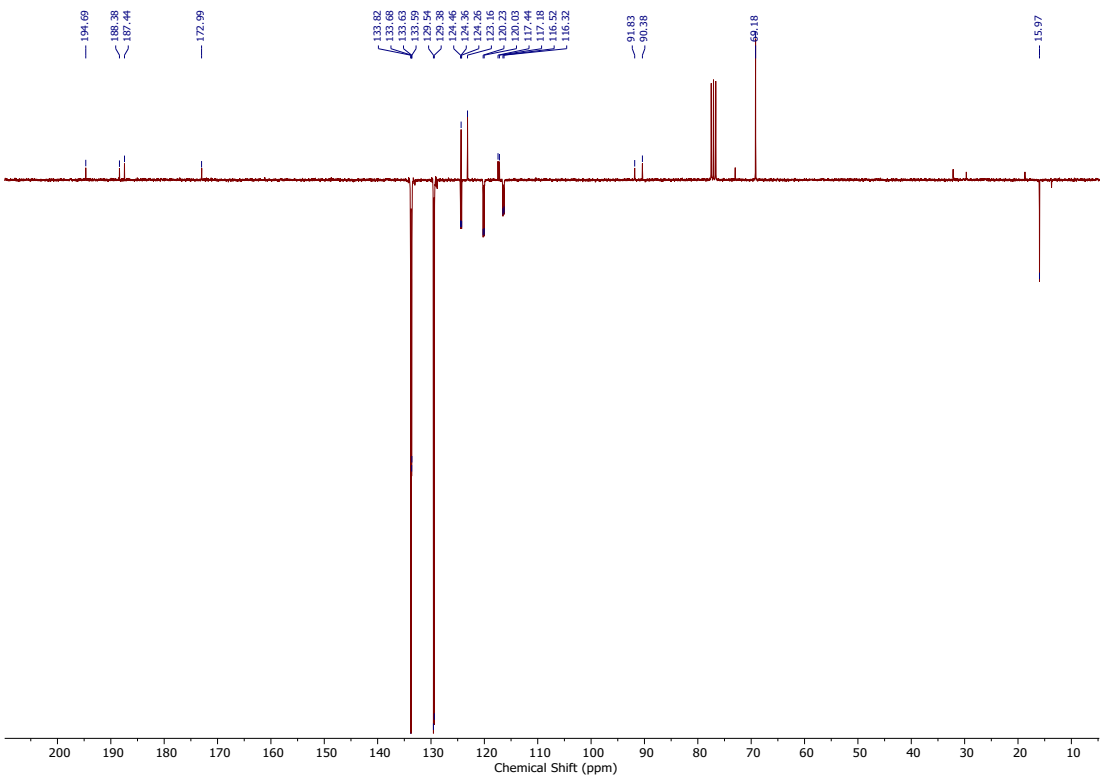

Figure S36: ^{13}C JMOD NMR (75 MHz) spectrum of **9** in $CDCl_3$

Theory

Methods

We have performed the DFT and TD-DFT calculations with Gaussian 16.[12] No structural simplification was performed. Default Gaussian16 thresholds and algorithms were used but for an improved optimization threshold (10^{-5} au on average residual forces), a stricter self-consistent field convergence criterion (10^{-10} a.u. for optimization/frequencies, 10^{-8} a.u. for single-point calculations), an increased two-electron accuracy level (10^{-14} a.u.) and the use of the *superfine* DFT integration grid, the largest pruned grid available in Gaussian.

Firstly, the S_0 geometries have been optimized with DFT and the vibrational frequencies have been analytically determined, using the M06-2X *meta*-GGA hybrid exchange-correlation functional.[13] These calculations were performed with the 6-311G(d,p) atomic basis set and account for solvent effects through the linear-response PCM approach considering CH_2Cl_2 as solvent.[14] We selected CH_2Cl_2, since this aprotic solvent is typically the one the best modeled by the PCM approach. These ground-state optimizations have been carried out starting with a series of chemically-sound conformers and we report below only the results obtained for the most stable ones (lowest free energy). Secondly, starting from the optimal ground-state geometries, we have used TD-DFT with the same functional and basis set to optimize the S_1 geometry and compute the vibrational frequencies. All optimized structures correspond to true minima of the potential energy surface. Thirdly, the vertical transition energies were determined with TD-DFT and the same functional, but a larger basis set, namely 6-311+G(2d,p), in gas-phase as well as in solution using the cLR[2] variant of the PCM,[15] in its *non-equilibrium* limit.

Partial atomic charges have been computed with the MK model, at the PCM-M06-2X/6-311+G(2d,p) level of theory.

As we are aware of the significant dependency of the TD-DFT results on the selected functional,[16] the obtained transition energies were also computed using CC2[17] with the Turbomole 7.3 code.[18] The CC2 energies were calculated in gas phase applying the resolution of identity scheme and the frozen-core approximations, and using the *aug*-cc-pVTZ atomic basis set. Combining the CC2 and TD-DFT data using a well-known protocol,[16] one can obtain accurate CC2-corrected estimates of the absorption, emission and 0-0 energies that can be straightforwardly compared to experimental values.

The vibrationally resolved spectrum was determined with the FCClasses 3.01 program.[19] We used the time-dependent formulation, applied the FC approximation (HT effects were neglected since the transitions are bright), and selected the so-called *Vertical Gradient* and *Vertical Hessian*[20] models for the calculations. We used a simulation temperature of 298K and internal coordinates, as build by default by FCClasses. The broadening function was a Gaussian with an HWM of $50cm^{-1}$.

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[12] M. J. Frisch, et al. Gaussian 16, revision A.03; Gaussian Inc.: Wallingford, CT, 2016.

[13] Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.,* 2008, **120**, 215−241

[14] J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev*., 2005, **105**, 2999−3094

[15] C. A. Guido, A. Chrayteh, G. Sclamani, B. Mennucci, D. Jacquemin *J. Chem. Theory Comput.,* 2021, **17,** 5155−5164.

[16] A. D. Laurent, D. Jacquemin, *Int. J. Quantum Chem.,* 2013, **113**, 2019−2039.

[17] O. Christiansen, H. Koch, P. Jørgensen *Chem. Phys. Lett.*, 1995, **243***,* 409−418.

[18] . Jacquemin, I. Duchemin, X. Blase, *J. Chem. Theory Comput.,* 2015, **11**, 5340−5359.

[19] J. Cerezo and F. Santoro, FCclasses 3.0, http://www.iccom.cnr.it/en/fcclasses/; J. Cerezo and F. Santoro, *J. Comput. Chem.*, 2023, **44**, 626–643

[20] F. Santoro and D. Jacquemin, *WIREs Comput. Mol. Sci.*, 2016, **6**, 460–486.

