

The photophysical properties of naphthalene bridged disilanes

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(i) NMR spectra

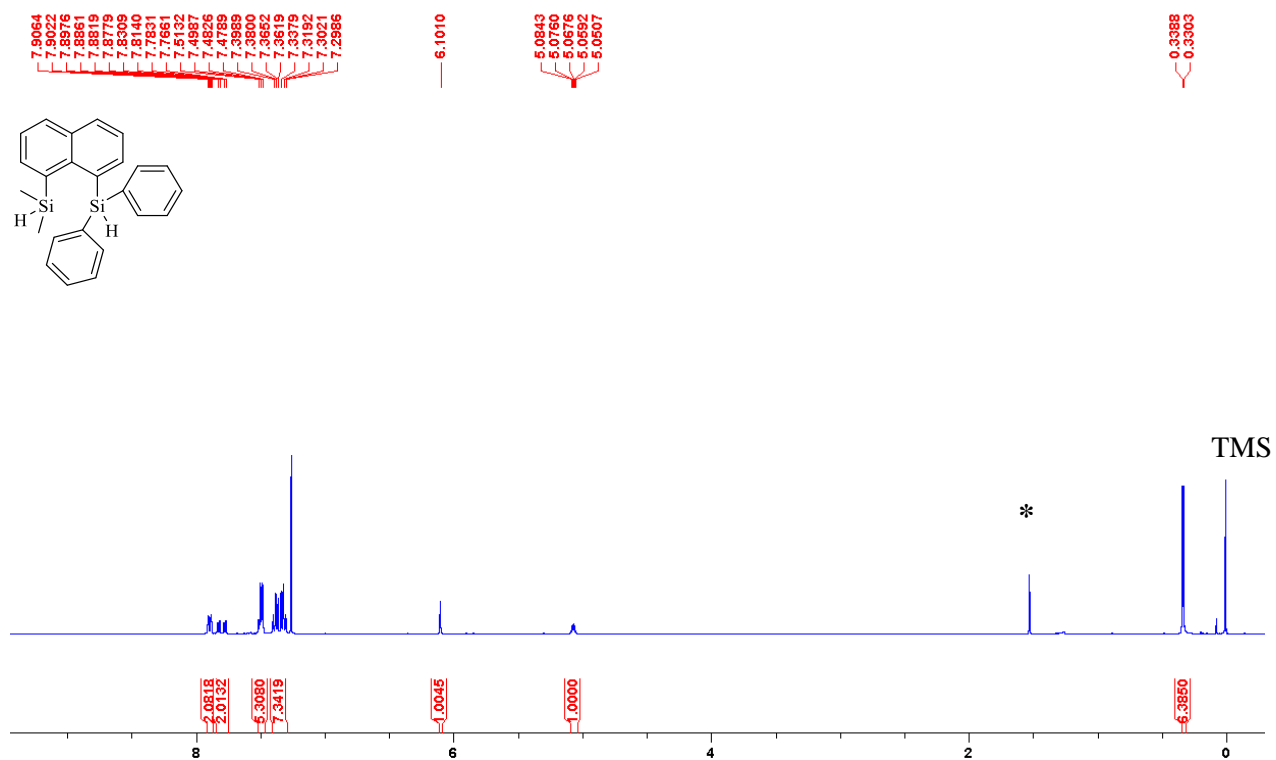


Figure S1 ¹H NMR spectrum of 1a, in CDCl₃ (* H₂O)

