Electronic Supporting Information

Amplified photomodulation of a bis(dithienylethene)-substituted phosphine

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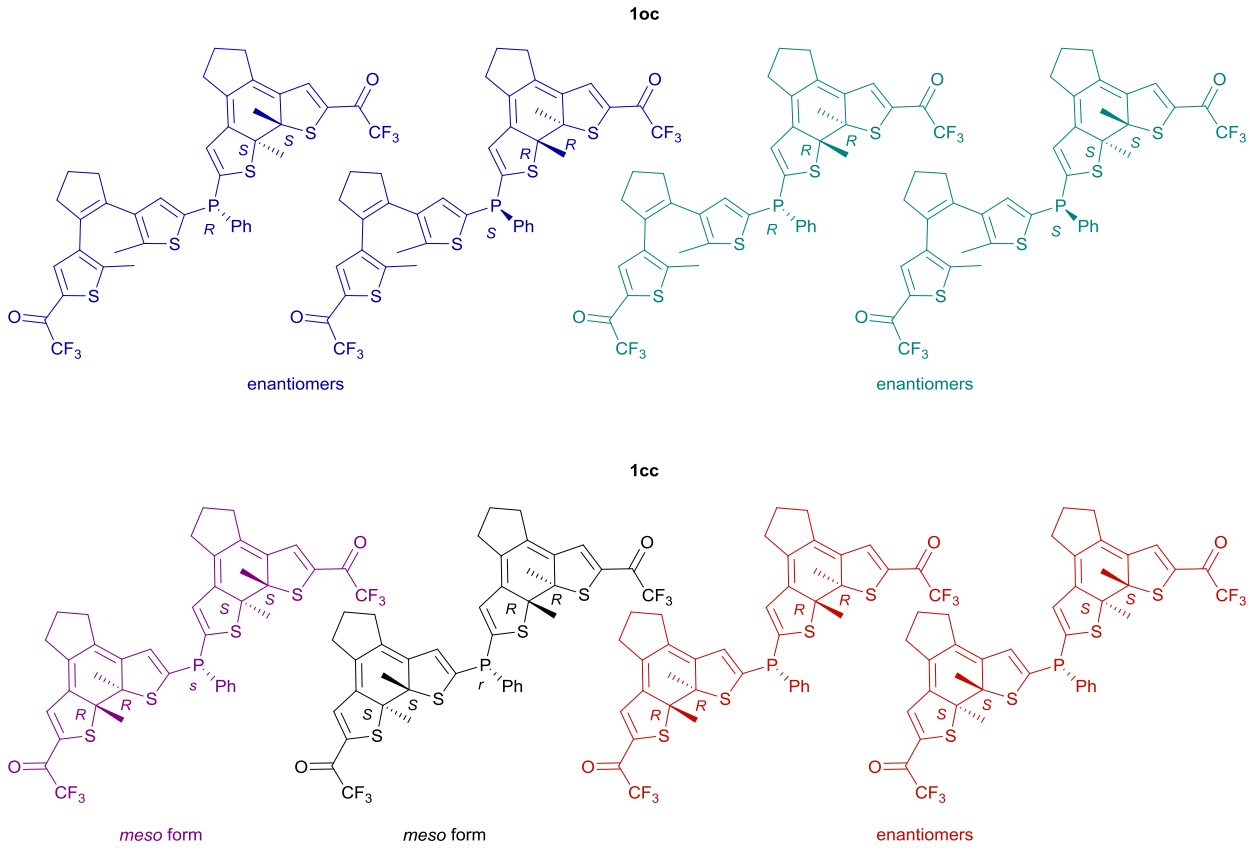
Contents

1 Experimental photochemical properties of ligand **1** and complex **4**



Scheme S1 Possible stereoisomers of **1** in the **oc** and **cc** states.

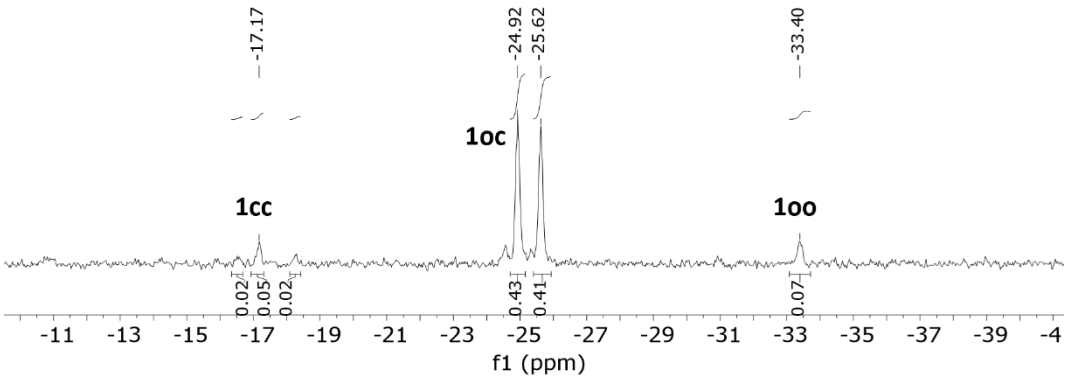


Fig. S1 ^{31}P NMR spectrum (toluene-d_8, 162 MHz) of the PSS@365 nm of **1**, where partial DTE photocyclization produces a mixture of **oo**, **oc** and **cc** isomers. The different signals detected for **oc** and **cc** isomers arise from the stereoisomers shown in Scheme S1.

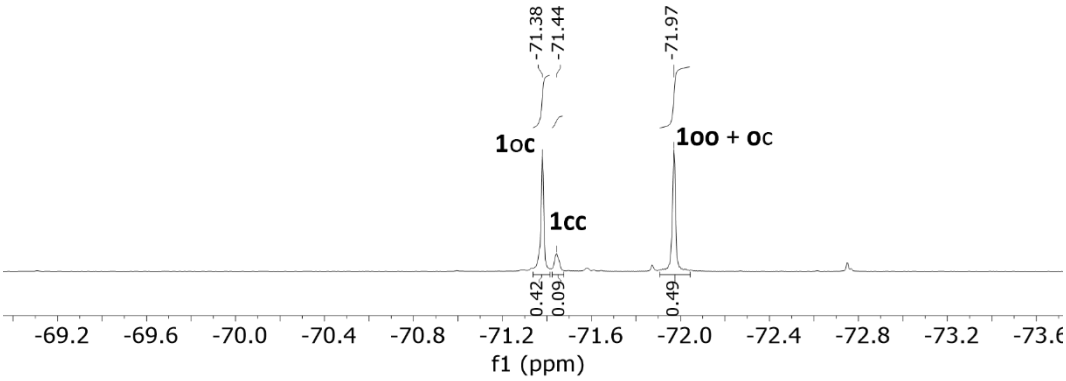


Fig. S2 ^{19}F NMR spectrum (toluene-d_8, 282 MHz) of the PSS@365 nm of **1**, where partial DTE photocyclization produces a mixture of **oo**, **oc** and **cc** isomers. Labels **o**c and o**c** are used to identify the ^{19}F NMR signals of the trifluoromethyl ketone group attached to the ring-open and ring-closed units of the **oc** isomer, respectively.

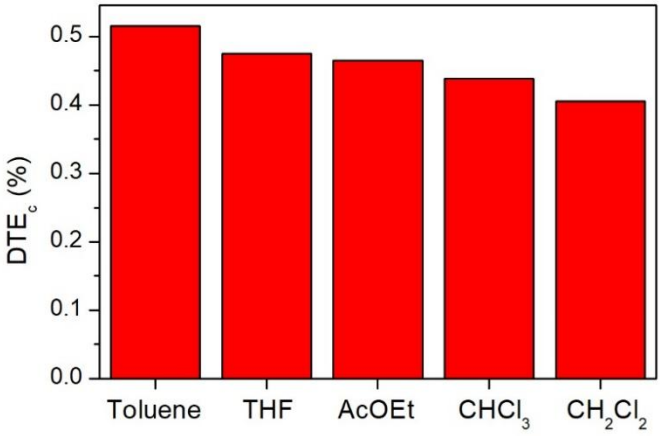


Fig. S3 Percentages of ring-closed DTE units (DTE_c) in the PSS@365 nm achieved for **1** in different solvents. These values were measured by adding an aliquot of the PSS@365 nm obtained in toluene (DTE_c = 52% according to ^{31}P NMR) to the desired solvent and then monitoring the UV-vis absorption changes observed upon irradiation at λ_{exc} = 365. Increasing solvent polarity relative to toluene resulted in a slight decrement in photocyclization efficiency, a common effect in electronically asymmetric DTEs because of the occurrence of UV-induced intramolecular charge transfer processes that compete with photoisomerization.[1]

[1] S. Qiu, A. T. Frawley, K. G. Leslie and H. L. Anderson, *Chem. Sci.*, 2023, **14**, 9123.

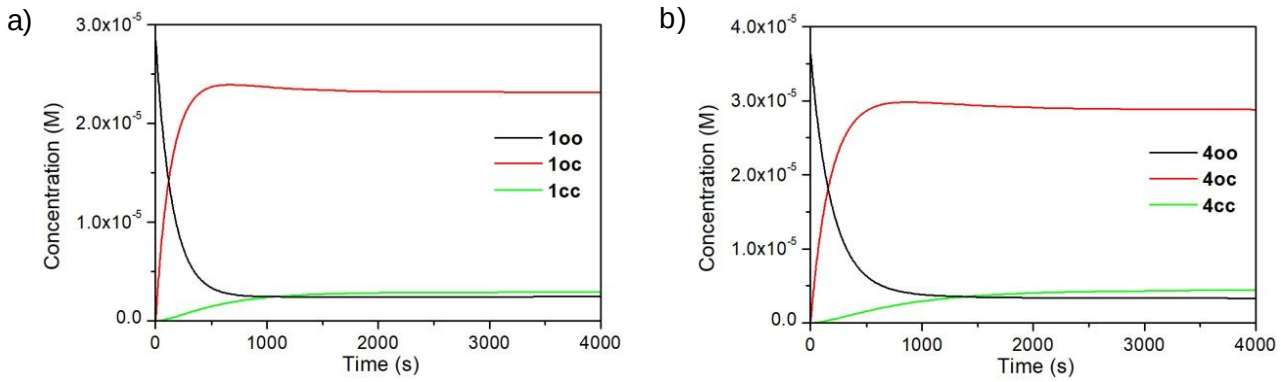


Fig. S4 Variation of the concentrations of the **oo**, **oc** and **cc** isomers of (a) **1** (c_1 = 28.7 10^{-6} M) and (b) **4** (c_1 = 36.5 10^{-6} M) during the photocyclization process in cyclohexane at λ_{exc} = 355 nm. These values were obtained from the analysis of the UV-vis absorption measurements conducted for quantum yield determination, which were fitted to a kinetic model previously reported that accounts for the sequential photoisomerization of the two DTE units in **1** and **4**.[2]

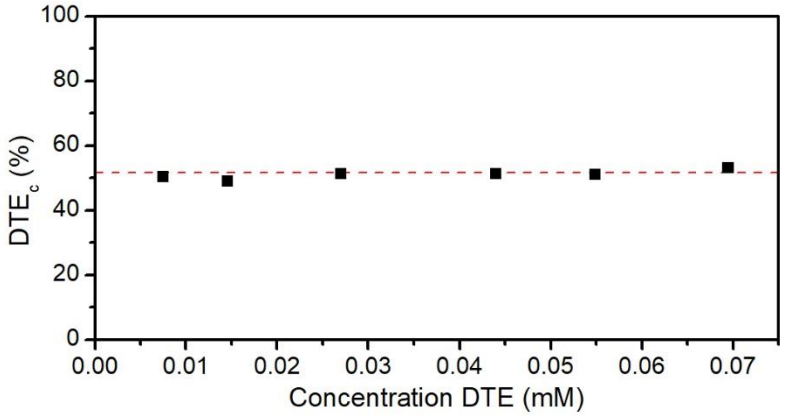


Fig. S5 Variation of the percentage of ring-closed DTE units (DTE$_c$) in the PSS@365 nm achieved for increasing concentrations of **1** in cyclohexane (from c_1 = 7.4 10^{-6} M to c_1 = 7.0 10^{-5} M). No significant changes in photocyclization efficiency were observed with concentration, as DTE$_c$ lies around 50% in all the cases. This suggests that the limited UV-induced photoisomerization determined for bisDTE **1** arises from an intramolecular interaction between its ring-open and ring-closed DTE units after partial cyclization. This is further proven by the fact that monoDTE **5** showed a much larger photocyclization conversion under the same concentration and irradiation conditions (DTE$_c$ ~ 90%) – i.e., no intermolecular effects occur between the ring-open and ring-closed isomers of **5** that could restrict its photoisomerization efficiency under UV excitation.

[2] L. Ordronneau, V. Aubert, R. Métivier, E. Ishow, J. Boixel, K. Nakatani, F. Ibersiene, D. Hammoutène, A. Boucekkine, H. Le Bozec and V. Guerchais, *Phys. Chem. Chem. Phys.*, 2012, **14**, 2599.

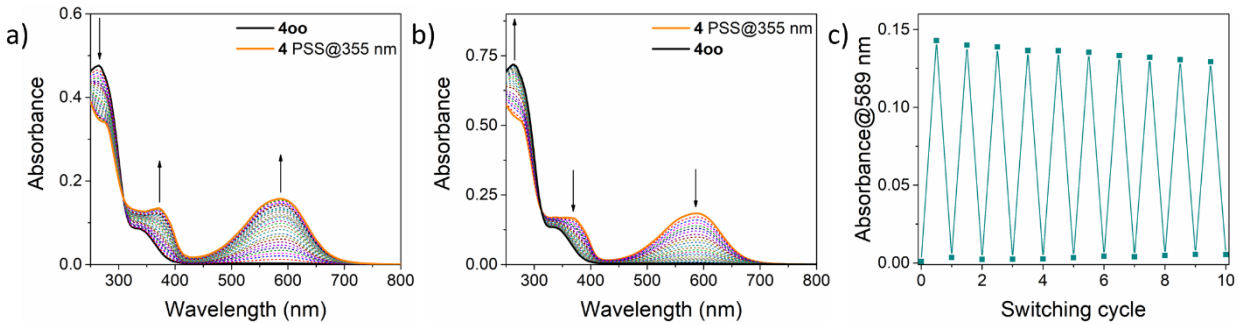


Fig. S6 Photochemical properties of complex **4** in cyclohexane solution. a) Variation of the UV-vis absorption spectrum of **4oo** (c = 1.29·10^{-5} M) upon 355 nm irradiation until a photostationary state is obtained (PSS@355 nm). b) Variation of the UV-vis spectrum of the PSS@355 nm of complex **4** (c = 1.98·10^{-5} M) upon 532 nm irradiation until the initial **4oo** isomer is recovered. c) Variation of the absorbance at the spectral maximum of the ring-closed isomer band of compound **4** (λ_{abs} = 589 nm, c = 2.23·10^{-5} M) upon 10 consecutive photoswitching cycles (λ_{exc} = 365 or 520 nm).

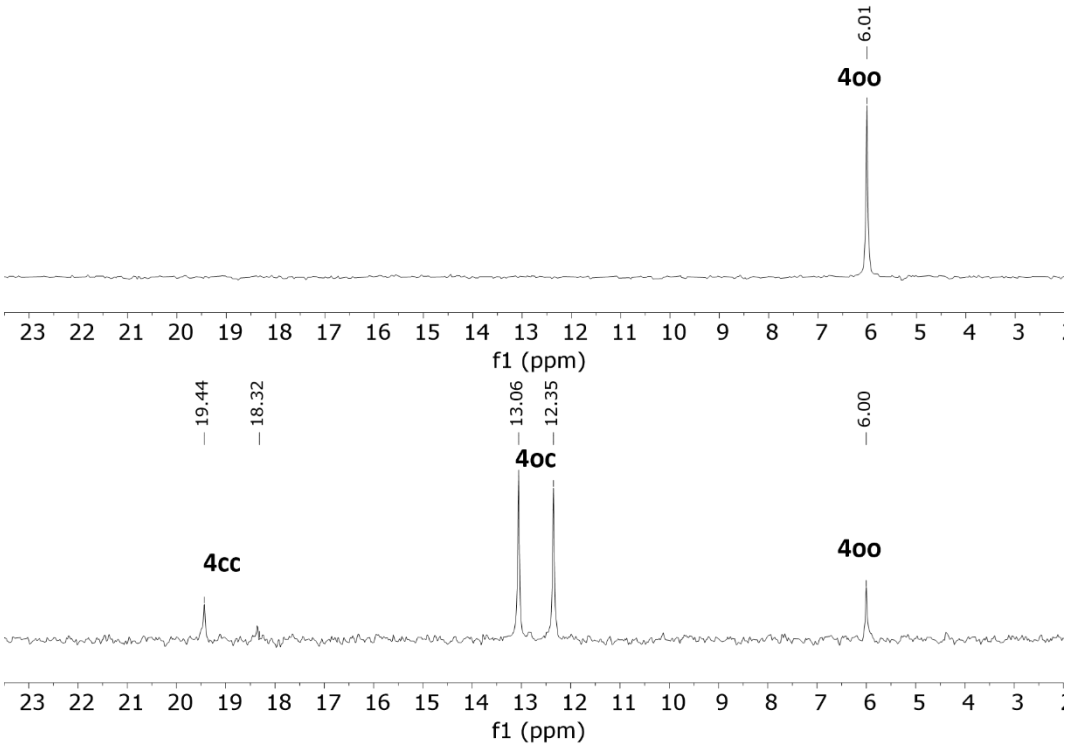


Fig. S7 $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz, $CDCl_3$) of complex **4oo** (top) and the PSS@365 nm (bottom), where partial DTE photocyclization produces a mixture of **oo**, **oc** and **cc** isomers. The different signals observed for the **oc** and **cc** isomers arise from the distinct stereoisomers produced during photocyclization, which are analogous to those shown for **1** in Scheme S1.