Optimal ground-state geometries

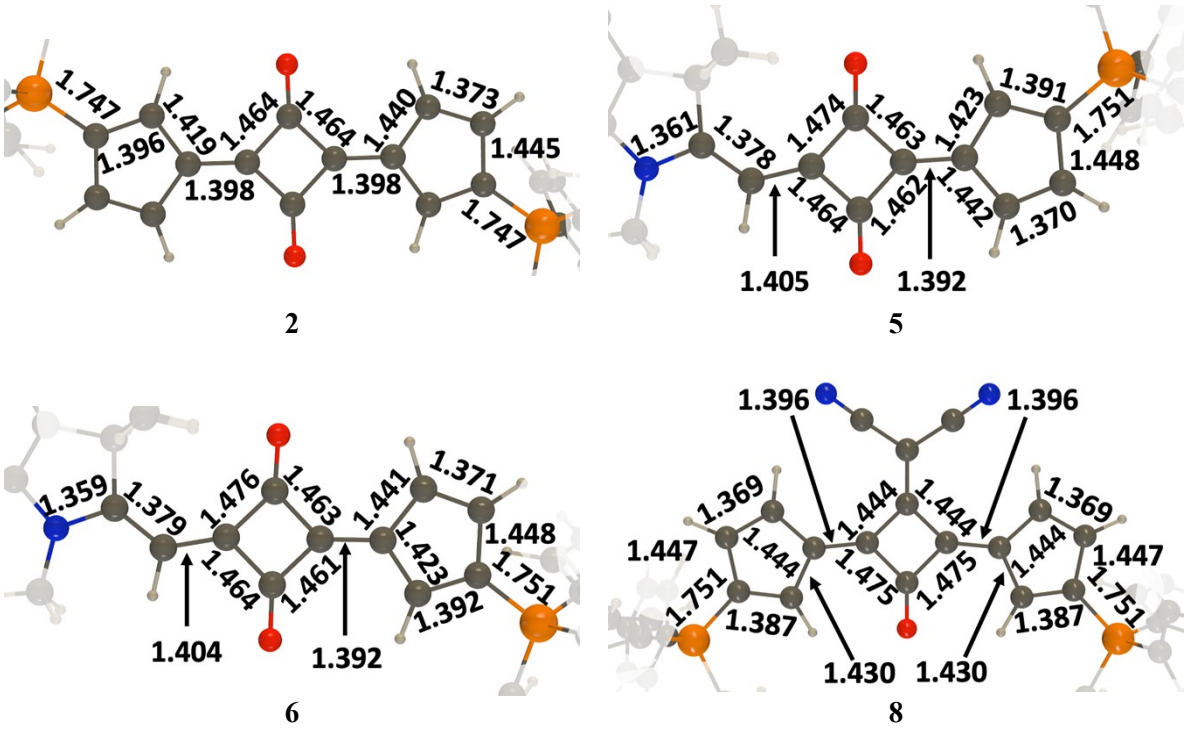
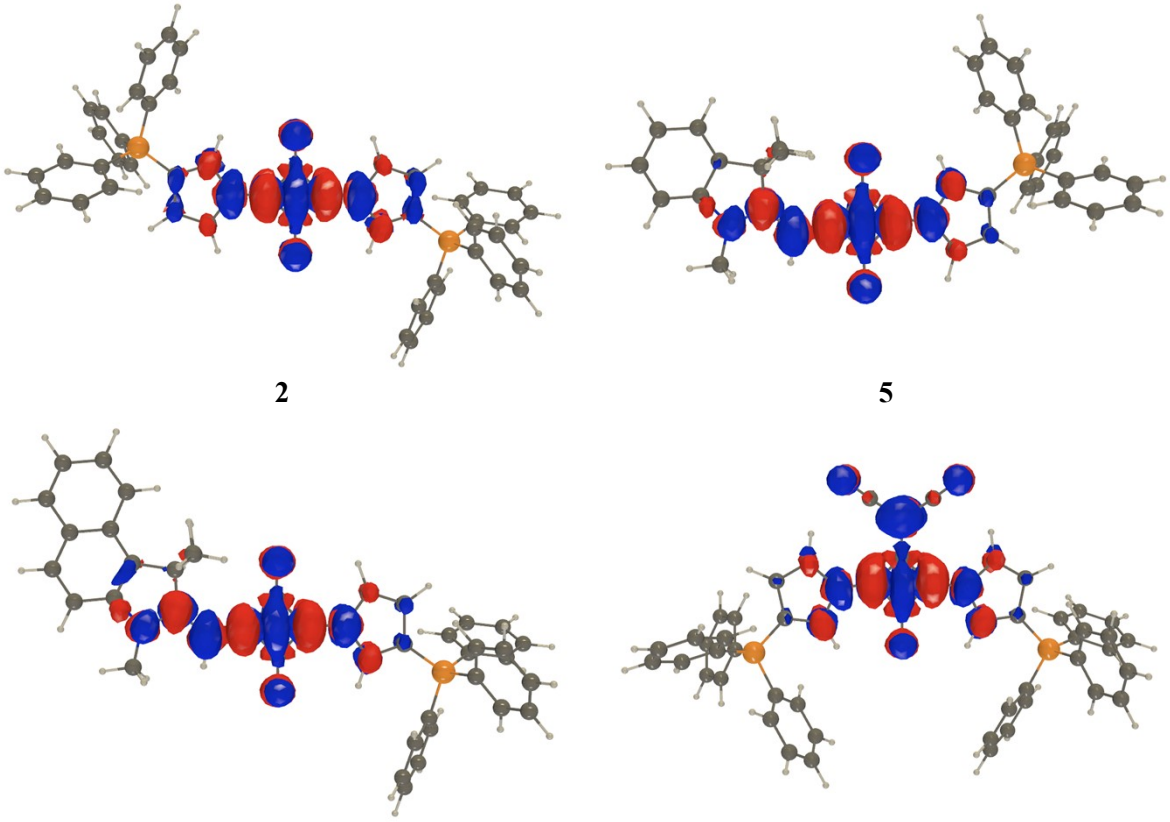


Figure S37: Bond lengths determined by DFT on the optimal ground-state structures along the conjugated pathway. The selected level of theory is PCM-M06-2X/6-311G(d,p). All values are in Å. The side groups are omitted for clarity.

EDD Plots



2 **5**

6 **8**

Figure S38: Electron density difference (EDD) plots corresponding to the absorption to the lowest state. The blue and red lobes represent regions of decrease and increase of density (threshold: 0.001 au). All EDD at the PCM-M06-2X/6-311+G(2d,p) level.