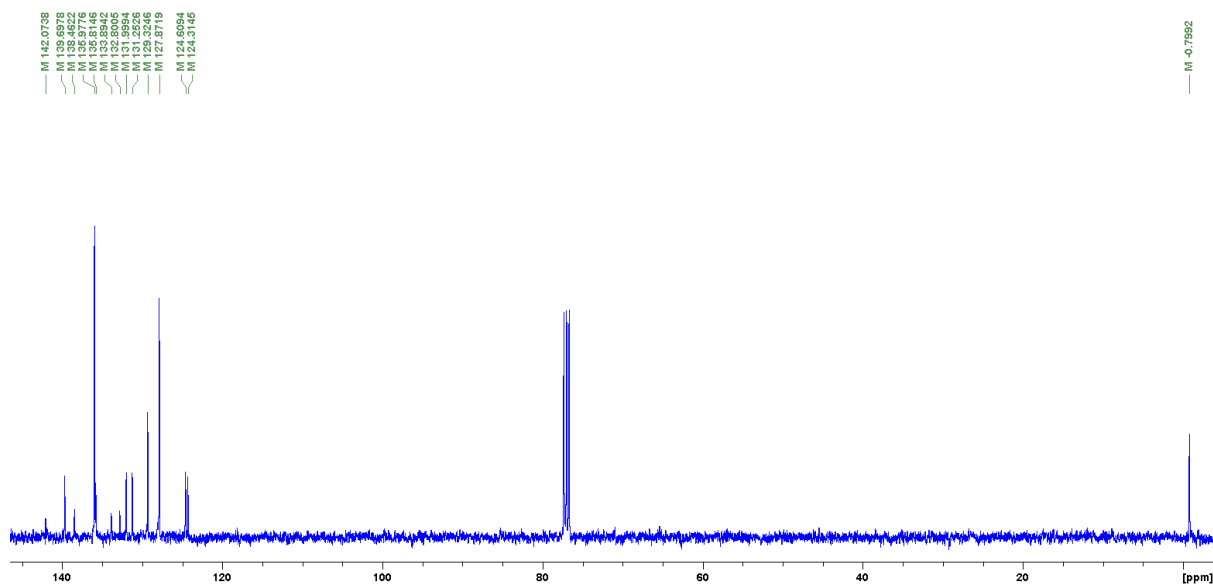


Figure S2 ¹³C{¹H} NMR spectrum of 1a, in CDCl₃

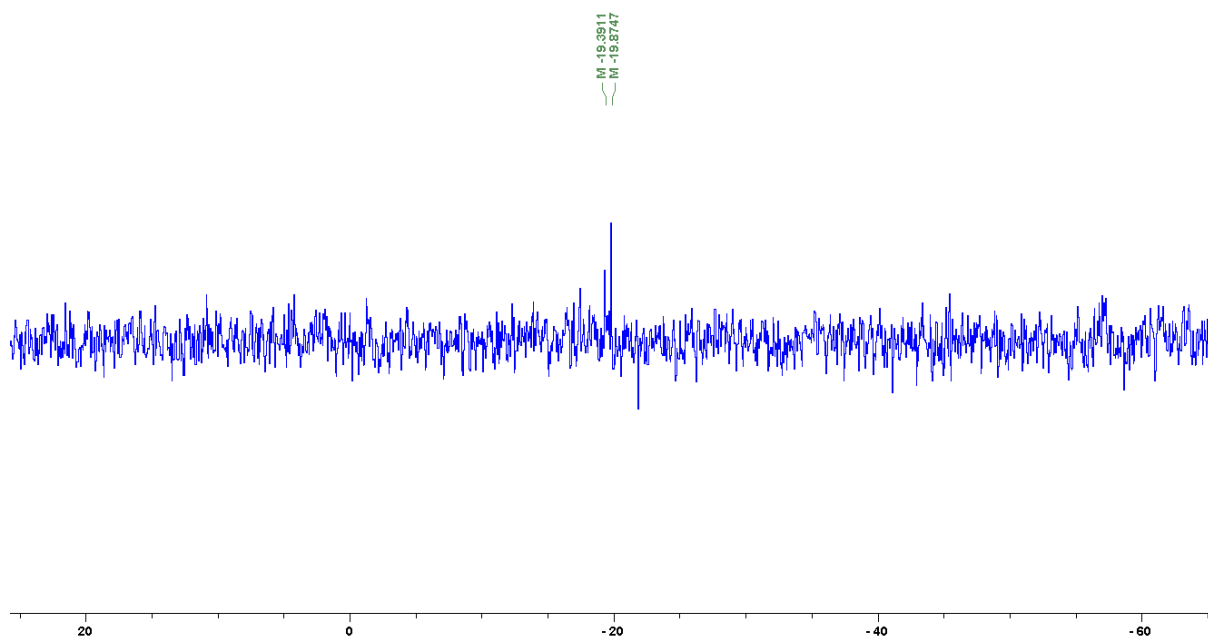


Figure S3 $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **1a**, in CDCl_3