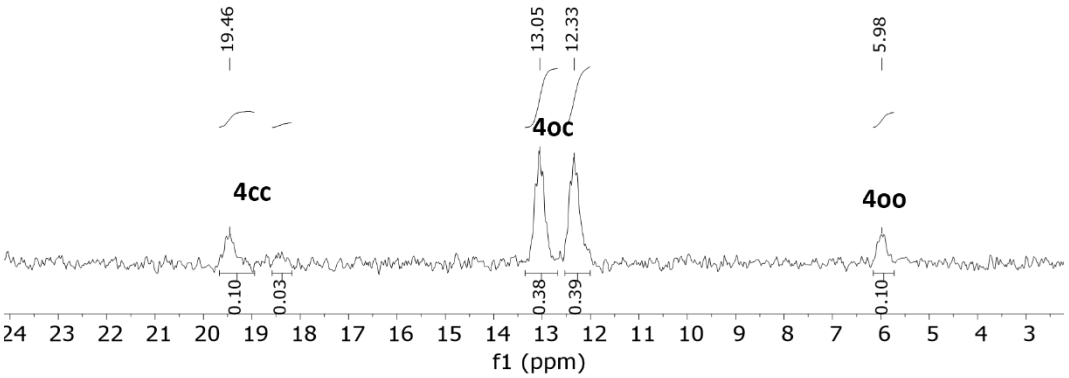


Fig. S8 ^{31}P NMR spectrum (toluene-d_8, 162 MHz) of the PSS@365 nm of complex **4**, where partial DTE photocyclization produces a mixture of **oo**, **oc** and **cc** isomers. The different signals observed for the **oc** and **cc** isomers arise from the distinct stereoisomers produced during photocyclization, which are analogous to those shown for **1** in Scheme S1.

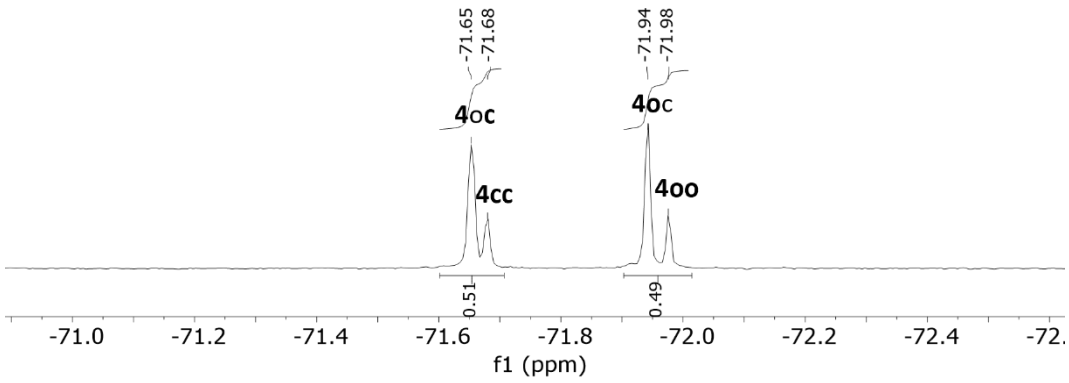


Fig. S9 ^{19}F NMR spectrum (toluene-d_8, 376 MHz) of the PSS@365 nm of complex **4**, where partial DTE photocyclization produces a mixture of **oo**, **oc** and **cc** isomers. Labels **o**c and o**c** are used to identify the ^{19}F NMR signals of the trifluoromethyl ketone group attached to the ring-open and ring-closed units of the **oc** isomer, respectively.

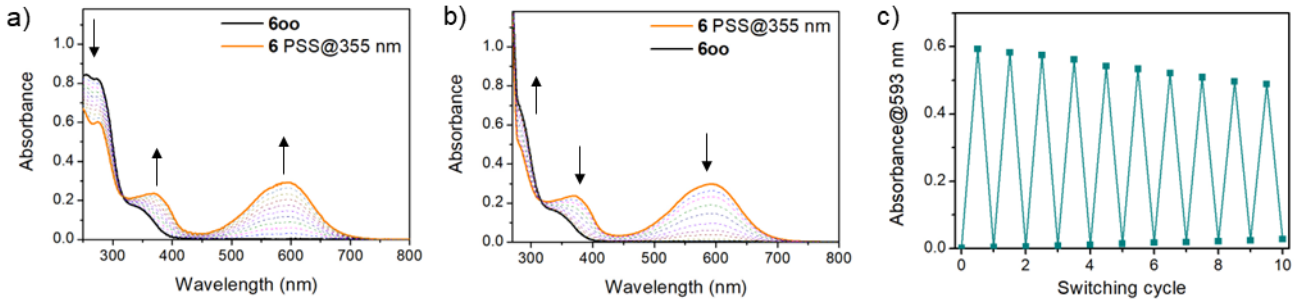


Fig. S10 Photochemical properties of phosphine selenide **6** in solution. a) Variation of the UV-vis absorption spectrum of **6oo** in cyclohexane (c = $1.94 \cdot 10^{-5}$ M) upon 355 nm irradiation until a photostationary state is obtained (PSS@355 nm). b) Variation of the UV-vis spectrum of the PSS@355 nm of **6** in cyclohexane ($c = 1.94 \cdot 10^{-5}$ M) upon 532 nm irradiation until the initial **6oo** isomer is recovered. c) Variation of the absorbance at the spectral maximum of the ring-closed isomer band of compound **6** (λ_{abs} = 593 nm, $c = 3.85 \cdot 10^{-5}$ M) upon 10 consecutive photoswitching cycles (λ_{exc} = 365 or 520 nm).

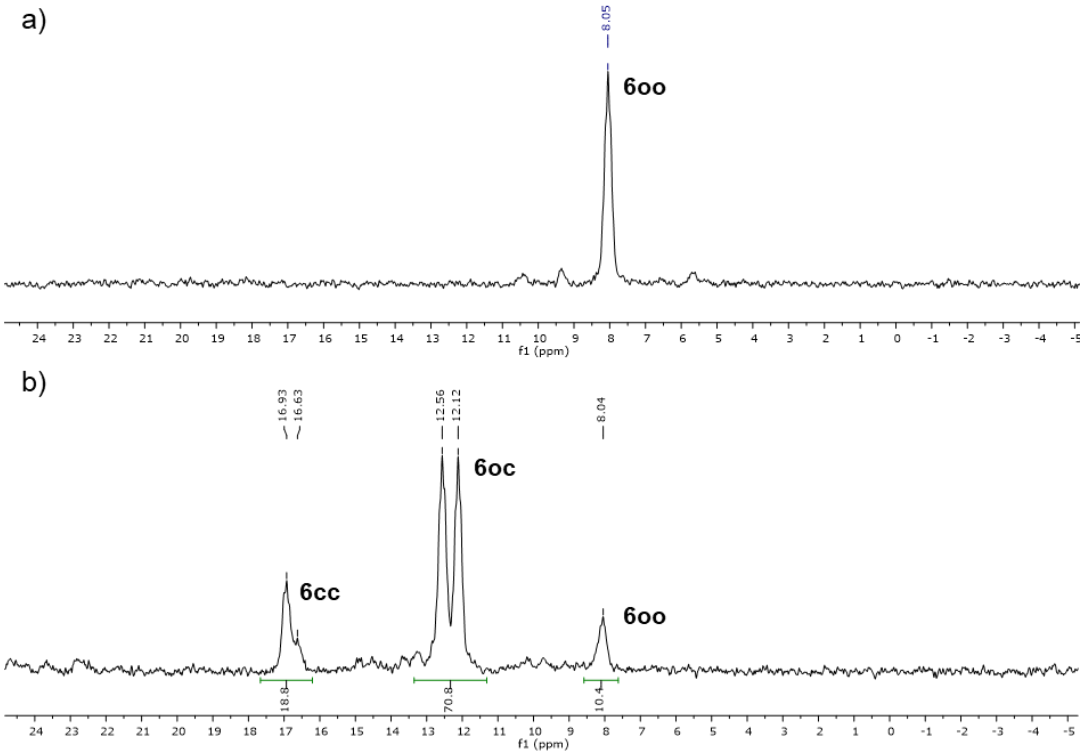


Fig. S11 a) ^{31}P NMR spectrum (toluene-d_8, 162 MHz) of **6oo**. b) ^{31}P NMR spectrum (toluene-d_8, 162 MHz) of the PSS@365 nm of **6**, where partial DTE photocyclization produces a mixture of **oo**, **oc** and **cc** isomers. The different signals observed for the **oc** and **cc** isomers arise from the distinct stereoisomers produced during photocyclization, which are analogous to those shown for **1** in Scheme S1.

2 DFT calculations of the optical properties of the ligand **1** and complex **4**

The optimized structures of ligands in their ground state exhibit distinctive geometric alterations during the isomerization process. Notably, the distance between the reactive carbon atoms changes from 3.48 Å in the open state to 1.54 Å in the closed state. For the ring-open state only the photocyclizable antiparallel conformation of the DTEs was considered.

2.1 Frontier molecular orbitals

Table S1 Selected frontier molecular orbitals of the **oo**, **oc** and **cc** forms of ligand **1** and complex **4**.

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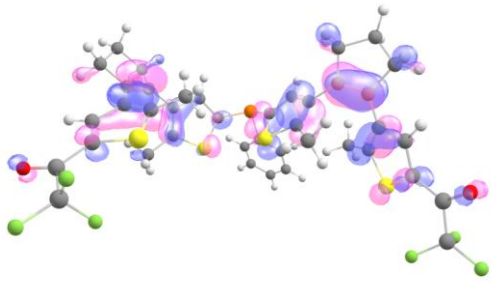	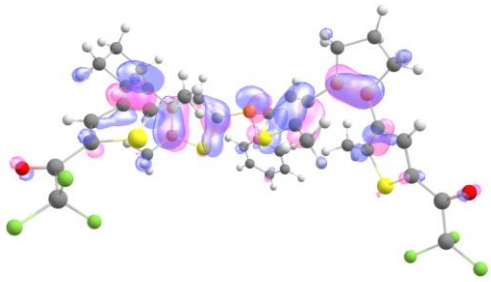
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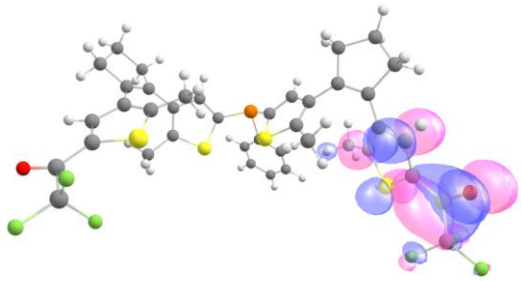
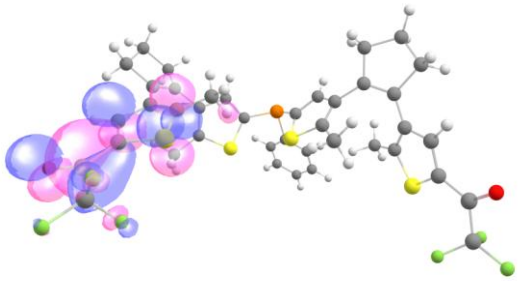
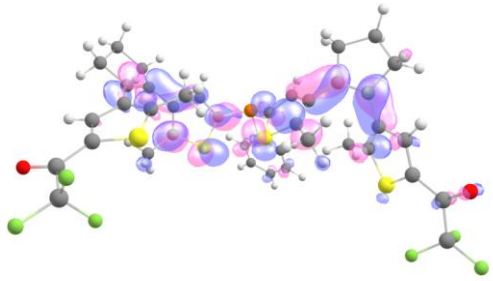
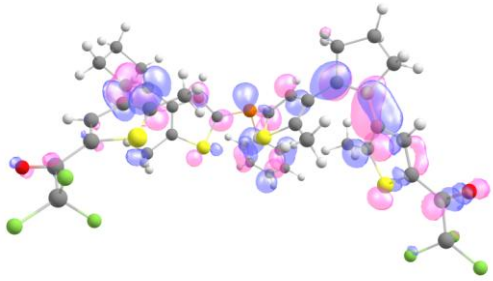
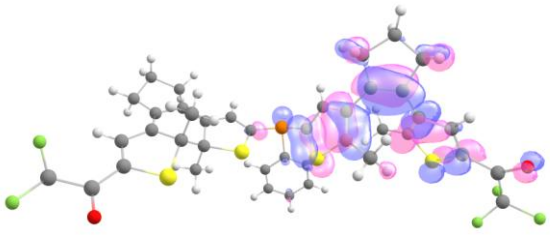
	
LUMO	LUMO+1
	
LUMO+3	LUMO+4
1oc	



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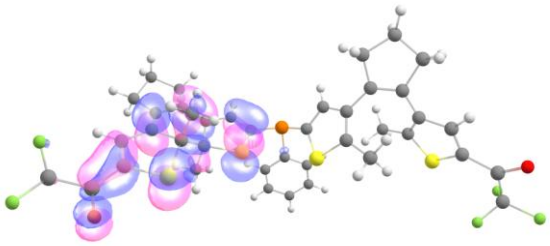

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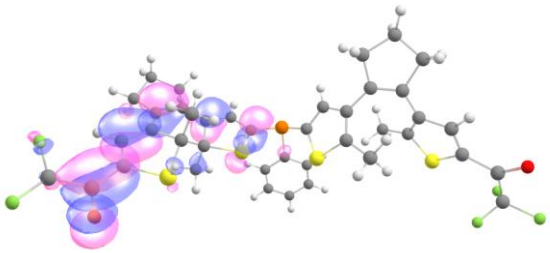

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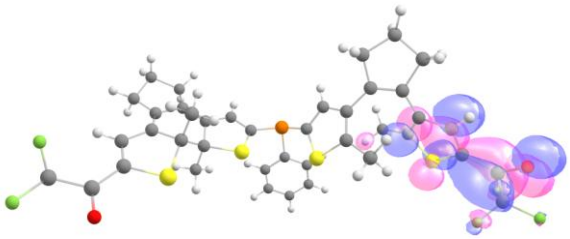

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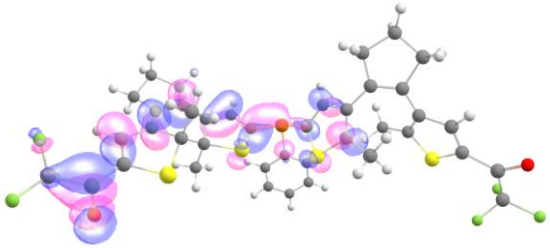

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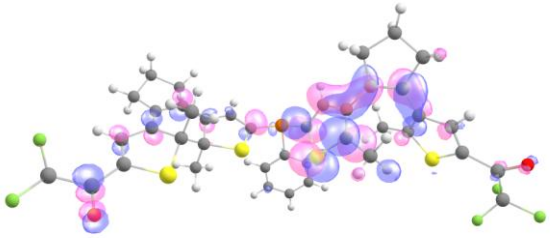

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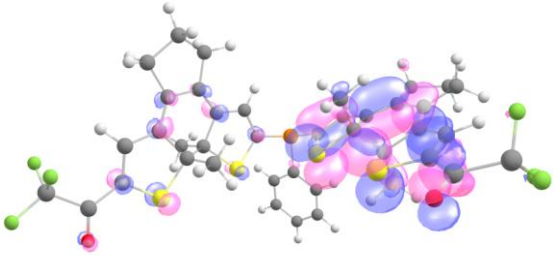

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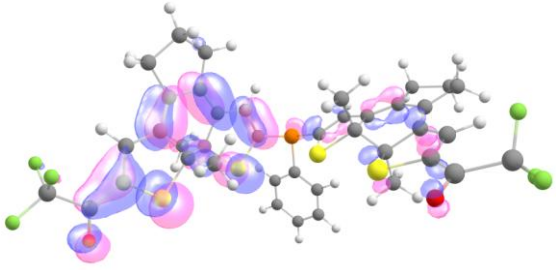

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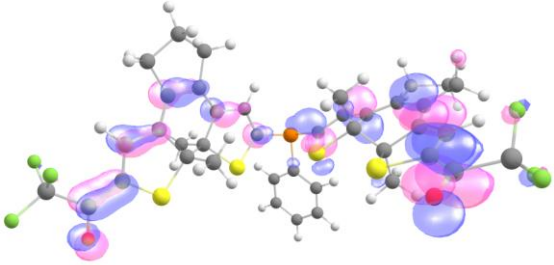

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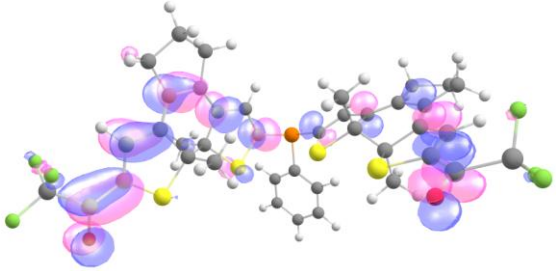

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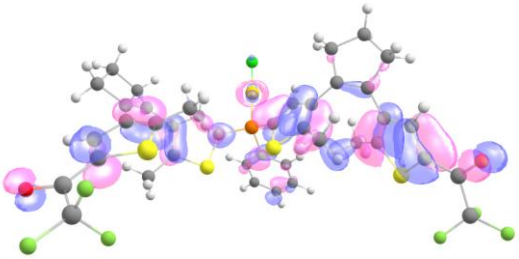

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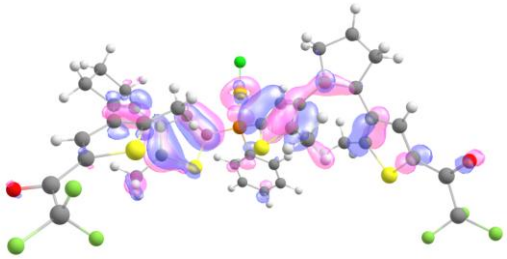