Frontier MOs

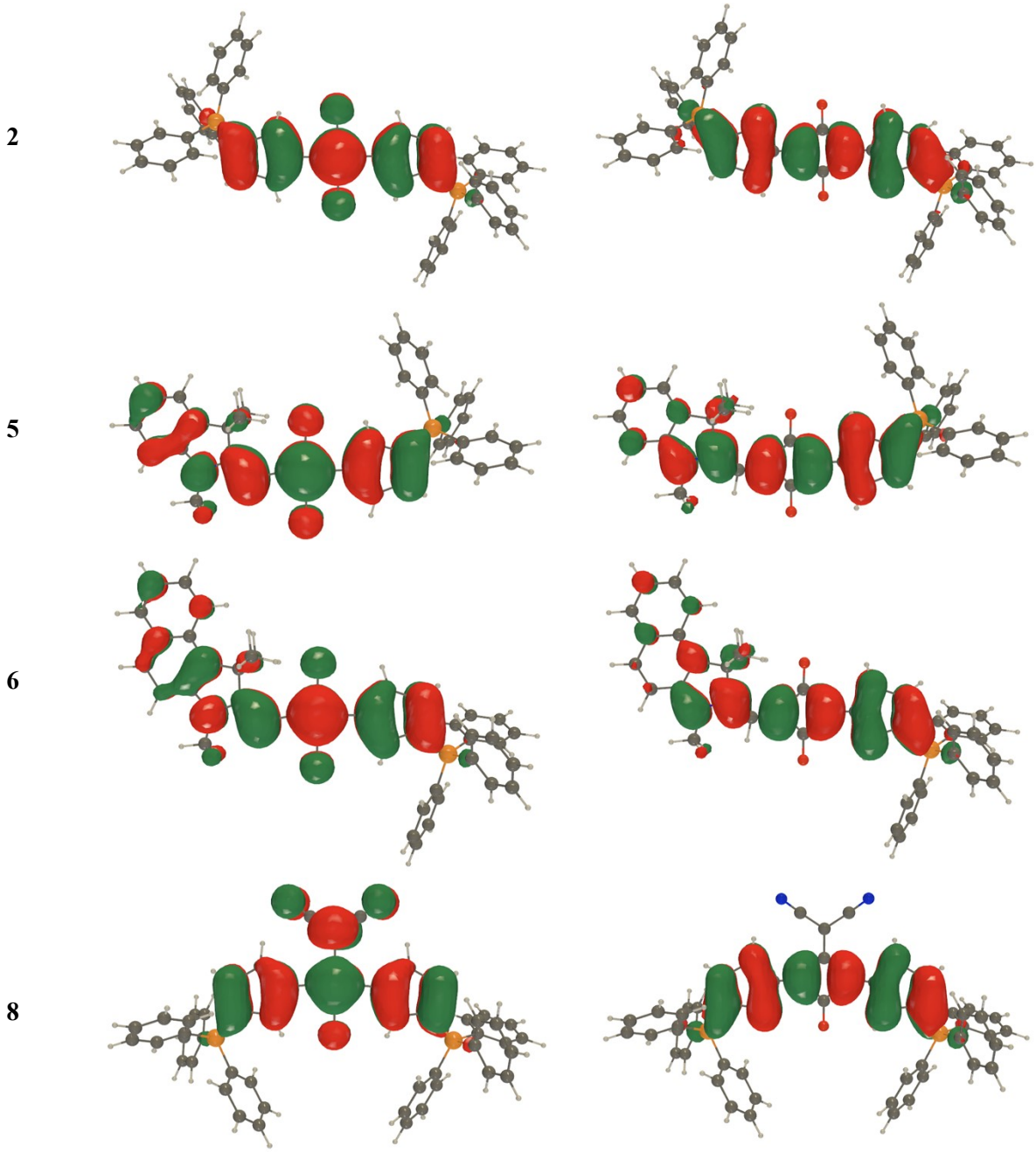
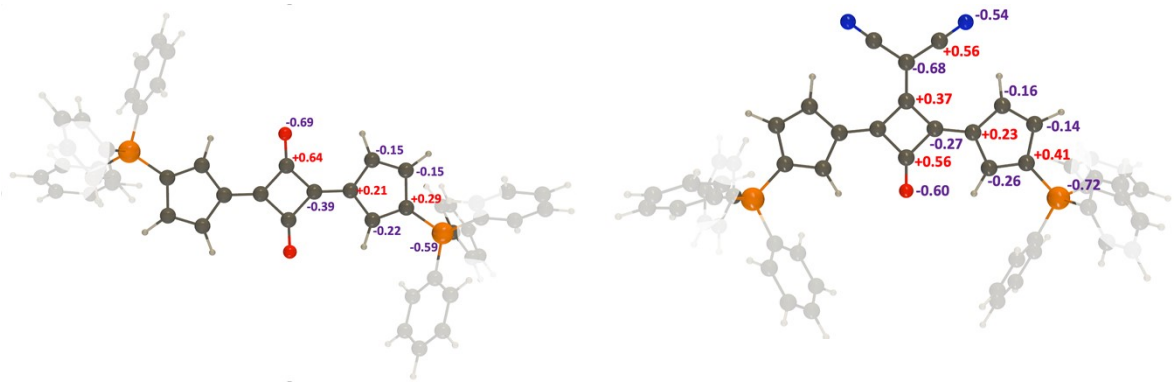


Figure S39: PCM-M06-2X/6-311+G(2d,p) frontier MOs for all four compounds (threshold: 0.02 au).

MK Charges



2 **8**

Figure S40: Computed MK charges in the ground electronic states. The charges of the H atoms are summed up in the charge of the vicinal C atom. In **2**, the total charges are -0.53 *e*, -0.10 e for the central squraine and (each) five member rings. In **8**, the total charges are -1.00 *e*, +0.08 e for the central squraine and (each) five member rings. Calculations at the PCM-M06-2X/6-311+G(2d,p) level.

Computed Optical Properties

Table. S4 TD-DFT absorption wavelength, dominant MO combination and oscillator strength for the lowest singlet absorption (S_0-S_1).

	$\lambda^{vert\text{-}abs}$ (nm)	MO composition	*f*
2	486	HO-LU (97.5%)	1.988
5	519	HO-LU (97.8%)	1.790
6	530	HO-LU (97.4%)	1.879
8	511	HO-LU (97.9%)	1.346

Table. S5 Theoretical best estimates of the vertical absorption and emission wavelengths (in nm) and 0-0 energies (in eV) for all compounds. In the rightmost column, we provide the experimental 0-0 energies for comparisons.

	$\lambda^{vert\text{-}abs}$ (nm)	$\lambda^{vert\text{-}flu}$ (nm)	ΔE^{0-0} (eV)	ΔE^{0-0} (eV), Exp.
2	532	560	2.196	2.175
5	565	588	2.064	2.060
6	579	604	2.012	1.990
8	560	606	2.089	2.009

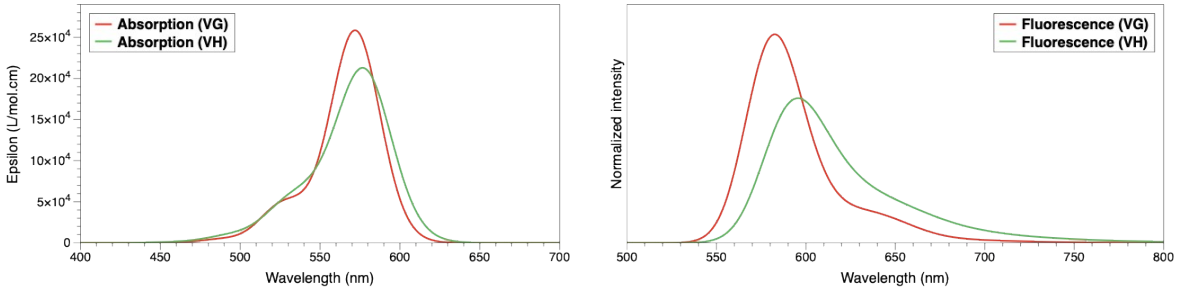


Figure S41: Computed vibrationally-resolved spectra for **5** for the absorption (left) and emission (right) using the VG and VHvibronic models. The integration of the emission spectra delivers estimated radiative rate constants (kr) of 2.7 and 3.0 x 10^8 s^{-1} for VH and VG, respectively

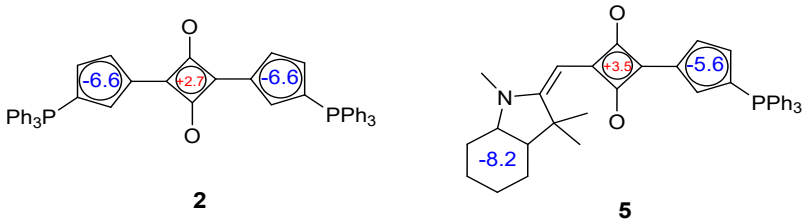


Figure S42: NICS(0) aromaticity pattern of **2** and **5** , PCM(CH2Cl2)-B3LYP/6-311+G(d,p).

Table S6: NBO, PCM(CH2Cl2)-M06-2X/6-311+G(2d,p).