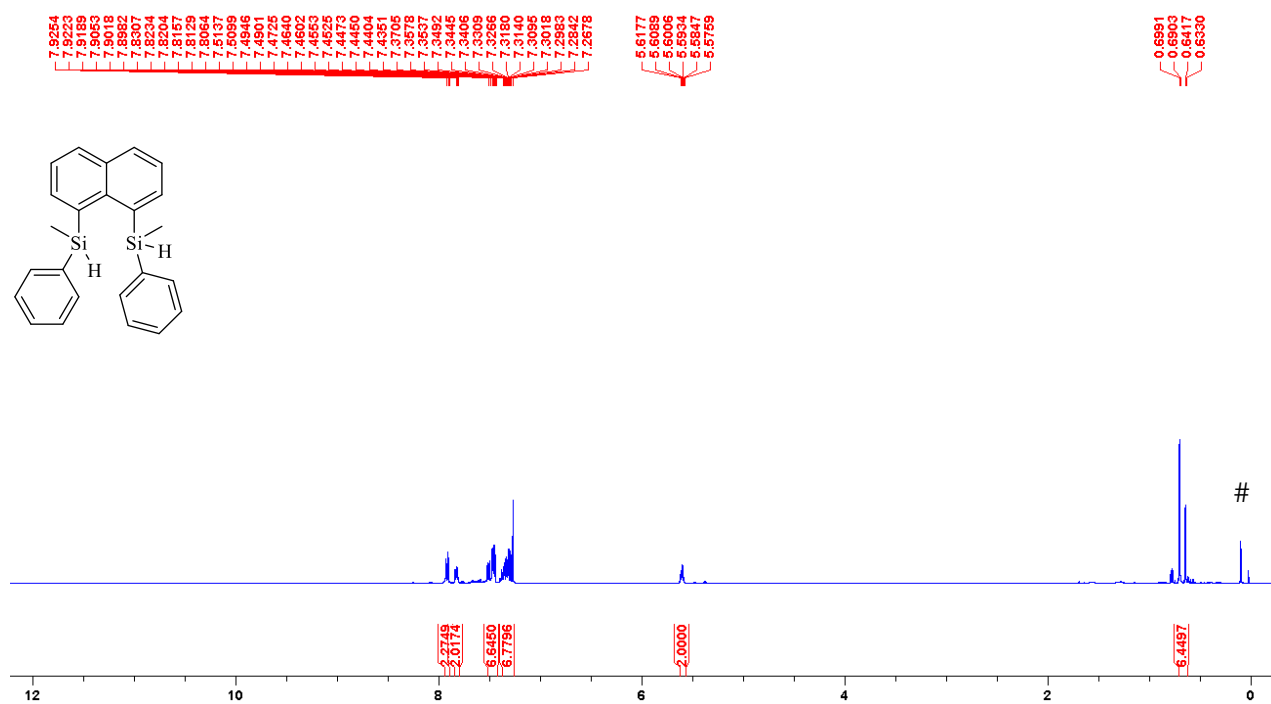


Figure S4 ^1H NMR spectrum of **2a**, in CDCl_3 (# grease)