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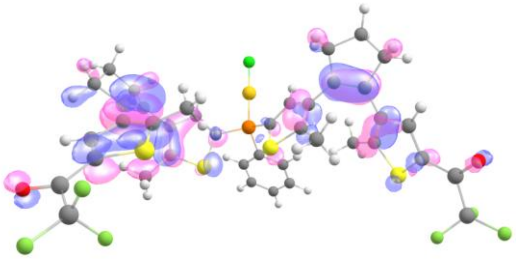

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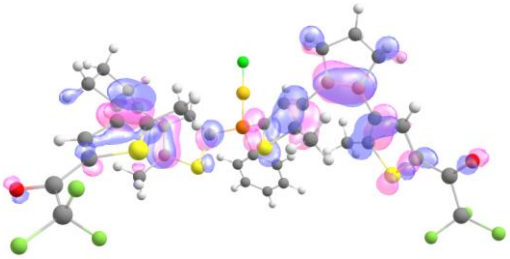

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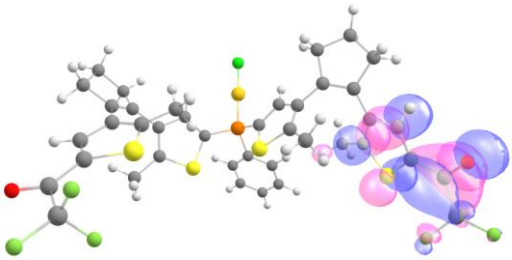

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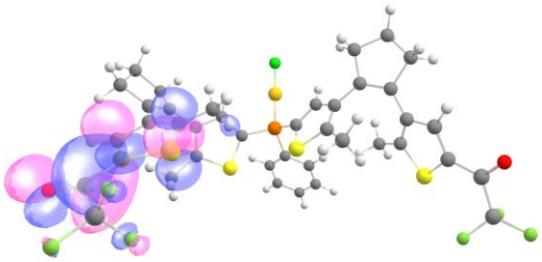

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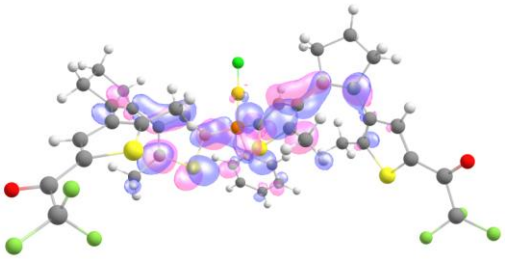

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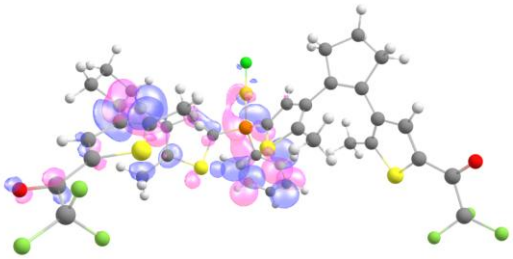

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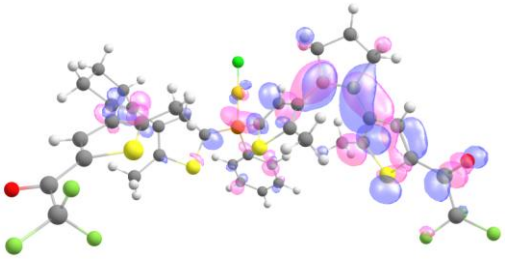

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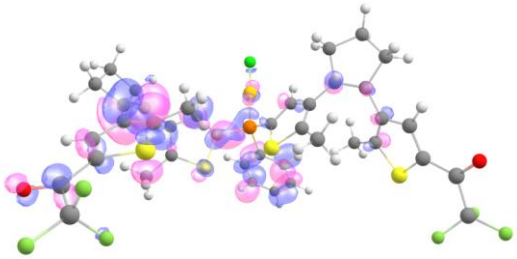

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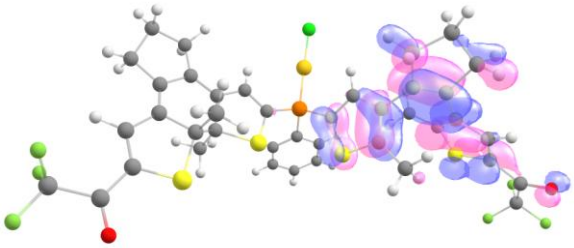

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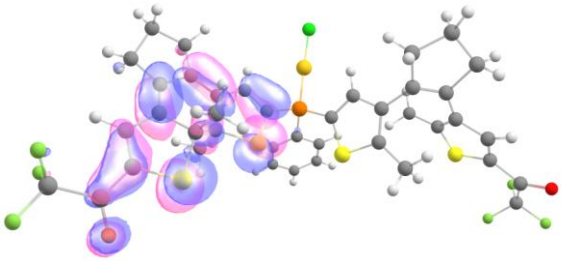

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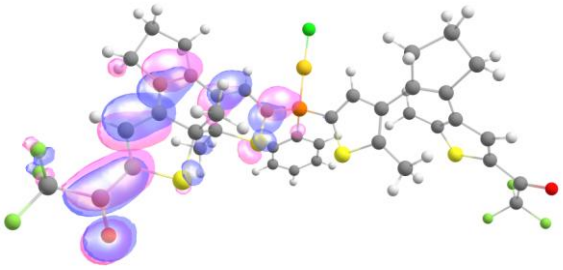

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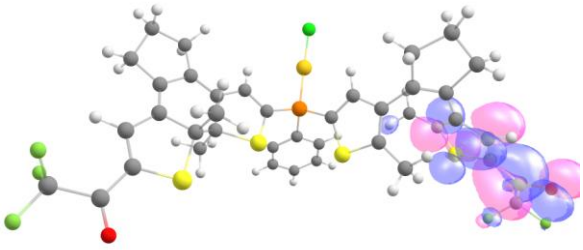

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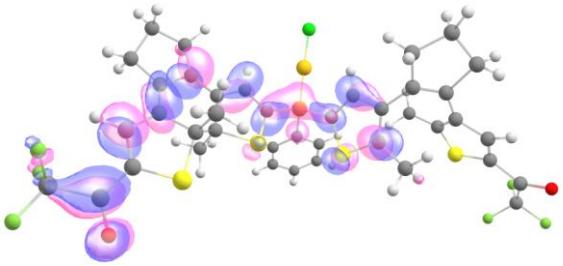

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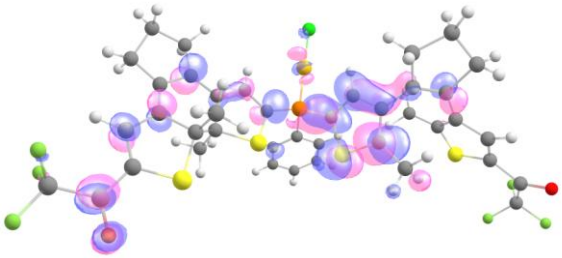

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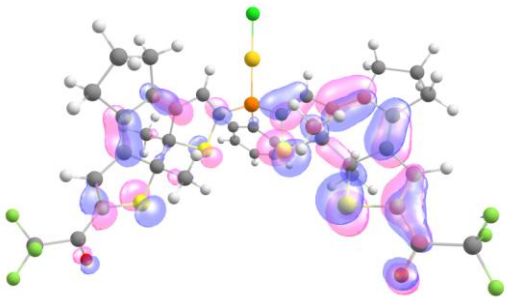

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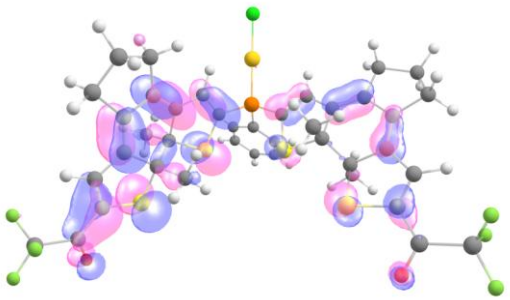
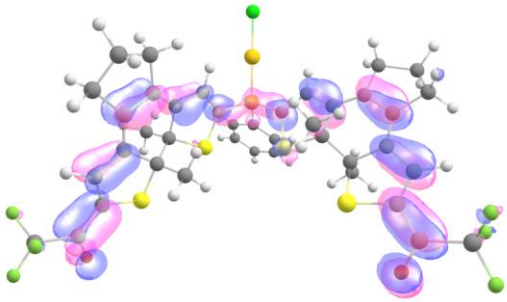
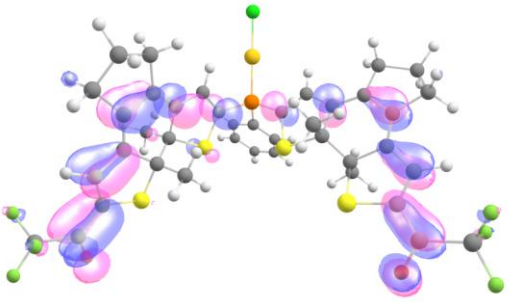


HOMO



LUMO



LUMO+1

2.2 Vertical transitions

Table S2 Calculated absorption wavelengths (λ), oscillator strengths (*f*) and assigned transitions for singlet state ligand **1** and complex **4** in toluene within the 250-800 nm range.

	λ (nm)	*f*	Assigned transition
1oo	317	0.1294	HOMO-1 – LUMO (56.5%), HOMO – LUMO (25.4%), HOMO-3 – LUMO (4.5%), HOMO-2 – LUMO (3.5%), HOMO-14 – LUMO (3.3%)
	312	0.1659	HOMO – LUMO+1 (46.4%), HOMO-1 – LUMO+1 (27.4%), HOMO-2 – LUMO+1 (14.2%), HOMO-13 – LUMO+1 (3.3%), HOMO-4 – LUMO+1 (2.7%)
	272	0.2008	HOMO – LUMO+2 (22.1%), HOMO-4 – LUMO+1 (12.9%), HOMO-6 – LUMO (9.8%), HOMO-1 – LUMO+3 (8.4%), HOMO-3 – LUMO (6.5%), HOMO-6 – LUMO+1 (5.8%), HOMO-5 – LUMO+1 (5.7%), HOMO-7 – LUMO (5.3%), HOMO – LUMO+1 (4.6%), HOMO-5 – LUMO (3.4%)
	270	0.5507	HOMO-6 – LUMO (22.1%), HOMO-7 – LUMO (12.6%), HOMO-3 – LUMO (11.7 %), HOMO-4 – LUMO+1 (7.8%), HOMO-5 – LUMO (6.9%), HOMO – LUMO+2 (6.5%), HOMO-9 – LUMO (5.1%), HOMO – LUMO+3 (4.9%), HOMO-6 – LUMO+1 (3.7%), HOMO-5 – LUMO+1 (3.2%), HOMO – LUMO+1 (2.0%)
	253	0.2924	HOMO-2 – LUMO+2 (34.9%), HOMO-1 – LUMO+3 (21.4%), HOMO – LUMO+4 (16.3%), HOMO – LUMO+3 (5.0%), HOMO – LUMO+5 (3.0%), HOMO-1 – LUMO+5 (2.4%)
1oc	568	0.3676	HOMO – LUMO (96.6%)
	368	0.2175	HOMO-2 – LUMO (61.3%), HOMO-3 – LUMO (29.7%), HOMO – LUMO+2 (2.3%)
	316	0.1605	HOMO – LUMO+1 (65.4%), HOMO – LUMO+2 (4.3%), HOMO-1 – LUMO (4.2%), HOMO-3 – LUMO+1 (4.0%), HOMO-2 – LUMO+1 (3.5%), HOMO-3 – LUMO (3.4%), HOMO-12 – LUMO+1 (3.2%), HOMO-2 – LUMO (2.4%)
	270	0.4423	HOMO-5 – LUMO+1 (44.2%), HOMO-6 – LUMO+1 (16.4%), HOMO-4 – LUMO+1 (10.3%), HOMO-1 – LUMO+3 (8.6%), HOMO-7 – LUMO+1 (8.3%), HOMO-1 – LUMO+1 (2.3%), HOMO-3 – LUMO+1 (2.0%)
1cc	597	0.3322	HOMO – LUMO (39.3%), HOMO – LUMO+1 (31.9%), HOMO-1 – LUMO+1 (14.0%), HOMO-1 – LUMO (11.4%)
	559	0.3949	HOMO-1 – LUMO (61.7%), HOMO – LUMO+1 (31.7%), HOMO-1 – LUMO+1 (3.0%)
	368	0.1822	HOMO-3 – LUMO (59.4%), HOMO-2 – LUMO+1 (22.0%), HOMO-3 – LUMO+1 (3.8%), HOMO-4 – LUMO (3.0%), HOMO-4 – LUMO+1 (2.0%)
	312	0.1483	HOMO-1 – LUMO+2 (55.0%), HOMO – LUMO+3 (17.4%), HOMO-1 – LUMO+3 (11.4%), HOMO-4 – LUMO (2.6%)
	281	0.1038	HOMO – LUMO+7 (24.7%), HOMO-7 – LUMO (19.4%), HOMO – LUMO+4 (8.6%), HOMO – LUMO+5 (5.9%), HOMO – LUMO+6 (4.2%), HOMO-1 – LUMO+7 (3.0%), HOMO-6 – LUMO (2.8%), HOMO-7 – LUMO+1 (2.6%), HOMO-3 – LUMO+1 (2.6%), HOMO – LUMO+3 (2.1%)
4oo	309	0.1042	HOMO-15 – LUMO+1 (42.3%), HOMO – LUMO+1 (23.4%), HOMO-1 – LUMO+1 (20.3%)
	269	0.4372	HOMO-1 – LUMO+2 (14.6%), HOMO-5 – LUMO (13.4%), HOMO-3 – LUMO (12.4%), HOMO – LUMO+3 (12.4%), HOMO-4 – LUMO (11.8%), HOMO-4 – LUMO+1 (8.0%), HOMO-3 – LUMO+1 (7.1%), HOMO-2 – LUMO (2.8%)
	264	0.2343	HOMO-1 – LUMO+2 (30.1%), HOMO – LUMO+3 (20.6%), HOMO-4 – LUMO+1 (8.9%), HOMO-3 – LUMO+1 (5.6%), HOMO-5 – LUMO (5.3%), HOMO-3 – LUMO (3.8%), HOMO-4 – LUMO (3.5%)
4oc	560	0.3713	HOMO – LUMO (97%)
	366	0.2097	HOMO-2 – LUMO (90.4%), HOMO – LUMO+2 (2.6%)
	317	0.1234	HOMO – LUMO+2 (75.7%), HOMO – LUMO+3 (11.8%), HOMO-2 – LUMO (2.9%)

	268	0.3919	HOMO-4 – LUMO+1 (49.5%), HOMO-1 – LUMO+3 (13.4%), HOMO-3 – LUMO+1 (10.8%), HOMO-1 – LUMO+2 (7.0%), HOMO-3 – LUMO (3.4%), HOMO-6 – LUMO+1 (2.1%)
4cc	587	0.3089	HOMO – LUMO (53.6%), HOMO-1 – LUMO+1 (23.0%), HOMO – LUMO+1 (15.2%), HOMO-1 – LUMO (5.1%)
	552	0.4254	HOMO-1 – LUMO (57.0%), HOMO – LUMO+1 (37.0%), HOMO-1 – LUMO+1 (2.7%)
	365	0.1805	HOMO-3 – LUMO (58.8%), HOMO-2 – LUMO+1 (24.9%), HOMO-3 – LUMO+1 (5.6%)
	314	0.1157	HOMO-1 – LUMO+2 (45.4%), HOMO – LUMO+3 (24.8%), HOMO-1 – LUMO+3 (14.2%), HOMO-3 – LUMO (2.7%)
	278	0.3306	HOMO-9 – LUMO (39.2%), HOMO-8 – LUMO+1 (20.8%), HOMO-4 – LUMO (5.5%), HOMO-3 – LUMO (5.0%), HOMO-3 – LUMO+2 (4.2%), HOMO-5 – LUMO+1 (2.1%)

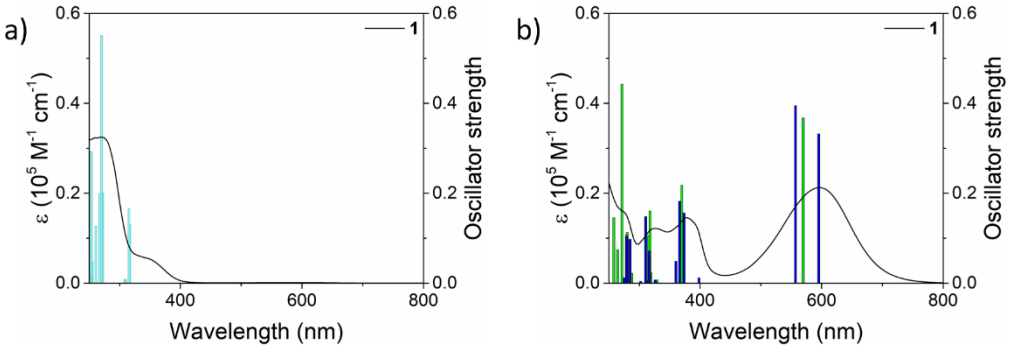


Fig. S12 Experimental absorption spectra (shown as lines) and vertical transitions computed (shown as bars) for **1** in toluene: a) **oo**; b) **oc** (green bars) and **cc** (blue bars).