Compound **2**, P-$C_{cyclopentadienyl}$ bond[23-11]

Natural charges: P: 1.67 e, C: -0.57 e,

Bonding (occupation: 1.97): C (s:29.8%, p: 70.0%), P (s:27.9%, p: 71.5%).

Anti-Bonding (occupation: 0.05) C (s:29.8%, p: 70.0%), P (s:27.9%, p: 71.5%)

Compound **5**, P-$C_{cyclopentadienyl}$ bond [16-11]

Natural charges: P: 1.67 e, C: -0.56 e

Bonding (occupation: 1.97): C (s:29.8%, p: 70.0%), P (s:27.6%, p: 71.8%).

Anti-Bonding (occupation: 0.05) C (s:29.8%, p: 70.0%), P (s:27.6%, p: 71.8%)

Cartesian coordinates

We produce below the Cartesian coordinates of all optimized geometries. All structures are true minima.

2 – S_0 – G= -2759.082576 au.

C	0.9838130	0.2858130	-0.1225010
C	0.3125560	-0.8954270	0.4233940
C	-0.9838110	-0.2858340	0.1224720
C	-0.3125560	0.8954050	-0.4234250
O	-0.6859360	1.9525720	-0.9229410
O	0.6859390	-1.9525940	0.9229100
C	-2.8103470	-1.8912190	0.8519120
C	-3.4404760	0.1205340	-0.1005940
C	-4.1825480	-1.8702080	0.8133670
H	-2.1817240	-2.6870820	1.2254040
C	-4.5828710	-0.6156600	0.2173270
H	-3.3926700	1.0950170	-0.5659370
H	-4.8581690	-2.6469380	1.1463000
C	2.8103470	1.8912000	-0.8519350
C	3.4404770	-0.1205490	0.1005790
C	4.1825480	1.8701930	-0.8133830
H	2.1817240	2.6870610	-1.2254310
C	4.5828700	0.6156450	-0.2173390
H	3.3926700	-1.0950320	0.5659230
H	4.8581690	2.6469250	-1.1463130
C	-2.3208790	-0.6610750	0.2865050
C	2.3208790	0.6610560	-0.2865290
P	-6.2302310	-0.0663220	0.0275240
P	6.2302360	0.0663240	-0.0275220
C	-7.2525670	-1.4198580	-0.6067090
C	-6.6704940	-2.3335700	-1.4904930
C	-8.6019510	-1.5303730	-0.2653610
C	-7.4453910	-3.3497630	-2.0367070
H	-5.6182510	-2.2519260	-1.7389730
C	-9.3681530	-2.5515500	-0.8152370
H	-9.0530560	-0.8349080	0.4323800
C	-8.7916820	-3.4574010	-1.7003730
H	-6.9955710	-4.0594670	-2.7197110
H	-10.4134740	-2.6416180	-0.5474530
H	-9.3918190	-4.2532640	-2.1245920
C	-6.9625080	0.5168040	1.5808310
C	-6.4285220	0.0781820	2.7930380
C	-8.0619620	1.3805390	1.5628550
C	-7.0055330	0.4951040	3.9877850
H	-5.5607260	-0.5723320	2.7996360
C	-8.6320350	1.7911330	2.7613770
H	-8.4645580	1.7378940	0.6208650
C	-8.1050670	1.3469020	3.9715420
H	-6.5901400	0.1598340	4.9299270
H	-9.4819250	2.4621380	2.7505030
H	-8.5490290	1.6729530	4.9043280
C	-6.3024800	1.3213960	-1.1287410
C	-5.8327320	2.5691400	-0.7063460
C	-6.7741190	1.1461320	-2.4294050
C	-5.8278920	3.6360600	-1.5948370
H	-5.4757870	2.7059140	0.3089420
C	-6.7708590	2.2229520	-3.3101720
H	-7.1446820	0.1808260	-2.7544210
C	-6.2970460	3.4624020	-2.8947920
H	-5.4600360	4.6019160	-1.2721570
H	-7.1391770	2.0908200	-4.3198020
H	-6.2944000	4.2978410	-3.5842840
C	6.3024860	-1.3214050	1.1287290

C	6.7741270	-1.1461570	2.4293940
C	5.8327390	-2.5691440	0.7063190
C	6.7708700	-2.2229880	3.3101470
H	7.1446900	-0.1808540	2.7544210
C	5.8279010	-3.6360750	1.5947960
H	5.4757930	-2.7059070	-0.3089700
C	6.2970570	-3.4624340	2.8947530
H	7.1391900	-2.0908700	4.3197790
H	5.4600450	-4.6019270	1.2721040
H	6.2944130	-4.2978800	3.5842340
C	7.2525440	1.4198660	0.6067370
C	8.6019260	1.5304180	0.2653910
C	6.6704510	2.3335480	1.4905390
C	9.3681050	2.5516010	0.8152870
H	9.0530450	0.8349770	-0.4323630
C	7.4453250	3.3497470	2.0367730
H	5.6182090	2.2518770	1.7390170
C	8.7916140	3.4574210	1.7004410
H	10.4134240	2.6416980	0.5475050
H	6.9954900	4.0594280	2.7197910
H	9.3917320	4.2532900	2.1246750
C	6.9625330	-0.5167820	-1.5808270
C	8.0620050	-1.3804930	-1.5628450
C	6.4285380	-0.0781780	-2.7930370
C	8.6320890	-1.7910790	-2.7613650
H	8.4646090	-1.7378350	-0.6208540
C	7.0055590	-0.4950940	-3.9877810
H	5.5607280	0.5723180	-2.7996390
C	8.1051120	-1.3468670	-3.9715320
H	9.4819950	-2.4620640	-2.7504870
H	6.5901600	-0.1598380	-4.9299270
H	8.5490820	-1.6729130	-4.9043170

2 – S_1 – G= -2759.001784 au.

C	1.0180760	0.3323640	-0.0234350
C	0.3050570	-0.9043700	0.3662610
C	-1.0056320	-0.2468630	0.1725440
C	-0.2926240	0.9907650	-0.2157010
O	-0.6501160	2.1093420	-0.5600070
O	0.6627330	-2.0239440	0.7075900
C	-2.8347880	-1.9663800	0.5501720
C	-3.4739840	0.1714500	-0.0943770
C	-4.2004610	-1.9596000	0.4559210
H	-2.2044550	-2.8038680	0.8139060
C	-4.6095600	-0.6268170	0.0453160
H	-3.4305930	1.2094200	-0.3930560
H	-4.8741390	-2.7871470	0.6350280
C	2.8624920	2.0216700	-0.4712750
C	3.4834660	-0.1116550	0.2047220
C	4.2300090	1.9935050	-0.4126100
H	2.2399080	2.8640490	-0.7377350
C	4.6279400	0.6637330	0.0185680
H	3.4298770	-1.1431780	0.5234160
H	4.9123240	2.8046140	-0.6298100
C	-2.3391720	-0.6470520	0.2097480
C	2.3544810	0.7182000	-0.0903800
P	-6.2620250	-0.0645960	-0.0077140
P	6.2671800	0.0623410	0.0082900
C	-7.3282870	-1.3947920	-0.6143330
C	-6.8417340	-2.2358910	-1.6206210
C	-8.6252100	-1.5605080	-0.1240540
C	-7.6576970	-3.2368050	-2.1336840
H	-5.8305560	-2.1104520	-1.9912310