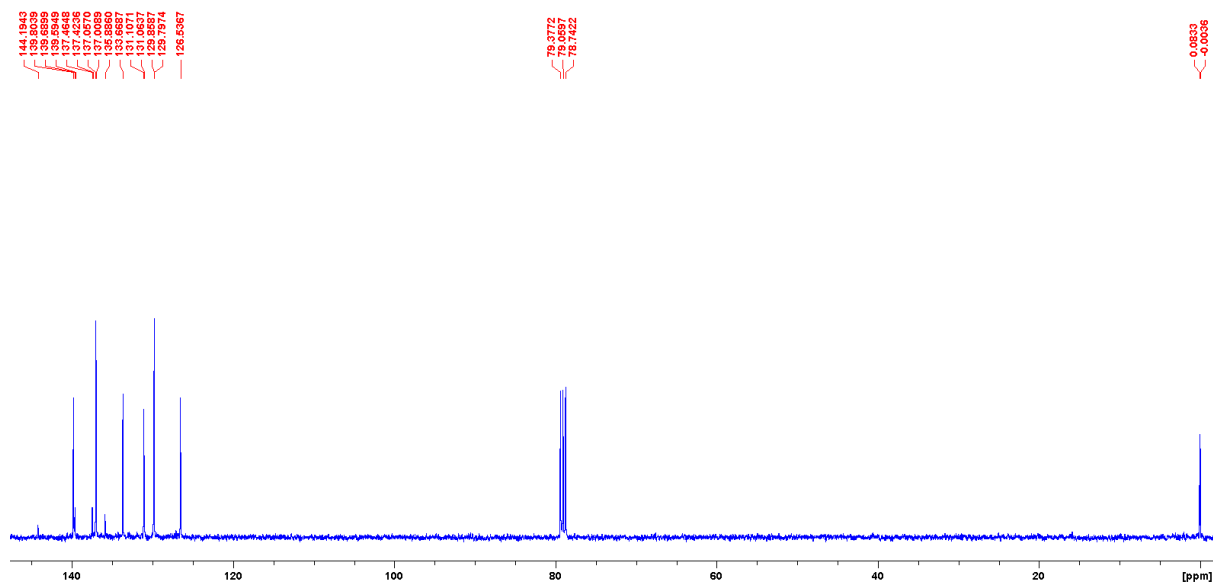


Figure S5 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2a**, in CDCl_3

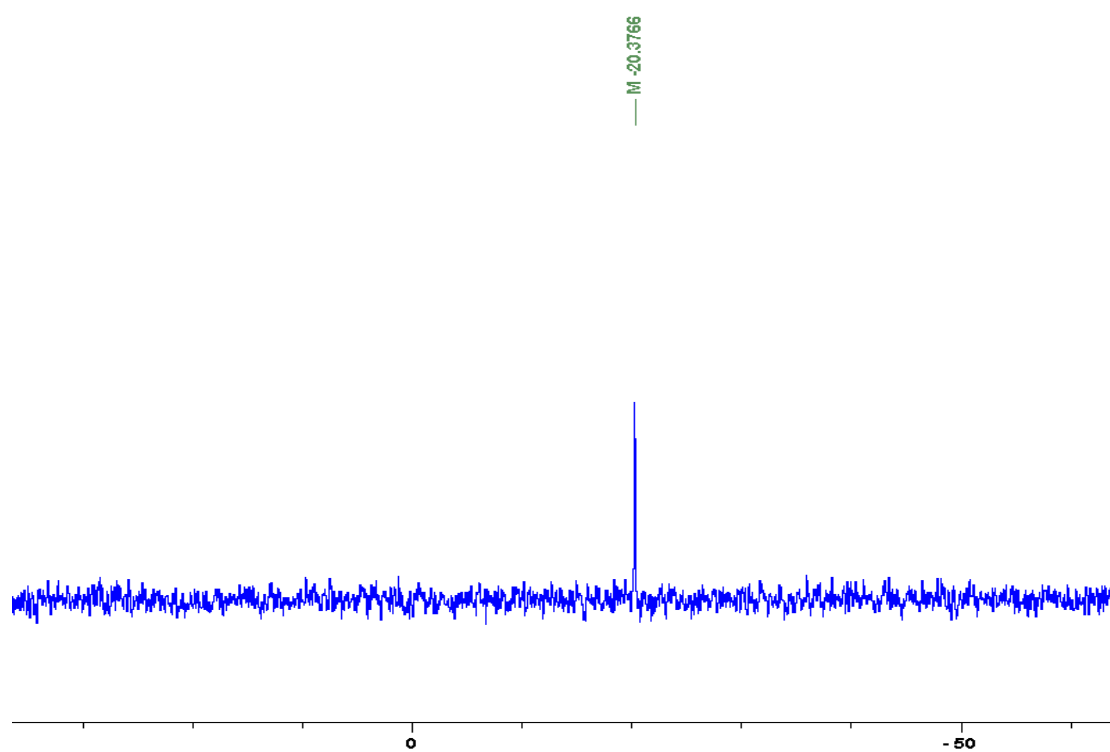


Figure S6 $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **2a**, in CDCl_3