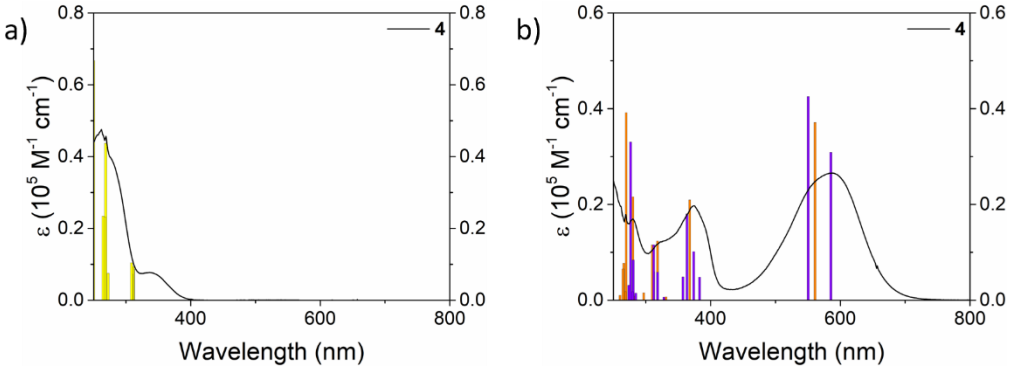


Fig. S13 Experimental absorption spectra (shown as lines) and vertical transitions computed (shown as bars) for **4** in toluene: a) **oo**; b) **oc** (orange bars) and **cc** (violet bars).

3 NMR spectra of the reported compounds

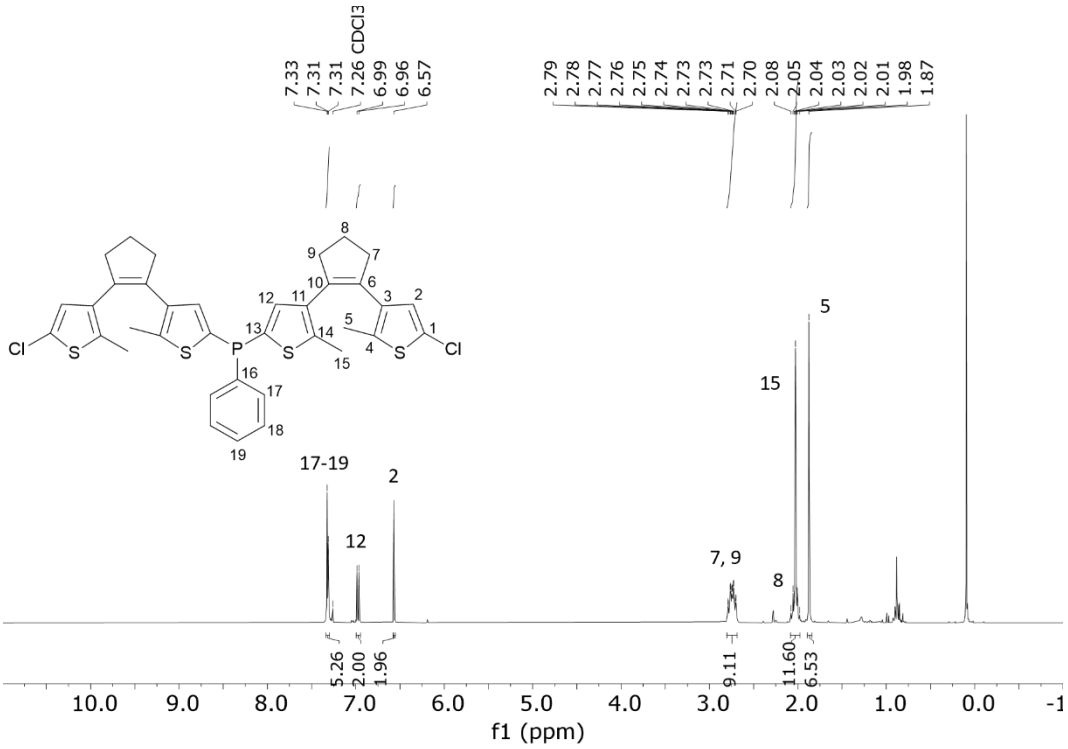


Fig. S14 ^{1}H NMR spectrum (300 MHz) of **3** in $CDCl_3$ recorded at 25 °C.

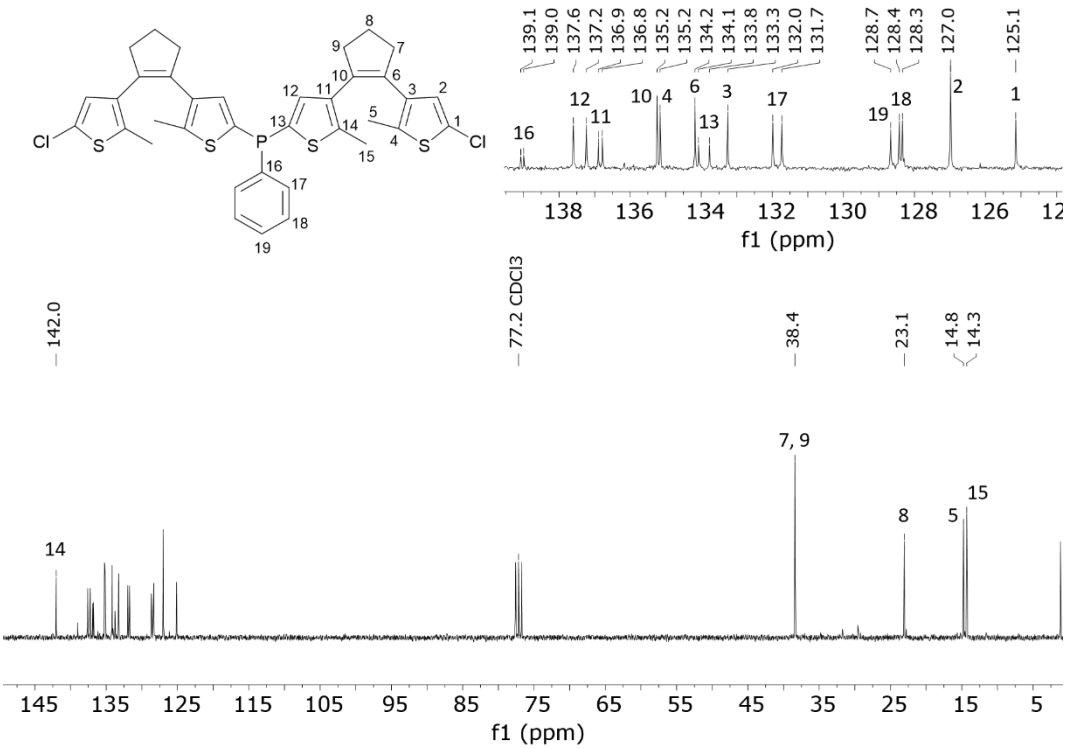


Fig. S15 $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz) of **3** in $CDCl_3$ recorded at 25 °C.

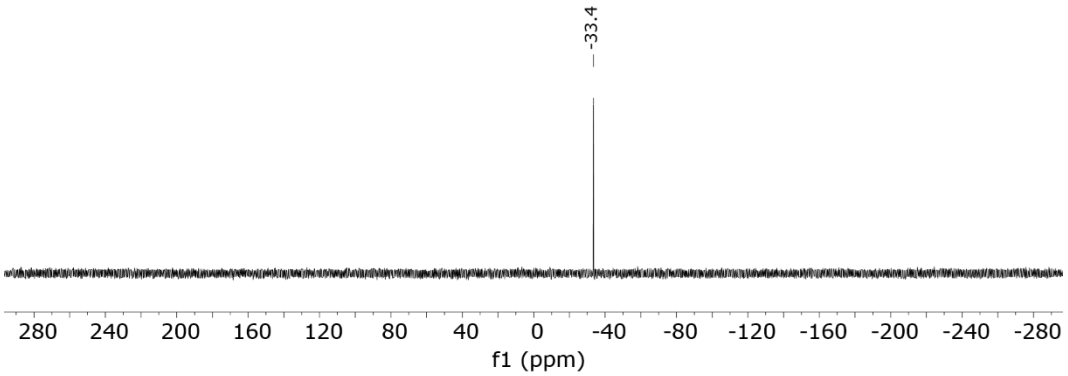


Fig. S16 $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz) of **3** in $CDCl_3$ recorded at 25 °C.

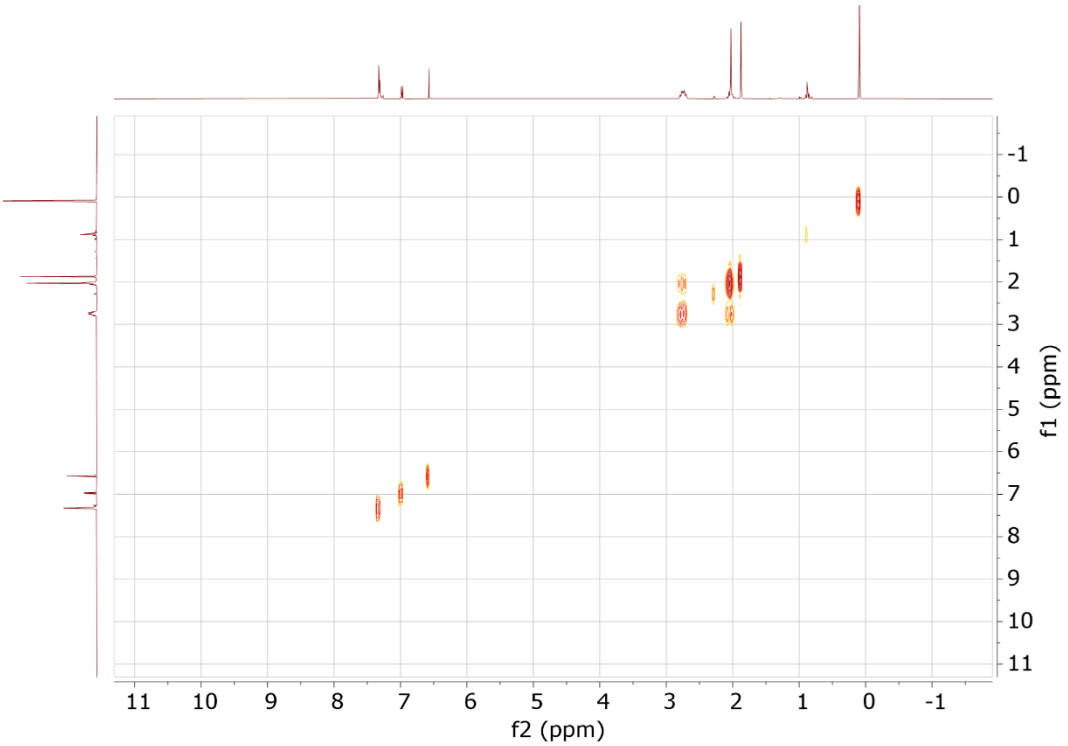


Fig. S17 ^{1}H-^{1}H COSY spectrum of **3** in $CDCl_3$ recorded at 25 °C.

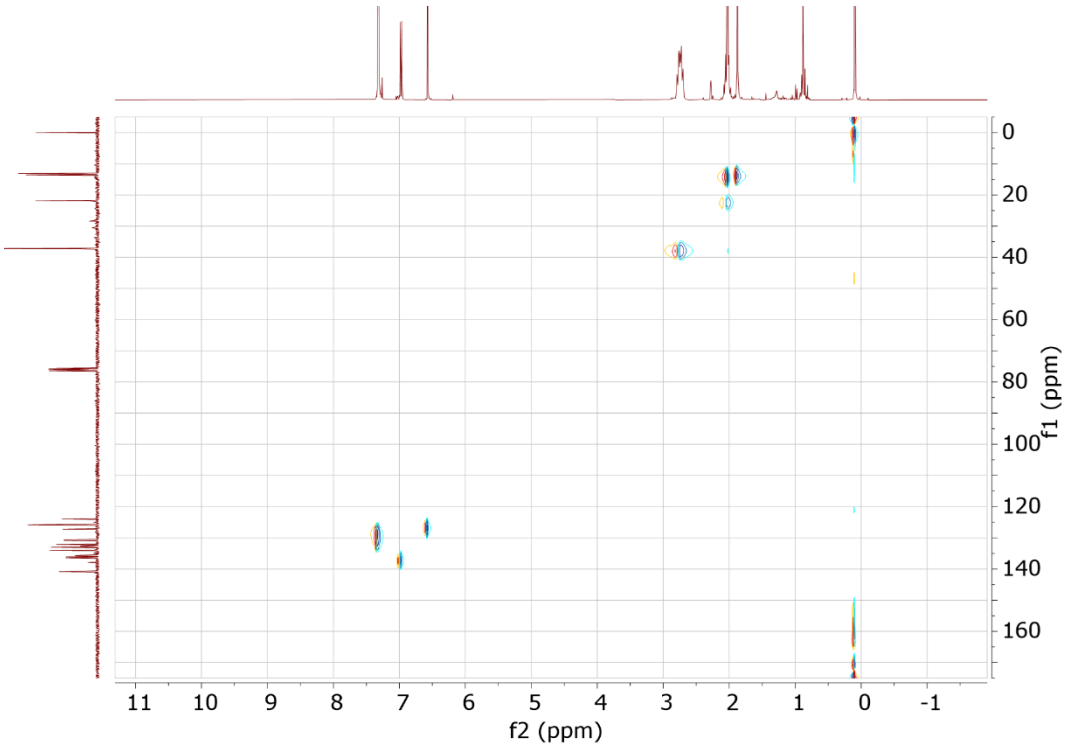


Fig. S18 ^{1}H-^{13}C HSQC spectrum of **3** in $CDCl_3$ recorded at 25 °C.

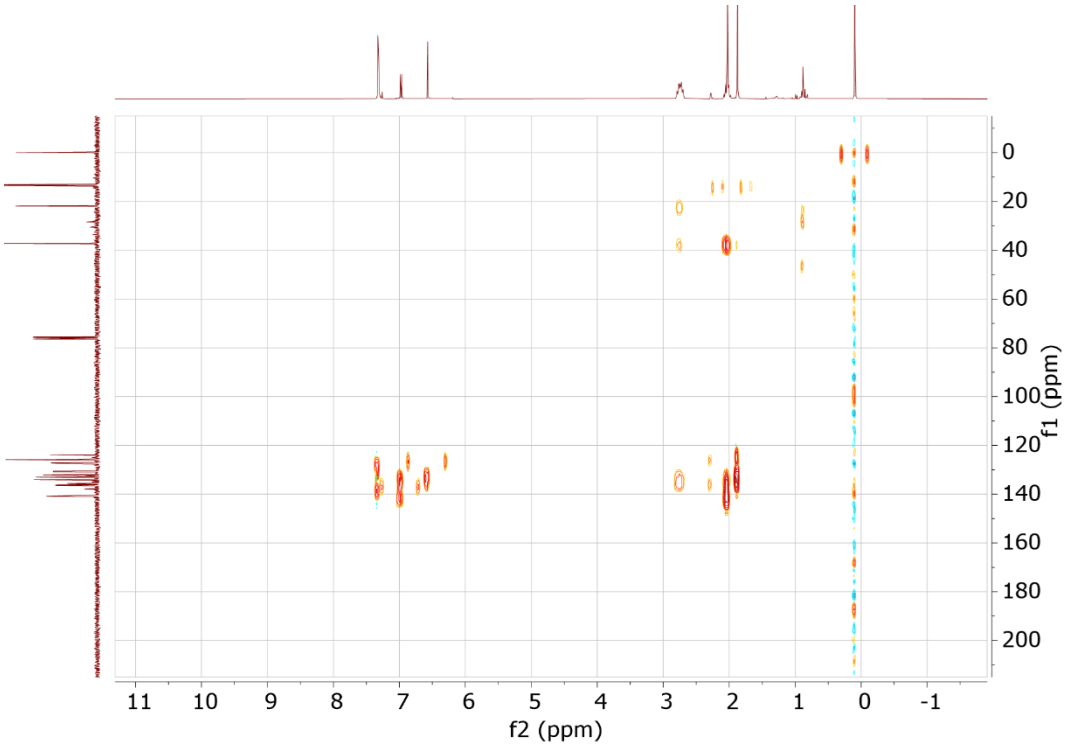


Fig. S19 ^{1}H-^{13}C HMBC spectrum of **3** in $CDCl_3$ recorded at 25 °C.

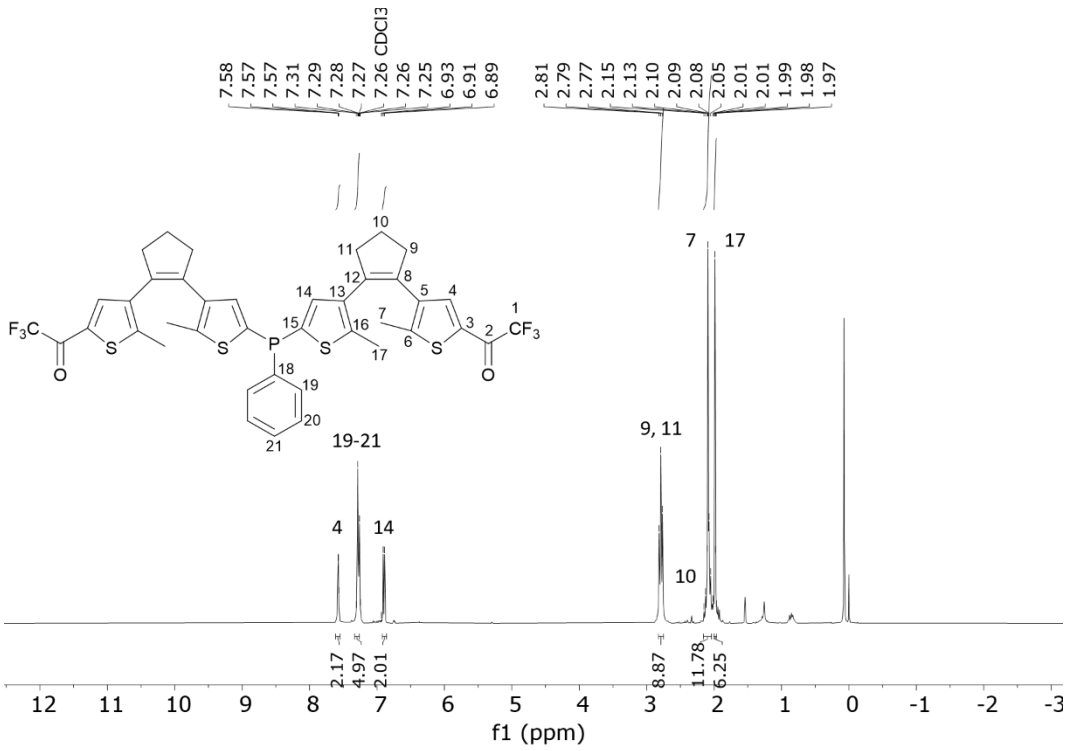


Fig. S20 ^{1}H NMR spectrum (300 MHz) of **1oo** in $CDCl_3$ recorded at 25 °C.