C	-9.4337150	-2.5647800	-0.6439870
H	-9.0009800	-0.9212220	0.6659530
C	-8.9516990	-3.3998100	-1.6470870
H	-7.2808520	-3.8906030	-2.9102670
H	-10.4376270	-2.6973010	-0.2603840
H	-9.5841670	-4.1828500	-2.0475460
C	-6.8816630	0.4605350	1.6174520
C	-6.2707140	-0.0448970	2.7654060
C	-7.9651670	1.3381290	1.7189460
C	-6.7535790	0.3206970	4.0173070
H	-5.4178520	-0.7097420	2.6764360
C	-8.4421990	1.6960440	2.9739080
H	-8.4289080	1.7447110	0.8262580
C	-7.8372970	1.1867970	4.1204770
H	-6.2783480	-0.0659170	4.9102310
H	-9.2806660	2.3764330	3.0567110
H	-8.2085960	1.4725860	5.0972400
C	-6.4108870	1.3773070	-1.0913940
C	-5.9219860	2.6084120	-0.6426490
C	-6.9561500	1.2574080	-2.3696690
C	-5.9712020	3.7133440	-1.4824340
H	-5.5108980	2.7043040	0.3566820
C	-7.0077710	2.3716860	-3.2006780
H	-7.3426610	0.3055760	-2.7152300
C	-6.5139330	3.5945650	-2.7595170
H	-5.5889660	4.6663300	-1.1386900
H	-7.4347160	2.2820430	-4.1917600
H	-6.5540250	4.4594640	-3.4104460
C	6.4479710	-1.3323890	1.1480940
C	7.0659370	-1.1670580	2.3877190
C	5.9092170	-2.5710180	0.7852430
C	7.1404700	-2.2430890	3.2660090
H	7.4911020	-0.2098380	2.6665590
C	5.9817360	-3.6371970	1.6721240
H	5.4418500	-2.7035470	-0.1847350
C	6.5971570	-3.4729180	2.9105810
H	7.6239420	-2.1182950	4.2268710
H	5.5610330	-4.5956280	1.3948440
H	6.6553630	-4.3078040	3.5983130
C	7.3961940	1.3920340	0.4873520
C	8.6627200	1.5069010	-0.0894210
C	6.9905230	2.2873280	1.4827670
C	9.5217710	2.5147900	0.3334990
H	8.9754710	0.8252070	-0.8714360
C	7.8564440	3.2914370	1.8983100
H	6.0022550	2.2012740	1.9203650
C	9.1202910	3.4037280	1.3256830
H	10.5020160	2.6077580	-0.1170810
H	7.5419380	3.9870650	2.6662610
H	9.7919450	4.1891790	1.6504540
C	6.7714420	-0.5543750	-1.6246620
C	7.8284510	-1.4602080	-1.7531740
C	6.0944510	-0.0919660	-2.7537010
C	8.2142390	-1.8884430	-3.0174660
H	8.3416100	-1.8350290	-0.8737190
C	6.4860530	-0.5280440	-4.0148740
H	5.2609900	0.5938140	-2.6414000
C	7.5443940	-1.4213760	-4.1457550
H	9.0320360	-2.5907540	-3.1212870
H	5.9594120	-0.1751380	-4.8927840
H	7.8444480	-1.7620280	-5.1293910

5 – S_0 – G= -2051.097240 au.

C	-3.0815380	-1.4781400	-0.0423690
C	-2.0943950	-2.5591940	-0.0755100
C	-1.0104360	-1.5794920	-0.0237600
C	-1.9880290	-0.4913830	0.0069000
O	-1.8746000	0.7311200	0.0538530
O	-2.1769200	-3.7796310	-0.1272590
C	1.2153140	-2.7960620	-0.0400540
C	1.2293810	-0.4792690	0.0272410
C	2.5252610	-2.3943670	-0.0140020
H	0.8464430	-3.8116700	-0.0624930
C	2.5396310	-0.9465350	0.0268490
H	0.8915090	0.5465800	0.0635040
H	3.4027090	-3.0271680	-0.0064540
C	0.3804730	-1.6210060	-0.0147610
C	-4.4721940	-1.6735930	-0.0656440
P	3.9741020	0.0570800	-0.0023490
C	5.1943640	-0.5990790	1.1621370
C	4.7348850	-1.2118000	2.3317190
C	6.5639550	-0.4576610	0.9298400
C	5.6504760	-1.6734380	3.2697720
H	3.6703270	-1.3316660	2.4992350
C	7.4716410	-0.9245640	1.8732240
H	6.9241520	0.0016450	0.0168700
C	7.0157120	-1.5288380	3.0409440
H	5.2967430	-2.1502720	4.1752900
H	8.5342200	-0.8206720	1.6926790
H	7.7267700	-1.8937190	3.7721960
C	4.7370420	0.1383110	-1.6440940
C	4.5042160	-0.8901120	-2.5582800
C	5.5692740	1.2102570	-1.9806960
C	5.1169270	-0.8501410	-3.8059230
H	3.8382890	-1.7064050	-2.3011590
C	6.1773120	1.2409020	-3.2295060
H	5.7332730	2.0203910	-1.2780450
C	5.9526890	0.2107750	-4.1391410
H	4.9343930	-1.6444550	-4.5188250
H	6.8199090	2.0713680	-3.4940210
H	6.4247720	0.2404040	-5.1136580
C	3.5594140	1.7525140	0.4648620
C	2.8544490	2.5444440	-0.4473590
C	3.8973640	2.2511720	1.7226310
C	2.4817860	3.8332250	-0.0901370
H	2.6014520	2.1580240	-1.4290120
C	3.5240240	3.5458710	2.0686900
H	4.4499000	1.6395390	2.4264440
C	2.8169600	4.3325270	1.1663410
H	1.9324390	4.4475140	-0.7923690
H	3.7873950	3.9372400	3.0433160
H	2.5271660	5.3397080	1.4401300
H	-4.7352610	-2.7268180	-0.1147640
C	-5.5131300	-0.7717270	-0.0346760
C	-5.4741260	0.7502570	0.0395960
C	-6.9475400	1.0901820	0.0453670
C	-7.6939870	-0.0855430	-0.0201510
C	-4.7844420	1.3463660	-1.1988230
H	-3.7234100	1.0998810	-1.1950120
H	-5.2519240	0.9772830	-2.1141280
H	-4.8855820	2.4343820	-1.1738840
C	-4.8011750	1.2216400	1.3391860
H	-4.8973540	2.3075380	1.4174970
H	-5.2834600	0.7687620	2.2079940
H	-3.7412690	0.9707200	1.3275710
N	-6.8121460	-1.1765820	-0.0671750

C	-7.2225490	-2.5654330	-0.1373530
H	-6.8289210	-3.0298410	-1.0438040
H	-6.8543300	-3.1125690	0.7329840
H	-8.3069650	-2.6190380	-0.1555020
C	-9.0819810	-0.0745160	-0.0315980
C	-9.7127750	1.1695750	0.0257640
H	-10.7953420	1.2094120	0.0185430
C	-7.5832010	2.3153440	0.1017720
C	-8.9808800	2.3515270	0.0918690
H	-9.4968160	3.3025110	0.1356820
H	-9.6681440	-0.9826850	-0.0822590
H	-7.0084860	3.2340740	0.1529480

5 – S_1 – G= -2051.021163 au.