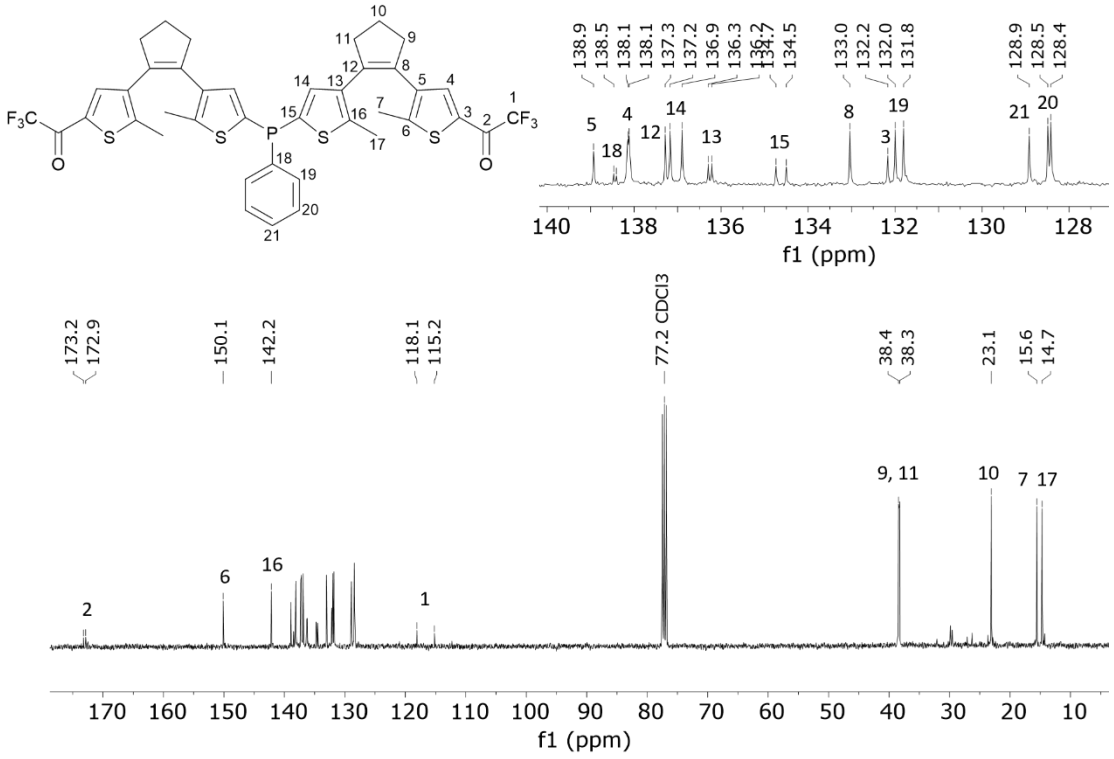


Fig. S21 $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of **1oo** in $CDCl_3$ recorded at 25 °C.

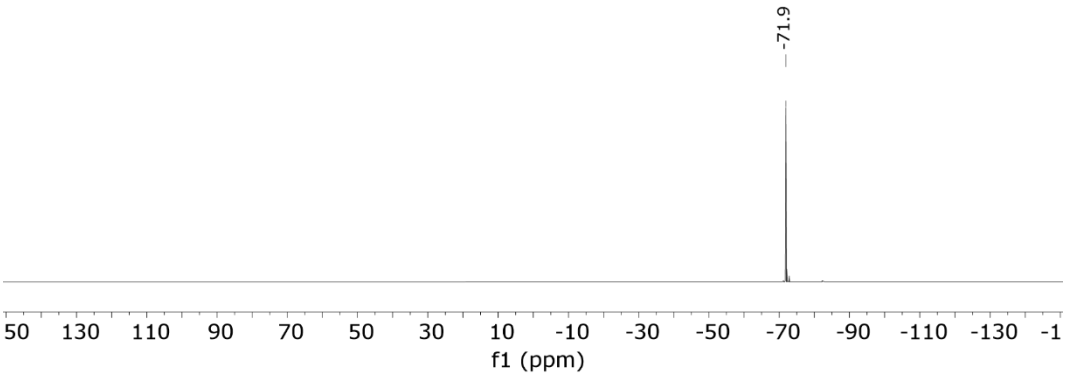


Fig. S22 ^{19}F NMR spectrum (376 MHz) of **1oo** in $CDCl_3$ recorded at 25 °C.

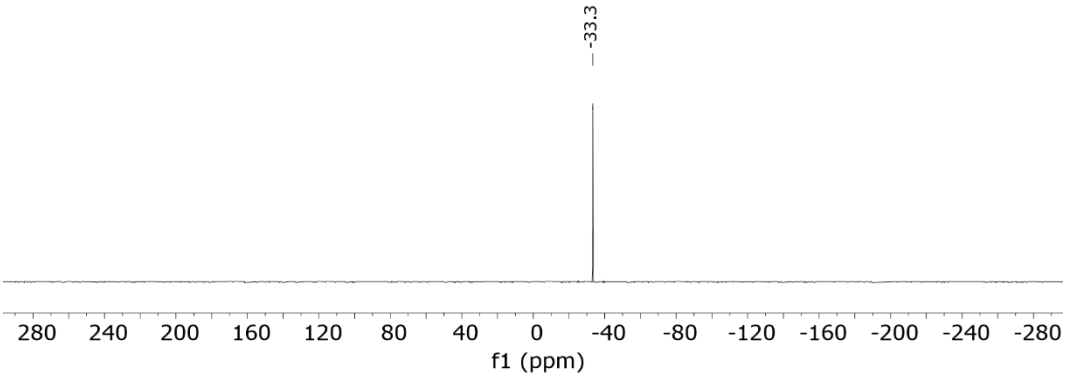


Fig. S23 $^{31}P\{^1H\}$ NMR spectrum (162 MHz) of **1oo** in $CDCl_3$ recorded at 25 °C.

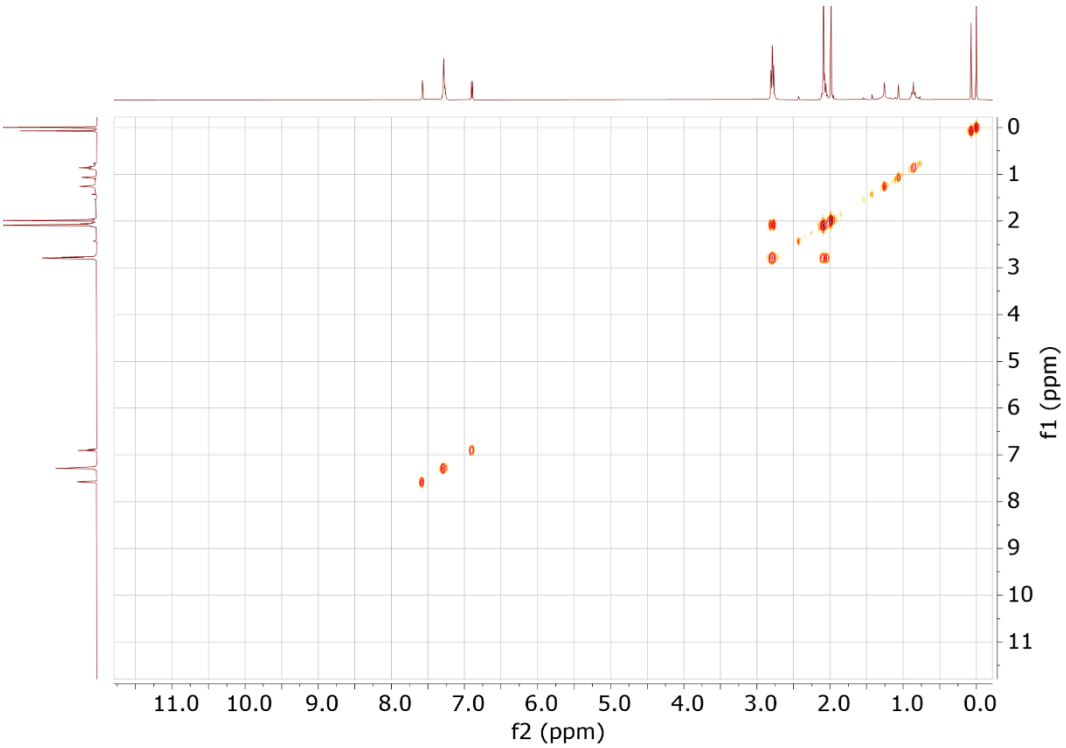


Fig. S24 ^1H-^1H COSY spectrum of **1oo** in $CDCl_3$ recorded at 25 °C.

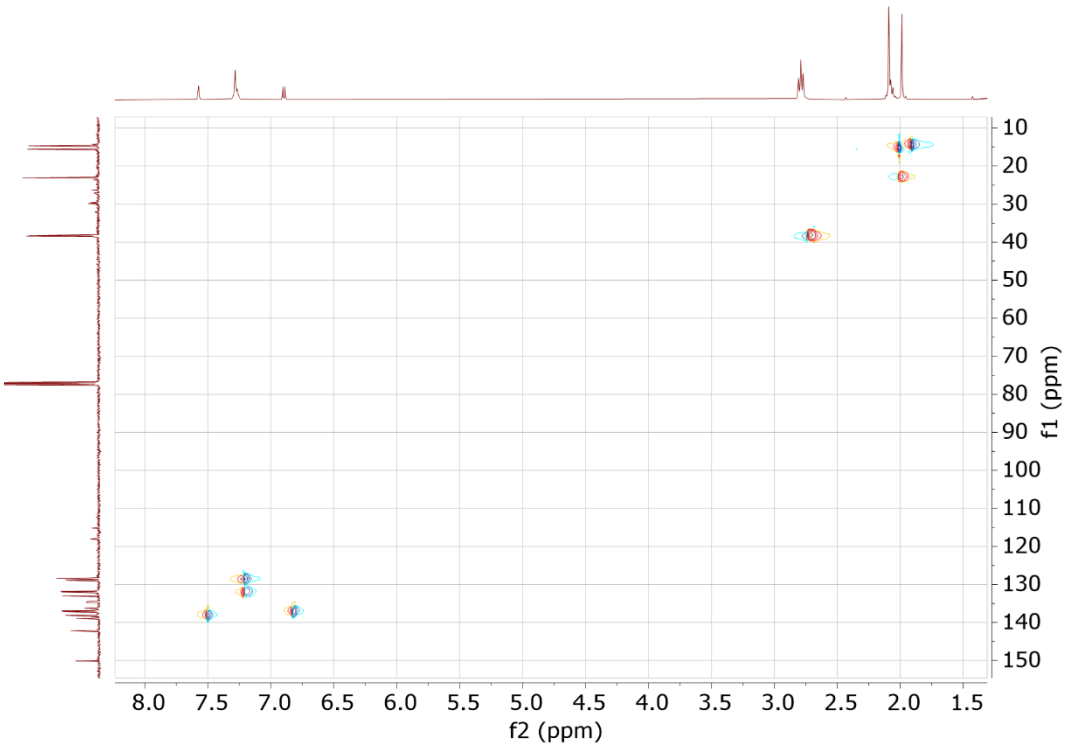


Fig. S25 ^{1}H-^{13}C HSQC spectrum of **1oo** in $CDCl_3$ recorded at 25 °C.

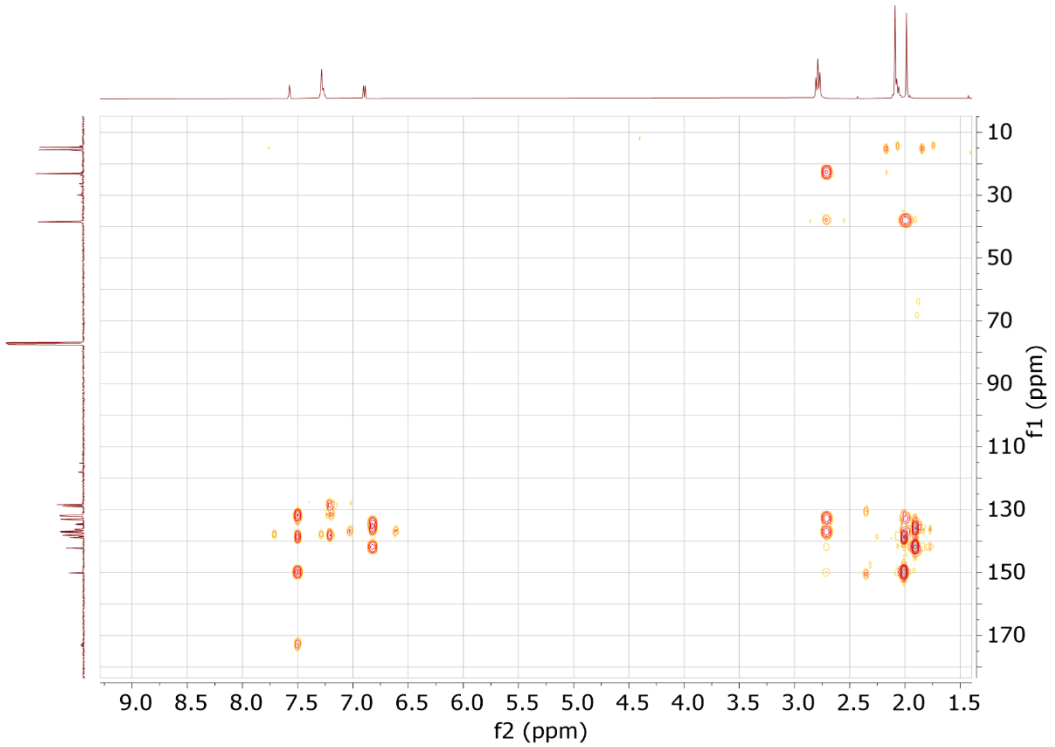


Fig. S26 ^{1}H-^{13}C HMBC spectrum of **1oo** in $CDCl_3$ recorded at 25 °C.

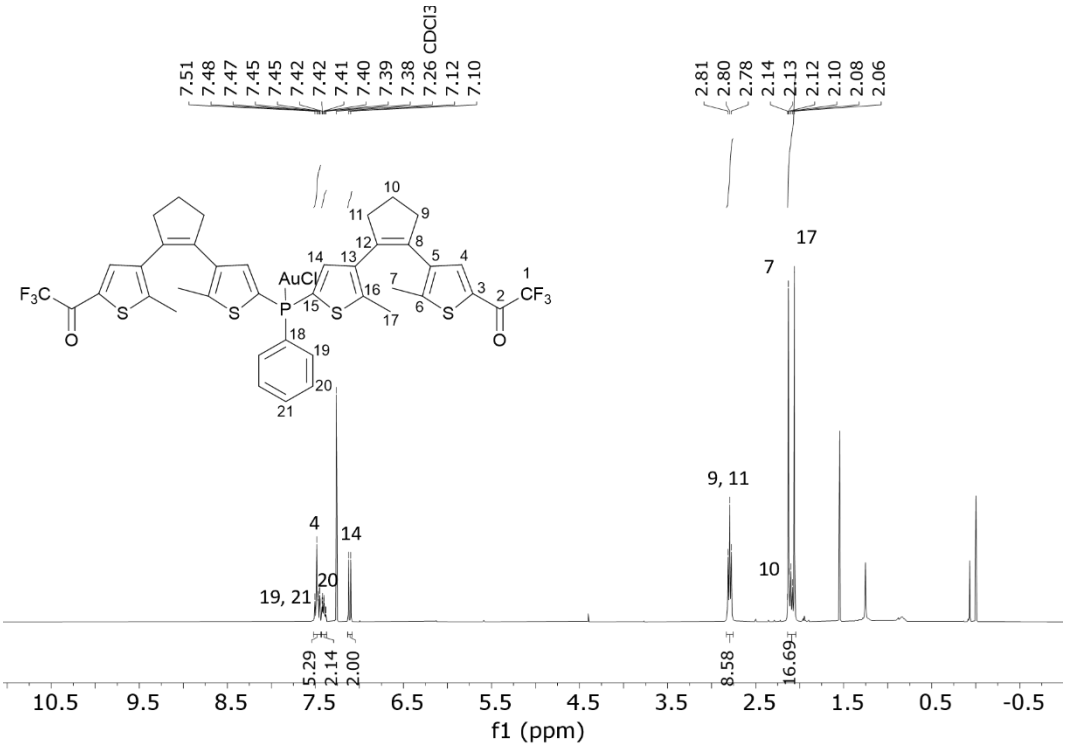


Fig. S27 ^{1}H NMR spectrum (400 MHz) of **4oo** in $CDCl_3$ recorded at 25 °C.