C	3.1218420	-1.4450700	-0.0066600
C	2.0919910	-2.5135100	0.0182030
C	1.0057780	-1.5264300	-0.0433620
C	2.0072300	-0.4487800	-0.0659770
O	1.9173780	0.7711080	-0.1134990
O	2.1622700	-3.7319890	0.0722890
C	-1.2196910	-2.7480570	-0.0479110
C	-1.2573220	-0.4276330	-0.1182180
C	-2.5326930	-2.3615470	-0.0904220
H	-0.8390230	-3.7593990	-0.0241690
C	-2.5649400	-0.9096880	-0.1401120
H	-0.9333530	0.6028320	-0.1490470
H	-3.4042910	-3.0025610	-0.1031330
C	-0.3887850	-1.5626210	-0.0652170
C	4.4948460	-1.6426310	0.0288910
P	-4.0108010	0.0652120	-0.0180350
C	-5.3422910	-0.7136700	-0.9639850
C	-5.0202990	-1.3638790	-2.1596090
C	-6.6702460	-0.6353470	-0.5393940
C	-6.0310220	-1.9281340	-2.9283700
H	-3.9863330	-1.4324820	-2.4786930
C	-7.6739850	-1.2035850	-1.3152840
H	-6.9223590	-0.1465300	0.3941960
C	-7.3552850	-1.8466140	-2.5073240
H	-5.7829050	-2.4343610	-3.8528680
H	-8.7036050	-1.1482810	-0.9846140
H	-8.1404380	-2.2901740	-3.1075520
C	-4.5766870	0.2665640	1.6951140
C	-4.2005820	-0.6832450	2.6454860
C	-5.3958600	1.3415830	2.0525870
C	-4.6557260	-0.5619410	3.9538610
H	-3.5479560	-1.5027600	2.3632770
C	-5.8467110	1.4536910	3.3620910
H	-5.6740270	2.0894820	1.3174480
C	-5.4778930	0.5022850	4.3099390
H	-4.3619410	-1.2950050	4.6947330
H	-6.4799370	2.2859680	3.6432840
H	-5.8274700	0.5959410	5.3309980
C	-3.7074490	1.7310200	-0.6543570
C	-2.9450180	2.6152510	0.1157360
C	-4.1834590	2.1150050	-1.9079900
C	-2.6530770	3.8792480	-0.3795490
H	-2.5865690	2.3207400	1.0964000
C	-3.8912090	3.3858310	-2.3922850
H	-4.7816300	1.4331730	-2.5013130
C	-3.1263200	4.2635110	-1.6318210
H	-2.0597700	4.5641960	0.2130930
H	-4.2633310	3.6879770	-3.3632370
H	-2.8999190	5.2517830	-2.0132010

H	4.7534060	-2.6991150	0.0787370
C	5.5668430	-0.7505470	0.0104690
C	5.5570870	0.7649350	-0.0574310
C	7.0366790	1.0722520	-0.0440030
C	7.7602230	-0.1253560	0.0236920
C	4.8576430	1.3766760	1.1711290
H	3.7963090	1.1308740	1.1606840
H	5.3152710	1.0139280	2.0934690
H	4.9594670	2.4646110	1.1371910
C	4.9032730	1.2619070	-1.3606860
H	5.0024310	2.3489620	-1.4200510
H	5.3951200	0.8204560	-2.2295790
H	3.8426210	1.0129170	-1.3677080
N	6.8642940	-1.1879300	0.0535670
C	7.2497830	-2.5842540	0.1179360
H	6.8436680	-3.0461110	1.0205490
H	6.8737210	-3.1191320	-0.7569610
H	8.3327570	-2.6578540	0.1391830
C	9.1543330	-0.1387210	0.0514880
C	9.8062050	1.0911030	0.0085040
H	10.8892490	1.1111200	0.0286940
C	7.6991760	2.2827700	-0.0864090
C	9.0975770	2.2903360	-0.0598540
H	9.6337300	3.2305500	-0.0923240
H	9.7235720	-1.0573240	0.1040230
H	7.1445370	3.2137090	-0.1396660

6 – S_0 – G= -2204.668464 au.

C	-2.2235120	0.7542170	-0.0543460
C	-0.8750280	1.3240340	-0.0359620
C	-0.2987980	-0.0171290	-0.0894460
C	-1.6399310	-0.5996940	-0.1214450
O	-2.0510560	-1.7553130	-0.1780190
O	-0.4347050	2.4663460	0.0114080
C	1.3715790	-1.9257830	-0.1308540
C	2.1824150	0.2430290	-0.0351280
C	2.7397090	-2.0003150	-0.0949380
H	0.6739690	-2.7499060	-0.1688440
C	3.2520730	-0.6469900	-0.0369160
H	2.2209260	1.3220940	0.0159580
H	3.3446770	-2.8971630	-0.0913190
C	0.9929700	-0.5356880	-0.0932080
C	-3.4072280	1.5071320	-0.0037510
P	4.9446990	-0.2003780	-0.0066440
C	5.8174150	-1.2273900	1.2017330
C	5.1254220	-1.6447080	2.3425160
C	7.1630990	-1.5585650	1.0309470
C	5.7876590	-2.3859410	3.3138100
H	4.0765450	-1.3968980	2.4615850
C	7.8159000	-2.3019260	2.0072220
H	7.6984470	-1.2508890	0.1403970
C	7.1301790	-2.7125960	3.1464530
H	5.2529760	-2.7120600	4.1971050
H	8.8580620	-2.5641280	1.8745410
H	7.6420530	-3.2942440	3.9035300
C	5.7549210	-0.3991590	-1.6154090
C	5.2224100	-1.2951820	-2.5434290
C	6.9162810	0.3207040	-1.9122090
C	5.8621000	-1.4792690	-3.7642670
H	4.3078150	-1.8323750	-2.3182430
C	7.5484490	0.1295340	-3.1345530
H	7.3189990	1.0334790	-1.2004320
C	7.0228260	-0.7709030	-4.0575000

H	5.4483280	-2.1705700	-4.4877150
H	8.4462210	0.6880260	-3.3683410
H	7.5158840	-0.9139410	-5.0113620
C	5.1192980	1.5373480	0.4561770
C	4.7658200	2.5167000	-0.4777150
C	5.5542420	1.8983640	1.7310620
C	4.8418420	3.8575140	-0.1257800
H	4.4360110	2.2335850	-1.4716950
C	5.6319390	3.2448940	2.0719420
H	5.8339780	1.1391490	2.4522260
C	5.2748580	4.2201380	1.1475740
H	4.5652160	4.6181140	-0.8449620
H	5.9721240	3.5288630	3.0598990
H	5.3354190	5.2673740	1.4176820
H	-3.2095680	2.5745940	0.0411660
C	-4.7317630	1.1228420	0.0022780
C	-5.3398810	-0.2746410	-0.0447900
C	-6.8249490	0.0375230	-0.0039900
C	-6.9924390	1.4022250	0.0557780
C	-4.8945490	-1.0720270	1.1953950
H	-3.8216630	-1.2543760	1.1544140
H	-5.1434030	-0.5236410	2.1064600
H	-5.4017380	-2.0371050	1.2290530
C	-4.9423530	-0.9645930	-1.3630600
H	-5.4480400	-1.9265860	-1.4562290
H	-5.2288810	-0.3443700	-2.2151110
H	-3.8681930	-1.1434060	-1.3792350
N	-5.7390520	2.0326900	0.0582560
C	-5.5266900	3.4664390	0.1145560
H	-4.9551540	3.7273570	1.0076080
H	-4.9801170	3.8003540	-0.7696890
H	-6.4852280	3.9745760	0.1488000
C	-8.2597110	2.0183620	0.1052400
C	-9.3612170	1.2046560	0.0919810
H	-10.3533890	1.6403730	0.1288360
C	-7.9529850	-0.8172040	-0.0188920
C	-9.2457820	-0.2089420	0.0308090
H	-8.3721270	3.0930660	0.1522520
C	-7.8820820	-2.2382210	-0.0799550
C	-9.0206540	-2.9994170	-0.0906500
H	-6.9186050	-2.7276630	-0.1186830
H	-8.9429480	-4.0791430	-0.1376030
C	-10.4028350	-1.0304590	0.0181510
C	-10.2986310	-2.3938230	-0.0410340
H	-11.3759430	-0.5526590	0.0565520
H	-11.1880180	-3.0118560	-0.0502290

6 – S_1 – G= -2204.592120 au.

C	2.2583130	0.7587530	-0.0132350
C	0.8894480	1.3288080	-0.0380620
C	0.2863040	-0.0094590	-0.0032710
C	1.6322440	-0.6005570	0.0267140
O	2.0381770	-1.7542600	0.0674820
O	0.4640580	2.4742140	-0.0745780
C	-1.3998790	-1.9107380	0.0148400
C	-2.2103690	0.2629200	-0.0690360
C	-2.7669220	-1.9849140	-0.0287080
H	-0.7033420	-2.7361970	0.0471610
C	-3.2823030	-0.6276300	-0.0859820
H	-2.2486630	1.3423000	-0.1102740
H	-3.3739180	-2.8806910	-0.0370870
C	-1.0133250	-0.5164860	-0.0116040
C	3.4398540	1.4860140	-0.0340590

P	-4.9731300	-0.1890270	-0.0098800
C	-5.9400520	-1.3379910	-1.0205190
C	-5.3690160	-1.8415590	-2.1933970
C	-7.2465600	-1.6826200	-0.6677060
C	-6.1111560	-2.6853290	-3.0110840
H	-4.3504680	-1.5795530	-2.4569340
C	-7.9805360	-2.5273330	-1.4921520
H	-7.6874880	-1.3061430	0.2477760
C	-7.4145320	-3.0262270	-2.6614050
H	-5.6691760	-3.0787090	-3.9179560
H	-8.9920370	-2.7992470	-1.2174480
H	-7.9889900	-3.6866510	-3.2996380
C	-5.6386370	-0.2299480	1.6788020
C	-5.0250510	-1.0492480	2.6273190
C	-6.7650810	0.5254170	2.0176770
C	-5.5479230	-1.1201240	3.9137540
H	-4.1386780	-1.6159620	2.3624540
C	-7.2807870	0.4475690	3.3056680
H	-7.2318650	1.1755260	1.2853200
C	-6.6735840	-0.3752300	4.2508430
H	-5.0712570	-1.7516190	4.6530630
H	-8.1518360	1.0331820	3.5722470
H	-7.0757240	-0.4295600	5.2552510
C	-5.2122080	1.4975140	-0.6164870
C	-4.8077590	2.5658890	0.1905390
C	-5.7457330	1.7309530	-1.8839050
C	-4.9302570	3.8659860	-0.2815450
H	-4.4045790	2.3839850	1.1811330
C	-5.8702800	3.0374100	-2.3449990
H	-6.0661060	0.9034140	-2.5062880
C	-5.4613270	4.1006540	-1.5475820
H	-4.6141570	4.6947060	0.3394860
H	-6.2877170	3.2217270	-3.3269590
H	-5.5585690	5.1164170	-1.9110830
H	3.2549930	2.5584460	-0.0660140
C	4.7807320	1.1009050	-0.0256740
C	5.3875770	-0.2896910	0.0126970
C	6.8701150	0.0317280	-0.0005130
C	7.0317230	1.4085920	-0.0419830
C	4.9588810	-1.0816930	-1.2408220
H	3.8799150	-1.2312630	-1.2318070
H	5.2493210	-0.5434910	-2.1451320
H	5.4360780	-2.0627450	-1.2554210
C	4.9647500	-1.0101500	1.3102950
H	5.4397220	-1.9901510	1.3763790
H	5.2616430	-0.4238280	2.1820290
H	3.8854220	-1.1573090	1.3153460
N	5.7907800	2.0243200	-0.0561510
C	5.5767870	3.4586640	-0.0999830
H	5.0174580	3.7266170	-0.9988540
H	5.0156440	3.7804510	0.7798190
H	6.5345010	3.9686810	-0.1142360
C	8.3038810	2.0283070	-0.0646000
C	9.4039030	1.2182910	-0.0435250
H	10.3955740	1.6566130	-0.0597030
C	8.0004760	-0.8141370	0.0214260
C	9.2936840	-0.2001490	-0.0005900
H	8.4152510	3.1035610	-0.0975560
C	7.9359190	-2.2368700	0.0640260
C	9.0785550	-2.9930430	0.0838840
H	6.9742230	-2.7306870	0.0810550
H	9.0051140	-4.0736410	0.1165050
C	10.4511400	-1.0142870	0.0207160

C	10.3531160	-2.3815530	0.0621680
H	11.4228540	-0.5323330	0.0035010
H	11.2457250	-2.9947200	0.0782520

8 – S_0 – G= -2907.615662 au.

C	0.0065980	1.0373230	-2.0907410
C	-0.0000000	-0.0000000	-1.0426690
C	-0.0065980	-1.0373230	-2.0907410
C	-0.0000000	-0.0000000	-3.0951140
O	0.0000000	0.0000000	0.1734300
C	-0.1398700	-3.4965100	-2.9173800
C	-0.0000000	-3.0222850	-0.6536740
C	-0.1654570	-4.6863680	-2.2401770
H	-0.2044010	-3.3805860	-3.9867640
C	-0.0731670	-4.3970770	-0.8254200
H	0.0614330	-2.4745870	0.2756600
H	-0.2588430	-5.6736050	-2.6725300
C	0.1398700	3.4965100	-2.9173800
C	0.0000000	3.0222850	-0.6536740
C	0.1654570	4.6863680	-2.2401770
H	0.2044010	3.3805860	-3.9867640
C	0.0731670	4.3970770	-0.8254200
H	-0.0614330	2.4745870	0.2756600
H	0.2588430	5.6736050	-2.6725300
C	-0.0356420	-2.4267000	-1.9531950
C	0.0356420	2.4267000	-1.9531950
P	-0.0117850	-5.5830450	0.4619830
P	0.0117850	5.5830450	0.4619830
C	-1.2917760	-6.8334230	0.1911080
C	-2.4871700	-6.4403150	-0.4178210
C	-1.1175580	-8.1504270	0.6212930
C	-3.5087990	-7.3674690	-0.5856440
H	-2.6106870	-5.4199810	-0.7633670
C	-2.1446010	-9.0704440	0.4472180
H	-0.1859620	-8.4629070	1.0783060
C	-3.3377490	-8.6790780	-0.1527840
H	-4.4344300	-7.0657740	-1.0595560
H	-2.0097110	-10.0935030	0.7752620
H	-4.1344520	-9.4002560	-0.2892670
C	1.5930520	-6.4171310	0.5674590
C	2.4124760	-6.4687850	-0.5611430
C	1.9937020	-7.0235780	1.7620510
C	3.6283460	-7.1402800	-0.4955750
H	2.1085610	-5.9760060	-1.4779800
C	3.2100620	-7.6925290	1.8172610
H	1.3673750	-6.9658240	2.6460520
C	4.0243110	-7.7522080	0.6892080
H	4.2677480	-7.1778920	-1.3685960
H	3.5243480	-8.1607460	2.7416870
H	4.9740460	-8.2709680	0.7374390
C	-0.2934190	-4.7810990	2.0561750
C	0.7242320	-3.9876620	2.5955100
C	-1.5151340	-4.9116870	2.7158500
C	0.5091220	-3.3196400	3.7933970
H	1.6766810	-3.8945160	2.0845780
C	-1.7184400	-4.2427350	3.9185160
H	-2.3010450	-5.5316700	2.3002850
C	-0.7106520	-3.4483020	4.4536170
H	1.2932900	-2.7011940	4.2115460
H	-2.6645360	-4.3445450	4.4351640
H	-0.8735710	-2.9282540	5.3897660
C	-1.5930520	6.4171310	0.5674590
C	-1.9937020	7.0235780	1.7620510