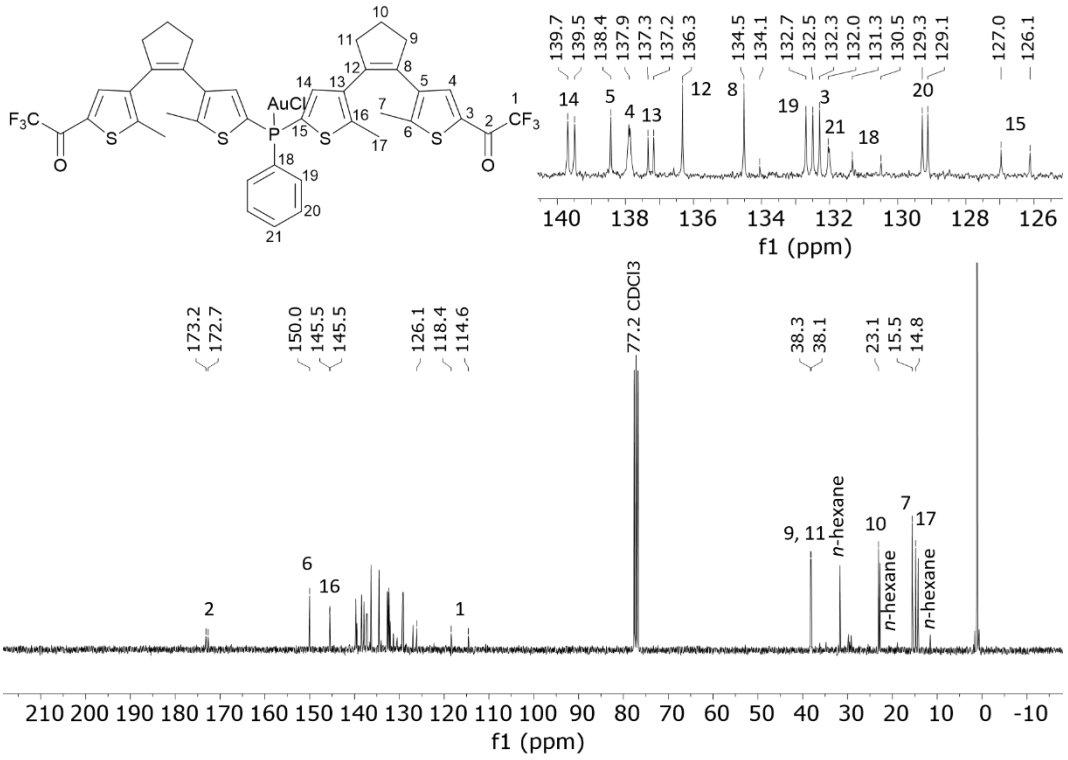


Fig. S28 $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz) of **4oo** in $CDCl_3$ recorded at 25 °C.

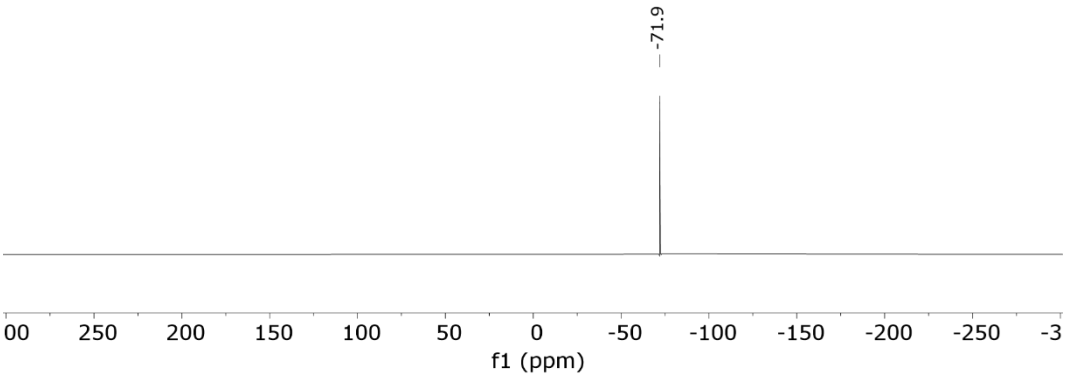


Fig. S29 ^{19}F NMR spectrum (376 MHz) of **4oo** in $CDCl_3$ recorded at 25 °C.

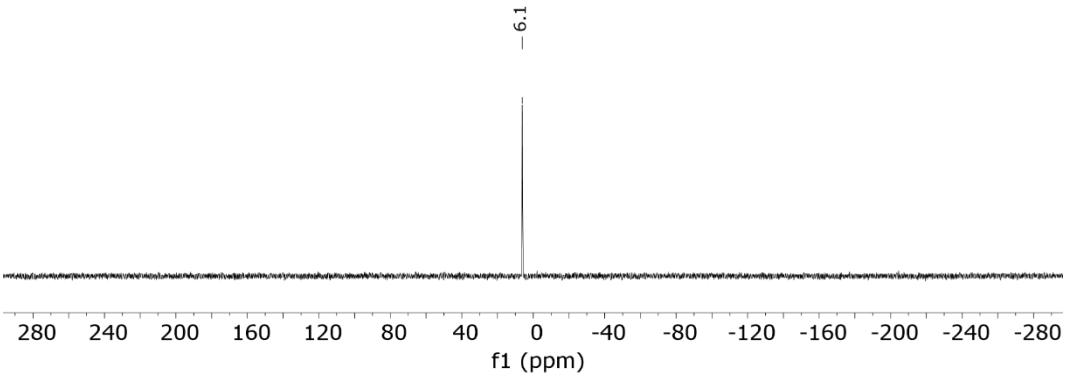


Fig. S30 $^{31}P\{^1H\}$ NMR spectrum (162 MHz) of **4oo** in $CDCl_3$ recorded at 25 °C.

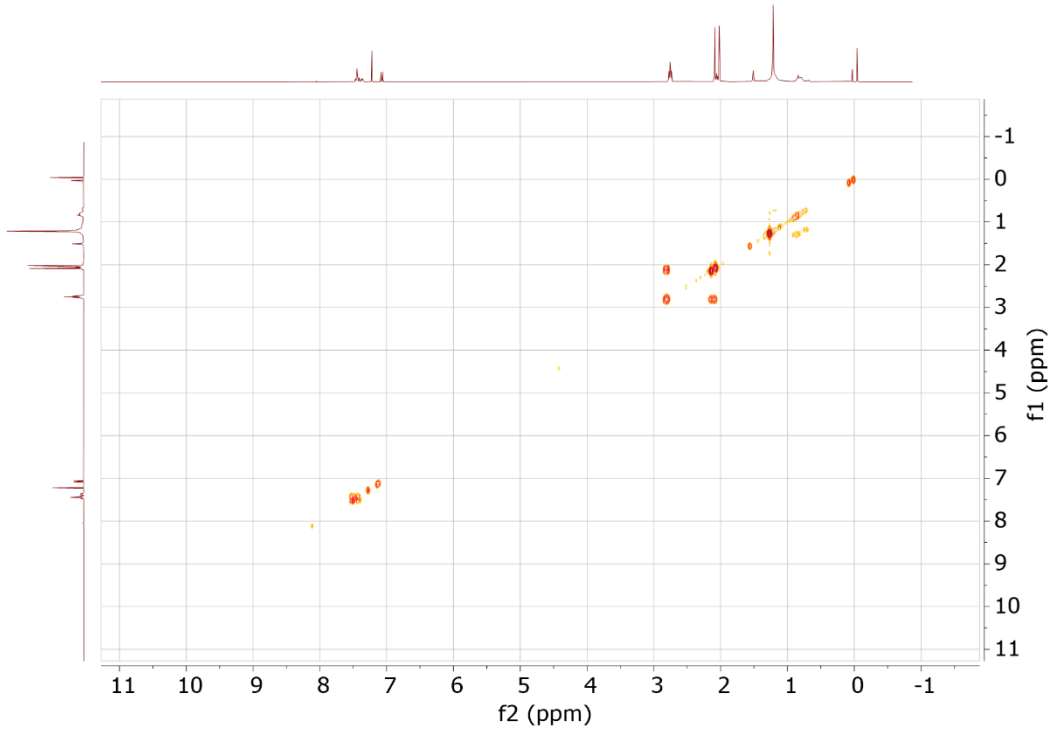


Fig. S31 ^1H-^1H COSY spectrum of **4oo** in $CDCl_3$ recorded at 25 °C.

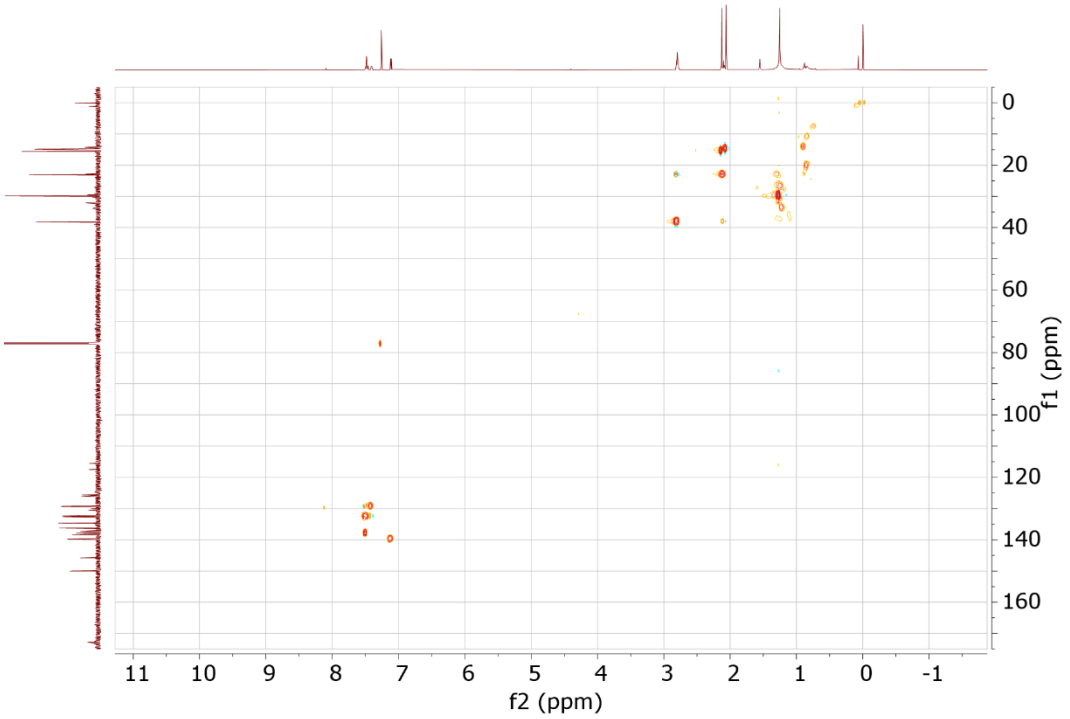


Fig. S32 ^{1}H-^{13}C HSQC spectrum of **4oo** in $CDCl_3$ recorded at 25 °C.

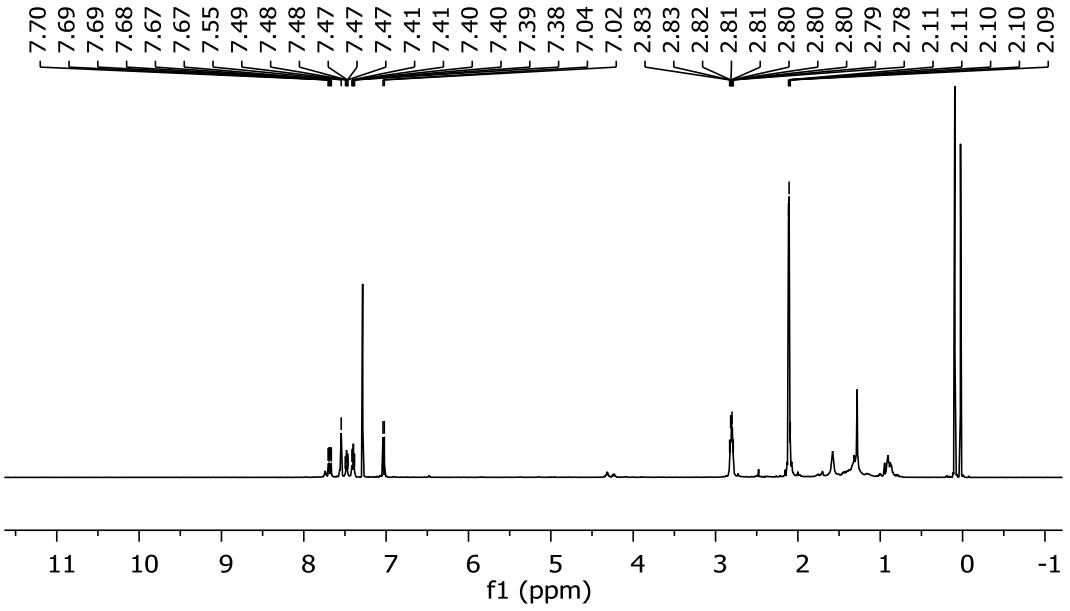


Fig. S33 ^{1}H NMR spectrum (400 MHz) of **6oo** in $CDCl_3$ recorded at 25 °C.

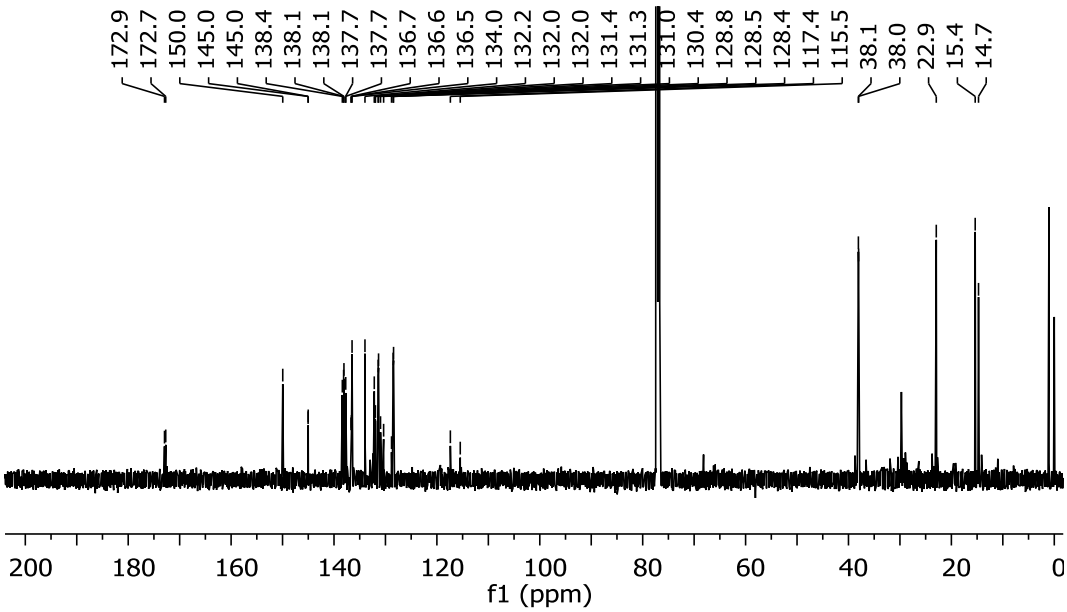


Fig. S34 ^{13}C NMR spectrum (151 MHz) of **6oo** in $CDCl_3$ recorded at 25 °C.

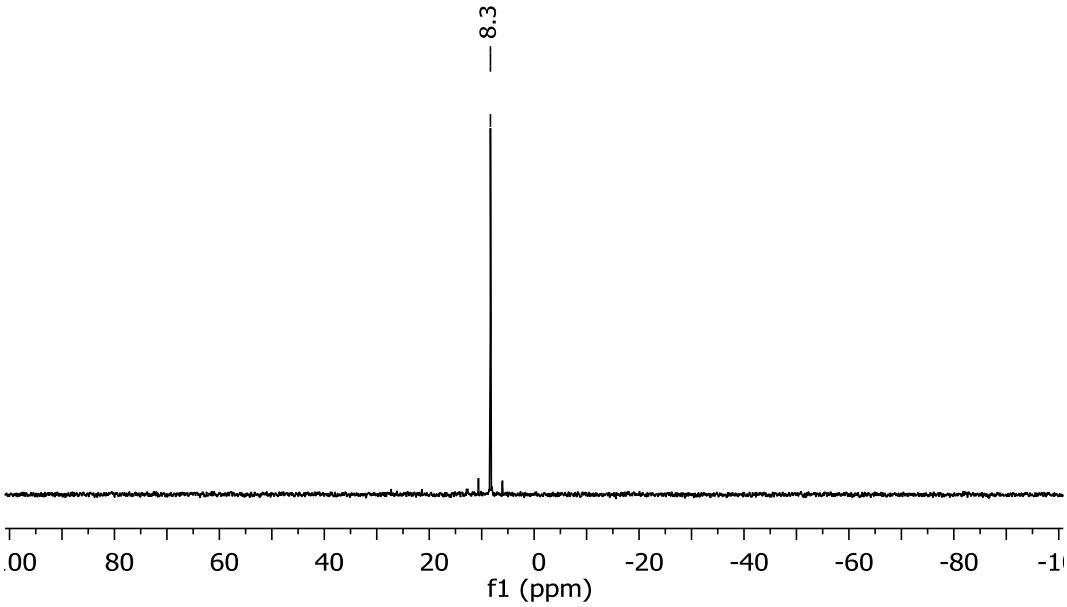


Fig. S35 $^{31}P\{^1H\}$ NMR spectrum (162 MHz) of **6oo** in $CDCl_3$ recorded at 25 °C.

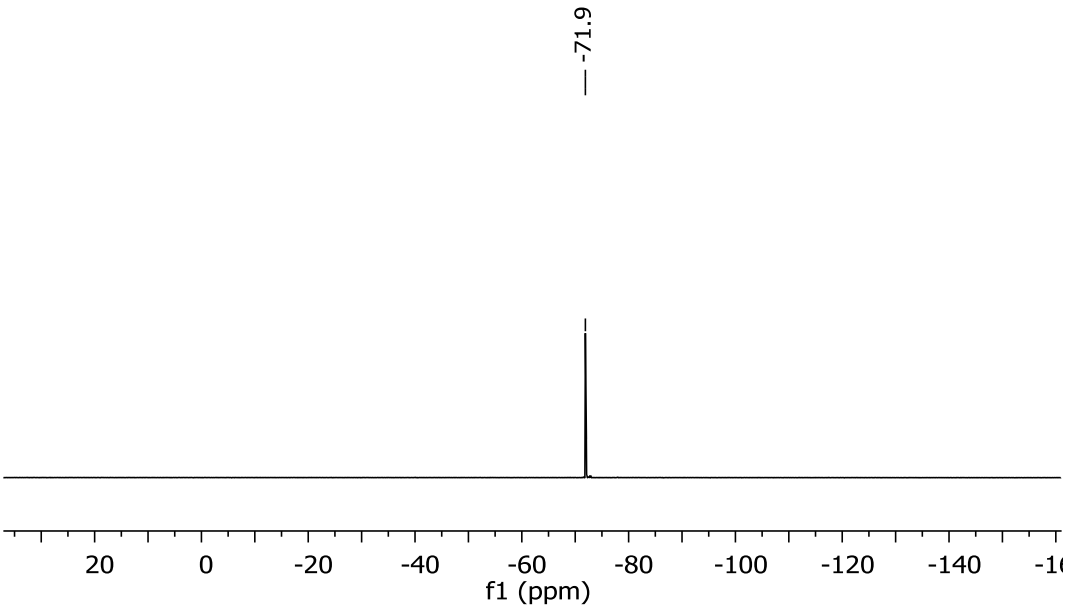


Fig. S36 ^{19}F NMR spectrum (376 MHz) of **6oo** in $CDCl_3$ recorded at 25 °C.

4 Cartesian coordinates

1oo

C	-5.206076000	0.129609000	1.391559000
C	-5.245031000	-0.473967000	0.136549000
S	-6.086581000	0.505179000	-1.022342000
C	-6.421350000	1.741112000	0.177617000
C	-5.894332000	1.373220000	1.399503000
H	-5.992557000	2.002972000	2.275795000
C	-4.677864000	-1.791093000	-0.287553000
H	-3.685776000	-1.659162000	-0.733313000
H	-4.566620000	-2.444786000	0.580277000
H	-5.316116000	-2.287354000	-1.024806000
C	-4.525758000	-1.367497000	4.807837000
C	-3.122854000	-1.438762000	4.168986000
C	-3.357431000	-0.993169000	2.734646000
C	-4.578464000	-0.423123000	2.600506000
C	-5.296201000	-0.349666000	3.939742000
H	-4.500782000	-1.096137000	5.866844000
H	-2.672256000	-2.435750000	4.232711000
H	-2.415132000	-0.748472000	4.651330000
H	-6.364697000	-0.576420000	3.856341000
H	-5.221317000	0.669052000	4.348461000
H	-5.010269000	-2.346929000	4.727035000
C	-1.586007000	-2.367770000	1.531347000
C	-0.650135000	-2.338636000	0.528582000
S	-0.607001000	-0.736987000	-0.192448000
C	-1.856597000	-0.140899000	0.869981000
C	-2.299134000	-1.135101000	1.723842000
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C	-2.287123000	1.291407000	0.782615000
H	-3.012792000	1.444058000	-0.024840000
H	-2.764473000	1.596320000	1.716826000
H	-1.436608000	1.954608000	0.594981000
P	0.357183000	-3.779093000	0.038485000
C	-0.294240000	-4.179812000	-1.646559000
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C	-1.606688000	-3.856664000	-2.022741000
C	-0.000422000	-5.319073000	-3.775265000
C	-2.106536000	-4.253150000	-3.264979000
C	-1.304533000	-4.980607000	-4.146973000
H	1.515150000	-5.200033000	-2.255794000
H	-2.240640000	-3.292473000	-1.346141000
H	0.630018000	-5.887782000	-4.453272000
H	-3.122712000	-3.987276000	-3.543588000
H	-1.692536000	-5.284416000	-5.115091000
C	1.974134000	-3.023712000	-0.337942000
C	3.010163000	-2.958049000	0.559465000
S	2.391661000	-2.130009000	-1.792857000
C	4.123831000	-2.163226000	0.126245000
C	3.942542000	-1.658811000	-1.148392000
C	4.878148000	-0.830313000	-1.974799000
H	4.871512000	-1.142829000	-3.023997000
H	4.608044000	0.231622000	-1.941913000
H	5.897299000	-0.923507000	-1.592239000
H	2.971982000	-3.432978000	1.534498000
C	5.296836000	-1.914808000	0.977662000
C	6.083422000	-3.055909000	1.597481000
H	6.638148000	-3.586015000	0.809340000
H	5.436071000	-3.801629000	2.073490000
C	7.027086000	-2.346676000	2.593383000
H	6.557552000	-2.324534000	3.583085000
H	7.993941000	-2.846939000	2.696703000
C	7.147409000	-0.901510000	2.059404000
H	7.257088000	-0.157189000	2.855684000
H	8.018168000	-0.785031000	1.397184000
C	5.864258000	-0.720693000	1.264418000
C	5.398471000	0.615360000	0.863621000
C	4.093073000	1.088666000	0.982962000
S	3.942571000	2.712043000	0.390740000
C	5.650151000	2.787679000	-0.008600000
C	6.268723000	1.596867000	0.318865000
H	7.326986000	1.437579000	0.147993000
C	2.894242000	0.393864000	1.546176000
H	2.304453000	-0.083330000	0.756030000
H	2.238035000	1.088482000	2.079327000
H	3.212352000	-0.390328000	2.236912000
C	6.340671000	3.919122000	-0.605310000
O	7.537424000	3.938511000	-0.849232000
C	5.495489000	5.170964000	-0.960338000
F	4.880744000	5.664374000	0.139548000
F	6.253163000	6.137130000	-1.484910000
F	4.529806000	4.856201000	-1.853656000
C	-7.144240000	2.982276000	-0.050109000
O	-7.369417000	3.811104000	0.818211000
C	-7.655254000	3.262373000	-1.488343000
F	-8.507280000	2.291080000	-1.890058000
F	-8.291709000	4.433768000	-1.559347000
F	-6.626919000	3.283858000	-2.366932000

1oc

C	5.901356000	-0.568951000	1.477025000
C	5.958782000	0.519547000	0.608955000
S	7.137319000	0.282083000	-0.641540000
C	7.591825000	-1.285740000	0.002643000
C	6.847760000	-1.570758000	1.130333000
H	6.974388000	-2.496565000	1.679108000
C	5.176847000	1.794289000	0.651189000
H	4.299619000	1.740185000	-0.003766000
H	4.818881000	1.974901000	1.667085000
H	5.782656000	2.648499000	0.333821000
C	4.428281000	-0.838278000	4.963983000
C	3.150831000	-0.709735000	4.106696000
C	3.683045000	-0.444379000	2.709051000
C	5.009759000	-0.702357000	2.638202000
C	5.532443000	-1.239653000	3.961232000
H	4.320263000	-1.547985000	5.788828000
H	2.475086000	0.079618000	4.455817000
H	2.562918000	-1.639357000	4.100623000
H	6.516556000	-0.833840000	4.219886000
H	5.647868000	-2.332091000	3.901925000
H	4.674016000	0.138217000	5.395933000
C	1.897987000	1.087440000	1.738803000
C	1.174416000	1.367774000	0.605895000
S	1.567267000	0.202567000	-0.649550000
C	2.698847000	-0.636687000	0.376893000
C	2.782707000	-0.035672000	1.620217000

H	1.830893000	1.689039000	2.639340000
C	3.431666000	-1.836001000	-0.141807000
H	4.285338000	-1.545745000	-0.765383000
H	3.817405000	-2.426209000	0.692589000
H	2.779207000	-2.474344000	-0.745914000
P	0.013585000	2.764829000	0.478493000
C	0.271702000	3.328260000	-1.266990000
C	-0.805374000	3.669011000	-2.098629000
C	1.581516000	3.533550000	-1.732919000
C	-0.577276000	4.182012000	-3.377308000
C	1.805974000	4.044996000	-3.011561000
C	0.727332000	4.368086000	-3.839392000
H	-1.825122000	3.532443000	-1.751697000
H	2.429581000	3.284484000	-1.100523000
H	-1.422288000	4.430895000	-4.013426000
H	2.824657000	4.188663000	-3.361180000
H	0.902893000	4.763405000	-4.835829000
C	8.592220000	-2.182502000	-0.553878000
O	8.920181000	-3.242205000	-0.042953000
C	9.260654000	-1.770702000	-1.892269000
F	9.859682000	-0.561864000	-1.783061000
F	10.181210000	-2.660457000	-2.270824000
F	8.334288000	-1.673539000	-2.872645000
C	-1.638505000	1.968413000	0.374063000
C	-2.730042000	2.526984000	0.973123000
H	-2.667094000	3.427148000	1.575987000
C	-3.954824000	1.805722000	0.794566000
C	-5.152841000	1.994414000	1.416387000
C	-6.253759000	1.085346000	1.184447000
C	-5.593628000	3.096231000	2.355322000
C	-6.928255000	2.564196000	2.933289000
C	-7.499191000	1.642065000	1.827713000
S	-1.990332000	0.456719000	-0.488027000
C	-3.840305000	0.725820000	-0.296449000
C	-4.351900000	1.338282000	-1.622078000
H	-3.819723000	2.271068000	-1.823127000
H	-5.420423000	1.559827000	-1.545848000
H	-4.196004000	0.660479000	-2.462639000
C	-4.628943000	-0.523097000	0.156980000
C	-4.021030000	-1.221905000	1.394990000
H	-3.918308000	-0.511584000	2.220589000
H	-4.851767000	3.321684000	3.127714000
H	-5.757376000	4.021998000	1.787017000
H	-7.618339000	3.364395000	3.212431000
H	-8.174673000	0.869878000	2.206119000
H	-8.057601000	2.233570000	1.088372000
H	-6.725414000	1.967717000	3.829685000
H	-4.683278000	-2.029935000	1.715443000
H	-3.038836000	-1.644129000	1.175005000
C	-6.064780000	-0.090053000	0.512839000
C	-7.040398000	-1.042046000	0.118884000
C	-6.573261000	-2.009916000	-0.734572000
S	-4.854853000	-1.828283000	-1.178219000
H	-8.073856000	-0.978561000	0.437672000
C	-7.322363000	-3.095997000	-1.329081000
O	-6.858325000	-3.911864000	-2.116140000
C	-8.819671000	-3.211197000	-0.937845000
F	-9.504461000	-2.100694000	-1.298916000
F	-9.392494000	-4.262846000	-1.532373000
F	-8.966982000	-3.353698000	0.399753000

1cc

C	-4.578370000	-0.853654000	1.076233000
C	-3.797061000	-0.152523000	-0.053561000
S	-4.926547000	-0.287789000	-1.550827000
C	-5.869998000	-1.571602000	-0.745502000
C	-5.587159000	-1.722712000	0.589779000
H	-6.114232000	-2.415365000	1.234898000
C	-3.430970000	-1.112106000	4.578029000
C	-2.844703000	0.259843000	4.162401000
C	-3.219609000	0.373292000	2.700741000
C	-4.208952000	-0.627555000	2.373405000
C	-4.642643000	-1.326947000	3.637474000
H	-3.705640000	-1.153698000	5.635117000
H	-1.765986000	0.333729000	4.333488000
H	-3.316606000	1.073247000	4.730402000
H	-4.897938000	-2.379195000	3.484699000
H	-5.534008000	-0.827642000	4.043010000
H	-2.689116000	-1.896827000	4.392785000
C	-1.736288000	2.223443000	1.853176000
C	-1.350931000	2.769574000	0.663157000
S	-2.286179000	2.207805000	-0.731276000
C	-3.489784000	1.295383000	0.388612000
C	-2.783540000	1.254500000	1.755599000
H	-1.236671000	2.449228000	2.790120000
P	0.114753000	3.874895000	0.553561000
C	0.057339000	4.458071000	-1.197408000
C	1.096592000	4.228983000	-2.111780000
C	-1.034314000	5.253220000	-1.589081000
C	1.032116000	4.765479000	-3.399600000
C	-1.099467000	5.777829000	-2.879891000
C	-0.066457000	5.534385000	-3.789086000
H	1.956055000	3.631182000	-1.826383000
H	-1.840236000	5.456329000	-0.888678000
H	1.840653000	4.575317000	-4.099899000
H	-1.955330000	6.379182000	-3.173070000
H	-0.116278000	5.945212000	-4.793404000
C	-4.744549000	2.188385000	0.532025000
H	-5.463915000	1.719524000	1.209786000
H	-4.455016000	3.156046000	0.949620000
H	-5.231547000	2.353381000	-0.430396000
C	-2.529514000	-0.989414000	-0.346977000
H	-1.855696000	-0.977560000	0.514628000
H	-2.818003000	-2.024438000	-0.546060000
H	-1.987845000	-0.607563000	-1.214109000
C	1.438003000	2.603798000	0.525433000
C	2.612247000	2.772477000	1.198996000
H	2.841235000	3.674208000	1.757767000
C	3.538612000	1.686448000	1.072614000
C	4.848934000	1.636598000	1.442853000
C	5.654638000	0.471859000	1.145663000
C	5.677538000	2.643775000	2.210109000
C	7.127533000	2.131396000	2.027920000
C	6.986336000	0.600406000	1.841871000
S	1.321394000	1.059736000	-0.346865000
C	2.874334000	0.423142000	0.495038000
C	2.416989000	-0.452632000	1.685980000
H	1.793835000	0.145184000	2.356185000
H	3.285521000	-0.810767000	2.246504000
H	1.839840000	-1.315405000	1.349733000
C	3.874170000	-0.276147000	-0.451542000

C	4.198918000	0.544633000	-1.721733000
H	4.560213000	1.540593000	-1.448608000
H	5.537884000	3.670116000	1.856765000
H	5.389174000	2.626534000	3.269995000
H	7.778771000	2.395754000	2.864818000
H	7.811763000	0.148238000	1.285165000
H	6.936336000	0.100157000	2.819343000
H	7.556474000	2.566098000	1.118266000
H	4.983105000	0.037434000	-2.289076000
H	3.322793000	0.655318000	-2.363266000
C	5.192420000	-0.507751000	0.312670000
C	5.804230000	-1.747455000	-0.009197000
C	4.994865000	-2.613087000	-0.700976000
S	3.349583000	-1.994613000	-1.005475000
H	6.810383000	-1.995574000	0.306886000
C	5.314056000	-3.951832000	-1.150747000
O	4.530724000	-4.694447000	-1.729143000
C	-6.856242000	-2.285906000	-1.524640000
O	-7.091668000	-2.078646000	-2.709443000
C	6.751545000	-4.463802000	-0.868646000
F	7.013376000	-4.478840000	0.459385000
F	6.920877000	-5.703957000	-1.338197000
F	7.675816000	-3.664684000	-1.449460000
C	-7.673168000	-3.380553000	-0.787887000
F	-8.384569000	-2.852221000	0.236015000
F	-8.530214000	-3.982272000	-1.619541000
F	-6.863276000	-4.328728000	-0.262626000

4oo

C	5.332587000	0.747120000	-1.314119000
C	5.391930000	0.316789000	0.009474000
S	6.339350000	1.387927000	0.991604000
C	6.689718000	2.427914000	-0.377662000
C	6.089574000	1.932826000	-1.517915000
H	6.185007000	2.431341000	-2.475349000
C	4.771642000	-0.894778000	0.629729000
H	3.809339000	-0.644125000	1.089674000
H	4.586528000	-1.651413000	-0.135997000
H	5.413527000	-1.325851000	1.403839000
C	4.403550000	-1.161688000	-4.458149000
C	3.030561000	-1.049115000	-3.761849000
C	3.361864000	-0.422688000	-2.417792000
C	4.619994000	0.076125000	-2.410920000
C	5.278295000	-0.090102000	-3.771750000
H	4.344209000	-1.035782000	-5.542605000
H	2.519191000	-2.013532000	-3.662232000
H	2.342777000	-0.388766000	-4.310310000
H	6.331932000	-0.379316000	-3.694563000
H	5.252655000	0.864777000	-4.317344000
H	4.828595000	-2.152038000	-4.261237000
C	1.588322000	-1.495432000	-0.948269000
C	0.705699000	-1.248848000	0.073393000
S	0.769624000	0.437759000	0.543012000
C	1.998347000	0.786702000	-0.646064000
C	2.348359000	-0.349437000	-1.354946000
H	1.708471000	-2.477510000	-1.392883000
C	2.510440000	2.186222000	-0.791141000
H	3.286532000	2.406450000	-0.049257000
H	2.952626000	2.318839000	-1.781157000
H	1.709643000	2.921698000	-0.665813000
P	-0.369021000	-2.478515000	0.839968000
C	0.261019000	-2.740504000	2.537231000
C	-0.580287000	-3.328008000	3.496032000
C	1.588492000	-2.434582000	2.866177000
C	-0.097509000	-3.585803000	4.778692000
C	2.065081000	-2.698152000	4.151488000
C	1.223826000	-3.269850000	5.108410000
H	-1.607545000	-3.576993000	3.245211000
H	2.247884000	-1.994280000	2.125325000
H	-0.753532000	-4.033244000	5.519475000
H	3.092876000	-2.453545000	4.403148000
H	1.596392000	-3.471265000	6.108523000
C	-1.978846000	-1.690805000	1.034397000
C	-2.996457000	-1.760993000	0.115719000
S	-2.378335000	-0.556380000	2.308024000
C	-4.092650000	-0.882614000	0.394231000
C	-3.909479000	-0.170113000	1.566565000
C	-4.828404000	0.812278000	2.224410000
H	-4.836642000	0.689574000	3.312022000
H	-4.529971000	1.844021000	2.005548000
H	-5.846108000	0.675580000	1.851814000
H	-2.951291000	-2.396320000	-0.762419000
C	-5.248552000	-0.758875000	-0.506774000
C	-6.056110000	-1.971037000	-0.933432000
H	-6.638535000	-2.340857000	-0.076878000
H	-5.422159000	-2.804311000	-1.258673000
C	-6.961939000	-1.422699000	-2.058356000
H	-6.477709000	-1.591785000	-3.026398000
H	-7.942552000	-1.905205000	-2.089753000
C	-7.044360000	0.097881000	-1.793367000
H	-7.111692000	0.690815000	-2.711909000
H	-7.923226000	0.358164000	-1.185107000
C	-5.772911000	0.381075000	-1.010668000
C	-5.274474000	1.753004000	-0.831888000
C	-3.954837000	2.165487000	-1.003535000
S	-3.765202000	3.858269000	-0.676102000
C	-5.474968000	4.042331000	-0.323962000
C	-6.123858000	2.831770000	-0.467542000
H	-7.188291000	2.728843000	-0.291843000
C	-2.769268000	1.359239000	-1.431783000
H	-2.186495000	1.019643000	-0.568292000
H	-2.101433000	1.937632000	-2.077465000
H	-3.101582000	0.472162000	-1.975702000
C	-6.139379000	5.273120000	0.074469000
O	-7.340054000	5.366477000	0.277112000
C	-5.257682000	6.535294000	0.268602000
F	-4.581745000	6.831183000	-0.865623000
F	-5.994180000	7.596420000	0.605820000
F	-4.340517000	6.327678000	1.240866000
C	7.488435000	3.643423000	-0.347960000
O	7.719343000	4.332360000	-1.329210000
C	8.070509000	4.087775000	1.020032000
F	8.862400000	3.122770000	1.541648000
F	8.792516000	5.204269000	0.901972000
F	7.075992000	4.316371000	1.908267000
Au	-0.512885000	-4.380370000	-0.407084000
Cl	-0.699135000	-6.346947000	-1.685350000