C	-2.4124760	6.4687850	-0.5611430
C	-3.2100620	7.6925290	1.8172610
H	-1.3673750	6.9658240	2.6460520
C	-3.6283460	7.1402800	-0.4955750
H	-2.1085610	5.9760060	-1.4779800
C	-4.0243110	7.7522080	0.6892080
H	-3.5243480	8.1607460	2.7416870
H	-4.2677480	7.1778920	-1.3685960
H	-4.9740460	8.2709680	0.7374390
C	0.2934190	4.7810990	2.0561750
C	-0.7242320	3.9876620	2.5955100
C	1.5151340	4.9116870	2.7158500
C	-0.5091220	3.3196400	3.7933970
H	-1.6766810	3.8945160	2.0845780
C	1.7184400	4.2427350	3.9185160
H	2.3010450	5.5316700	2.3002850
C	0.7106520	3.4483020	4.4536170
H	-1.2932900	2.7011940	4.2115460
H	2.6645360	4.3445450	4.4351640
H	0.8735710	2.9282540	5.3897660
C	1.2917760	6.8334230	0.1911080
C	2.4871700	6.4403150	-0.4178210
C	1.1175580	8.1504270	0.6212930
C	3.5087990	7.3674690	-0.5856440
H	2.6106870	5.4199810	-0.7633670
C	2.1446010	9.0704440	0.4472180
H	0.1859620	8.4629070	1.0783060
C	3.3377490	8.6790780	-0.1527840
H	4.4344300	7.0657740	-1.0595560
H	2.0097110	10.0935030	0.7752620
H	4.1344520	9.4002560	-0.2892670
C	-0.0000000	-0.0000000	-4.4988450
C	-0.1779630	1.1740670	-5.2674180
N	-0.3360470	2.1019180	-5.9396300
C	0.1779630	-1.1740670	-5.2674180
N	0.3360470	-2.1019180	-5.9396300

8 – S_1 – G= -2907.534423 au.

C	0.1998200	-1.0411690	-1.9933830
C	0.0000000	-0.0000000	-0.9422020
C	-0.1998200	1.0411690	-1.9933830
C	0.0000000	-0.0000000	-2.9840150
O	-0.0000000	0.0000000	0.2694610
C	-0.2674600	3.4980140	-2.8392270
C	-0.4396280	3.0469380	-0.5706510
C	-0.3804150	4.6968710	-2.1853560
H	-0.1502090	3.3732150	-3.9033130
C	-0.4832570	4.4246190	-0.7655730
H	-0.4821970	2.5101900	0.3662850
H	-0.3777340	5.6819410	-2.6327380
C	0.2674600	-3.4980140	-2.8392270
C	0.4396280	-3.0469380	-0.5706510
C	0.3804150	-4.6968710	-2.1853560
H	0.1502090	-3.3732150	-3.9033130
C	0.4832570	-4.4246190	-0.7655730
H	0.4821970	-2.5101900	0.3662850
H	0.3777340	-5.6819410	-2.6327380
C	-0.3025240	2.4317360	-1.8593830
C	0.3025240	-2.4317360	-1.8593830
P	-0.8522360	5.6149350	0.4593960
P	0.8522360	-5.6149350	0.4593960
C	-0.0000000	7.1616430	0.0655150
C	1.2793580	7.0953380	-0.4958100

C	-0.5817650	8.3988450	0.3497350
C	1.9729830	8.2688300	-0.7652310
H	1.7218170	6.1326290	-0.7260580
C	0.1201510	9.5670930	0.0758710
H	-1.5789830	8.4551990	0.7698680
C	1.3946310	9.5020980	-0.4785180
H	2.9621660	8.2188790	-1.2028530
H	-0.3321770	10.5272170	0.2905360
H	1.9368770	10.4150300	-0.6930380
C	-2.6300660	5.9596230	0.5824260
C	-3.4448920	5.6955590	-0.5190900
C	-3.1719730	6.5017950	1.7515950
C	-4.8030220	5.9870440	-0.4530480
H	-3.0197460	5.2546910	-1.4146520
C	-4.5298270	6.7910190	1.8076060
H	-2.5417450	6.6895600	2.6144940
C	-5.3427150	6.5351990	0.7060340
H	-5.4387670	5.7791330	-1.3046160
H	-4.9535650	7.2096570	2.7119950
H	-6.4018160	6.7574870	0.7552470
C	-0.3312820	5.0338480	2.0915990
C	-1.0828770	4.0365980	2.7214700
C	0.8239910	5.5339200	2.6924690
C	-0.6663720	3.5360470	3.9480110
H	-1.9890320	3.6579410	2.2605690
C	1.2288950	5.0309060	3.9244670
H	1.4021970	6.3126680	2.2088140
C	0.4877020	4.0333720	4.5483650
H	-1.2443880	2.7611180	4.4356440
H	2.1228580	5.4207390	4.3950010
H	0.8071640	3.6432510	5.5070980
C	2.6300660	-5.9596230	0.5824260
C	3.1719730	-6.5017950	1.7515950
C	3.4448920	-5.6955590	-0.5190900
C	4.5298270	-6.7910190	1.8076060
H	2.5417450	-6.6895600	2.6144940
C	4.8030220	-5.9870440	-0.4530480
H	3.0197460	-5.2546910	-1.4146520
C	5.3427150	-6.5351990	0.7060340
H	4.9535650	-7.2096570	2.7119950
H	5.4387670	-5.7791330	-1.3046160
H	6.4018160	-6.7574870	0.7552470
C	0.3312820	-5.0338480	2.0915990
C	1.0828770	-4.0365980	2.7214700
C	-0.8239910	-5.5339200	2.6924690
C	0.6663720	-3.5360470	3.9480110
H	1.9890320	-3.6579410	2.2605690
C	-1.2288950	-5.0309060	3.9244670
H	-1.4021970	-6.3126680	2.2088140
C	-0.4877020	-4.0333720	4.5483650
H	1.2443880	-2.7611180	4.4356440
H	-2.1228580	-5.4207390	4.3950010
H	-0.8071640	-3.6432510	5.5070980
C	-0.0000000	-7.1616430	0.0655150
C	-1.2793580	-7.0953380	-0.4958100
C	0.5817650	-8.3988450	0.3497350
C	-1.9729830	-8.2688300	-0.7652310
H	-1.7218170	-6.1326290	-0.7260580
C	-0.1201510	-9.5670930	0.0758710
H	1.5789830	-8.4551990	0.7698680
C	-1.3946310	-9.5020980	-0.4785180
H	-2.9621660	-8.2188790	-1.2028530
H	0.3321770	-10.5272170	0.2905360

H	-1.9368770	-10.4150300	-0.6930380
C	0.0000000	-0.0000000	-4.3800320
C	0.4256590	-1.1140740	-5.1466210
N	0.7849990	-1.9906710	-5.8068500
C	-0.4256590	1.1140740	-5.1466210
N	-0.7849990	1.9906710	-5.8068500