4oc

C	-5.765281000	-1.070335000	-1.557425000
C	-5.866798000	-0.300949000	-0.400376000
S	-7.075876000	-0.921305000	0.677854000
C	-7.479082000	-2.222784000	-0.428318000
C	-6.698283000	-2.141687000	-1.564206000
H	-6.791004000	-2.856018000	-2.373796000
C	-5.106664000	0.932960000	-0.027214000
H	-4.241982000	0.690063000	0.601163000
H	-4.731365000	1.422613000	-0.928805000
H	-5.733477000	1.641466000	0.522500000
C	-4.172426000	-0.190833000	-4.890754000
C	-2.926611000	-0.360540000	-3.993714000
C	-3.512545000	-0.570002000	-2.608907000
C	-4.838950000	-0.825330000	-2.672711000
C	-5.313489000	-0.887111000	-4.115530000
H	-4.031568000	-0.593391000	-5.897510000
H	-2.245831000	0.497777000	-4.035808000
H	-2.331885000	-1.242087000	-4.274643000
H	-6.286440000	-0.404506000	-4.257563000
H	-5.433744000	-1.936192000	-4.423903000
H	-4.404325000	0.875377000	-4.988685000
C	-1.806170000	0.555110000	-1.099224000
C	-1.142623000	0.430120000	0.096934000
S	-1.542958000	-1.093814000	0.862740000
C	-2.609756000	-1.539575000	-0.442458000
C	-2.661848000	-0.549763000	-1.408949000
H	-1.715217000	1.431557000	-1.731889000
C	-3.334677000	-2.848778000	-0.396208000
H	-4.216209000	-2.793797000	0.252787000
H	-3.676622000	-3.117467000	-1.398155000
H	-2.691562000	-3.650889000	-0.020949000
P	-0.002381000	1.651292000	0.772654000
C	-0.267427000	1.616084000	2.582788000
C	0.813728000	1.635687000	3.473917000
C	-1.582306000	1.650892000	3.074171000
C	0.578526000	1.671396000	4.849480000
C	-1.808663000	1.686755000	4.449547000
C	-0.729487000	1.694470000	5.338181000
H	1.832779000	1.620378000	3.101069000
H	-2.424248000	1.644592000	2.387688000
H	1.419120000	1.677562000	5.537066000
H	-2.827042000	1.707539000	4.826089000
H	-0.908943000	1.719938000	6.409017000
C	-8.478144000	-3.256543000	-0.207497000
O	-8.743849000	-4.132584000	-1.015689000
C	-9.238220000	-3.244524000	1.145043000
F	-9.886853000	-2.070638000	1.322164000
F	-10.134184000	-4.232111000	1.208597000
F	-8.374577000	-3.386896000	2.176534000
C	1.677620000	1.015937000	0.503905000
C	2.696021000	1.781773000	0.020843000
H	2.559914000	2.816409000	-0.276153000
C	3.945126000	1.092059000	-0.105802000
C	5.080175000	1.508131000	-0.731758000
C	6.223767000	0.626124000	-0.846240000
C	5.411555000	2.848961000	-1.347456000
C	6.705505000	2.567493000	-2.150142000
C	7.393881000	1.402891000	-1.396019000
S	2.120093000	-0.668096000	0.849703000
C	3.946564000	-0.256850000	0.636688000
C	4.529349000	-0.019185000	2.049035000
H	3.989013000	0.797907000	2.533535000
H	5.584044000	0.261609000	1.976310000
H	4.448276000	-0.910381000	2.673043000
C	4.734460000	-1.286773000	-0.203034000
C	4.054052000	-1.645407000	-1.544780000
H	3.857047000	-0.739520000	-2.125586000
H	4.600391000	3.248388000	-1.963887000
H	5.599786000	3.580091000	-0.549525000
H	7.346835000	3.447543000	-2.240759000
H	8.053698000	0.801164000	-2.026959000
H	7.997860000	1.791207000	-0.563889000
H	6.443042000	2.236980000	-3.161123000
H	4.718809000	-2.289718000	-2.125337000
H	3.110500000	-2.171375000	-1.388681000
C	6.122349000	-0.695897000	-0.520757000
C	7.155989000	-1.670553000	-0.478735000
C	6.787643000	-2.856349000	0.101786000
S	5.106738000	-2.897777000	0.691902000
H	8.157075000	-1.467863000	-0.839612000
C	7.616434000	-4.026218000	0.321805000
O	7.236721000	-5.046508000	0.879900000
C	9.084286000	-3.952822000	-0.177394000
F	9.757971000	-2.960313000	0.448183000
F	9.727000000	-5.101723000	0.053236000
F	9.138057000	-3.699460000	-1.504989000
Au	-0.329620000	3.703669000	-0.167017000
Cl	-0.704360000	5.817912000	-1.126826000

4cc

C	4.861665000	-1.419499000	-1.065715000
C	3.913038000	-1.232086000	0.135863000
S	4.857534000	-1.953580000	1.592461000
C	5.962642000	-2.798280000	0.478062000
C	5.851496000	-2.411696000	-0.832630000
H	6.489210000	-2.790898000	-1.622074000
C	4.169312000	-0.253176000	-4.498267000
C	3.462152000	0.835823000	-3.654467000
C	3.647671000	0.355577000	-2.232553000
C	4.647493000	-0.692064000	-2.201119000
C	5.270145000	-0.821530000	-3.568538000
H	4.570374000	0.133841000	-5.438202000
H	2.410862000	0.975402000	-3.924884000
H	3.958227000	1.807915000	-3.779264000
H	5.566501000	-1.844848000	-3.814377000
H	6.172383000	-0.195800000	-3.619051000
H	3.455803000	-1.048898000	-4.739166000
C	1.957815000	1.690418000	-0.935235000
C	1.411891000	1.709733000	0.313366000
S	2.202525000	0.652157000	1.492806000
C	3.584096000	0.270894000	0.268777000
C	3.051054000	0.778600000	-1.083738000
H	1.555438000	2.269622000	-1.760068000
P	-0.122238000	2.608689000	0.691703000
C	-0.112550000	2.865181000	2.499144000
C	-1.179870000	2.451941000	3.307825000
C	0.975928000	3.549986000	3.064454000
C	-1.148448000	2.711472000	4.679530000
C	0.999999000	3.801307000	4.435078000
C	-0.061055000	3.381471000	5.243385000

H	-2.028791000	1.930740000	2.877591000
H	1.801066000	3.878902000	2.438575000
H	-1.974108000	2.385953000	5.305280000
H	1.845676000	4.324444000	4.871256000
H	-0.039856000	3.579143000	6.311091000
C	4.792197000	1.149725000	0.665699000
H	5.614180000	0.996271000	-0.039446000
H	4.502082000	2.203081000	0.633853000
H	5.147511000	0.914576000	1.670238000
C	2.667425000	-2.119088000	-0.098607000
H	2.104491000	-1.764595000	-0.966979000
H	2.986384000	-3.146488000	-0.289815000
H	2.004112000	-2.117236000	0.768054000
C	-1.438913000	1.407056000	0.345838000
C	-2.576407000	1.734091000	-0.330850000
H	-2.780497000	2.739526000	-0.683910000
C	-3.496439000	0.649058000	-0.495514000
C	-4.785854000	0.692781000	-0.930293000
C	-5.600699000	-0.505116000	-0.940498000
C	-5.580385000	1.849713000	-1.493052000
C	-7.035696000	1.320854000	-1.495148000
C	-6.898418000	-0.213896000	-1.651558000
S	-1.347828000	-0.288381000	0.865168000
C	-2.853149000	-0.714280000	-0.183819000
C	-2.325109000	-1.302955000	-1.512653000
H	-1.677492000	-0.570664000	-2.001911000
H	-3.160887000	-1.527798000	-2.181692000
H	-1.755071000	-2.218427000	-1.347294000
C	-3.892907000	-1.604464000	0.531434000
C	-4.284528000	-1.092947000	1.937647000
H	-4.635329000	-0.058163000	1.881186000
H	-5.457627000	2.772994000	-0.918619000
H	-5.241689000	2.060135000	-2.516623000
H	-7.647994000	1.771030000	-2.280277000
H	-7.747214000	-0.773341000	-1.249089000
H	-6.800875000	-0.481805000	-2.713052000
H	-7.506732000	1.544276000	-0.531577000
H	-5.094567000	-1.709648000	2.334514000
H	-3.442751000	-1.139389000	2.630951000
C	-5.172003000	-1.647393000	-0.328090000
C	-5.791106000	-2.926799000	-0.326170000
C	-5.007170000	-3.929480000	0.182624000
S	-3.385566000	-3.406503000	0.703948000
H	-6.780679000	-3.092070000	-0.734855000
C	-5.337240000	-5.338024000	0.289750000
O	-4.577204000	-6.195105000	0.718845000
C	6.894514000	-3.756865000	1.038734000
O	6.972032000	-4.031112000	2.228777000
C	-6.751086000	-5.765689000	-0.186306000
F	-6.928499000	-5.480217000	-1.496951000
F	-6.937635000	-7.078105000	-0.017415000
F	-7.714279000	-5.110610000	0.500819000
C	7.858692000	-4.461003000	0.047231000
F	8.644752000	-3.559736000	-0.586147000
F	8.650654000	-5.329720000	0.683154000
F	7.174044000	-5.134320000	-0.905255000
Au	-0.325207000	4.515072000	-0.536563000
Cl	-0.539704000	6.480005000	-1.807655000

[AuCl(**5o**)]

C	3.891249000	1.380627000	-0.093867000
C	3.621485000	0.316959000	-0.951421000
S	4.990606000	-0.735339000	-1.121488000
C	5.961080000	0.258253000	-0.048816000
C	5.227138000	1.341270000	0.391204000
H	5.644869000	2.078744000	1.066331000
C	2.361519000	0.009545000	-1.696048000
H	1.760501000	-0.725721000	-1.149429000
H	1.762254000	0.915934000	-1.805086000
H	2.568573000	-0.397906000	-2.690316000
C	2.129100000	4.713378000	0.313305000
C	1.085700000	3.752409000	0.920654000
C	1.665213000	2.373878000	0.646992000
C	2.962533000	2.460653000	0.269573000
C	3.443188000	3.903529000	0.302410000
H	2.211180000	5.656392000	0.860530000
H	0.084274000	3.881900000	0.494646000
H	0.980238000	3.891248000	2.006683000
H	4.092910000	4.147718000	-0.544968000
H	4.034287000	4.078341000	1.213641000
H	1.844979000	4.950866000	-0.717817000
C	-0.481258000	1.044602000	0.368253000
C	-1.087061000	-0.149379000	0.668799000
S	-0.020282000	-1.152666000	1.628585000
C	1.240502000	0.053889000	1.602007000
C	0.854695000	1.168026000	0.875736000
H	-0.969395000	1.815344000	-0.218553000
C	2.519756000	-0.196554000	2.339204000
H	3.214221000	-0.797431000	1.740708000
H	3.011822000	0.752706000	2.562751000
H	2.344214000	-0.727217000	3.280138000
P	-2.714422000	-0.676506000	0.095370000
C	-2.424410000	-1.782238000	-1.336605000
C	-3.480168000	-2.585844000	-1.797009000
C	-1.200086000	-1.783194000	-2.016145000
C	-3.300860000	-3.393427000	-2.919203000
C	-1.028084000	-2.592057000	-3.141701000
C	-2.074907000	-3.398213000	-3.592604000
H	-4.433691000	-2.586826000	-1.275997000
H	-0.386471000	-1.153856000	-1.672282000
H	-4.118119000	-4.017594000	-3.268546000
H	-0.074974000	-2.590884000	-3.662570000
H	-1.938929000	-4.027344000	-4.467448000
C	-3.375543000	-1.745164000	1.422320000
C	-2.984289000	-3.089348000	1.530866000
C	-4.236859000	-1.188825000	2.379953000
C	-3.448357000	-3.863876000	2.594735000
C	-4.696813000	-1.969641000	3.440926000
C	-4.302706000	-3.305682000	3.549260000
H	-2.330281000	-3.533741000	0.786856000
H	-4.546173000	-0.150806000	2.292856000
H	-3.144584000	-4.903439000	2.674861000
H	-5.366212000	-1.535763000	4.177819000
H	-4.664814000	-3.912995000	4.373769000
C	7.337306000	-0.000791000	0.345416000
O	7.990688000	0.734545000	1.068753000
C	8.000289000	-1.303520000	-0.175045000
F	7.989486000	-1.344235000	-1.527481000
F	9.266053000	-1.403901000	0.236772000
F	7.322178000	-2.387838000	0.265567000
Au	-4.035595000	1.103630000	-0.438668000

Cl	-5.398743000	2.931356000	-1.025325000

[AuCl(**5c**)]

C	3.831529000	-1.001954000	0.104303000
C	2.973199000	0.249202000	0.378189000
S	4.092070000	1.691141000	-0.072061000
C	5.517738000	0.622123000	-0.025491000
C	5.222018000	-0.714139000	0.053424000
H	5.973714000	-1.493986000	0.036429000
C	2.664341000	-4.483123000	0.491663000
C	1.363467000	-3.769052000	0.048733000
C	1.772153000	-2.315837000	-0.040645000
C	3.217218000	-2.215861000	-0.009779000
C	3.809150000	-3.601627000	-0.066236000
H	2.719820000	-5.516655000	0.141331000
H	0.526286000	-3.936374000	0.733337000
H	1.044379000	-4.120242000	-0.941932000
H	4.746327000	-3.695201000	0.489111000
H	4.018493000	-3.865997000	-1.112359000
H	2.719583000	-4.495422000	1.585798000
C	-0.423268000	-1.091471000	-0.125973000
C	-0.888569000	0.187069000	-0.053516000
S	0.376079000	1.433163000	-0.038863000
C	1.685462000	0.149555000	-0.468718000
C	1.004462000	-1.199450000	-0.173401000
H	-1.079909000	-1.955049000	-0.108265000
P	-2.654394000	0.613068000	0.038928000
C	-2.840522000	1.519974000	1.618341000
C	-3.916729000	2.406059000	1.784566000
C	-1.972010000	1.268979000	2.690629000
C	-4.108677000	3.045644000	3.009107000
C	-2.171293000	1.912810000	3.913093000
C	-3.236206000	2.801898000	4.073518000
H	-4.596131000	2.605397000	0.961126000
H	-1.141616000	0.579395000	2.575362000
H	-4.938864000	3.735295000	3.129941000
H	-1.490819000	1.720376000	4.737304000
H	-3.387226000	3.303125000	5.025143000
C	-2.924534000	1.833464000	-1.295395000
C	-2.513381000	3.169319000	-1.157326000
C	-3.499805000	1.401834000	-2.500145000
C	-2.676769000	4.059249000	-2.218479000
C	-3.658720000	2.297907000	-3.558442000
C	-3.247281000	3.625093000	-3.418558000
H	-2.079490000	3.519424000	-0.226088000
H	-3.824019000	0.370354000	-2.607603000
H	-2.359071000	5.091673000	-2.106950000
H	-4.107694000	1.958893000	-4.487301000
H	-3.374141000	4.322522000	-4.241524000
C	1.923946000	0.236546000	-1.993843000
H	2.644173000	-0.525931000	-2.304426000
H	0.982344000	0.057540000	-2.519270000
H	2.306114000	1.216083000	-2.285145000
C	2.709172000	0.320771000	1.900491000
H	2.101989000	-0.530787000	2.221384000
H	3.661604000	0.285333000	2.434864000
H	2.191322000	1.241545000	2.175073000
C	6.830140000	1.231593000	-0.119572000
O	7.027858000	2.435563000	-0.212429000
C	8.052112000	0.274735000	-0.116062000
F	8.004637000	-0.575106000	-1.167699000
F	9.197536000	0.959827000	-0.186401000
F	8.080122000	-0.478438000	1.007339000
Au	-3.981820000	-1.236610000	-0.111501000
Cl	-5.360082000	-3.137230000	-0.284264000