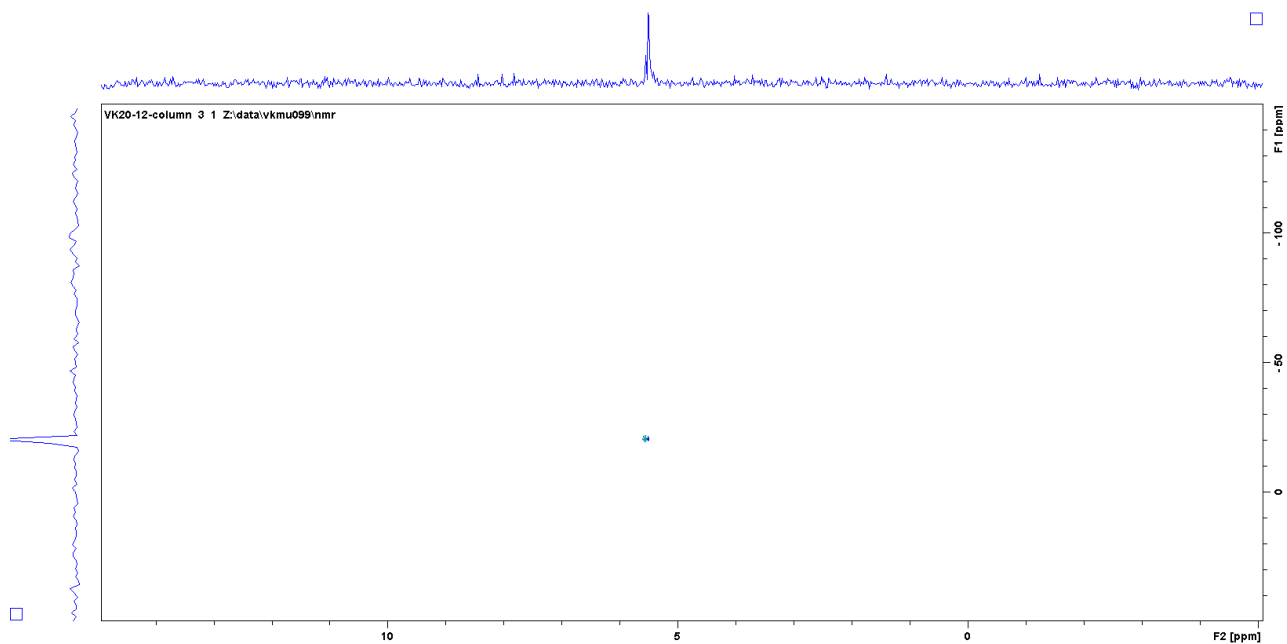


Figure S7 $^{29}\text{Si}\{^1\text{H}\}$ -HSQC 2D-NMR spectrum of **2a**, in CDCl_3

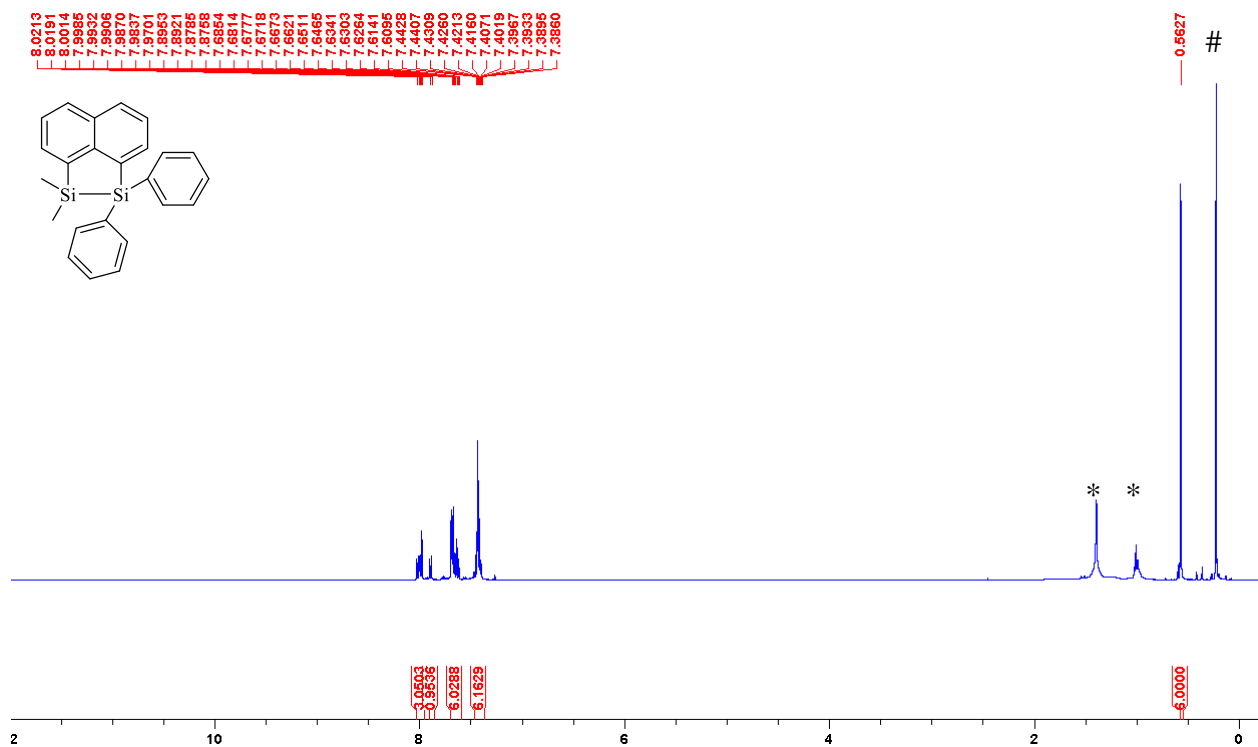


Figure S8 ^1H NMR spectrum of **1b**, in CDCl_3 (**n*-hexane, # grease).

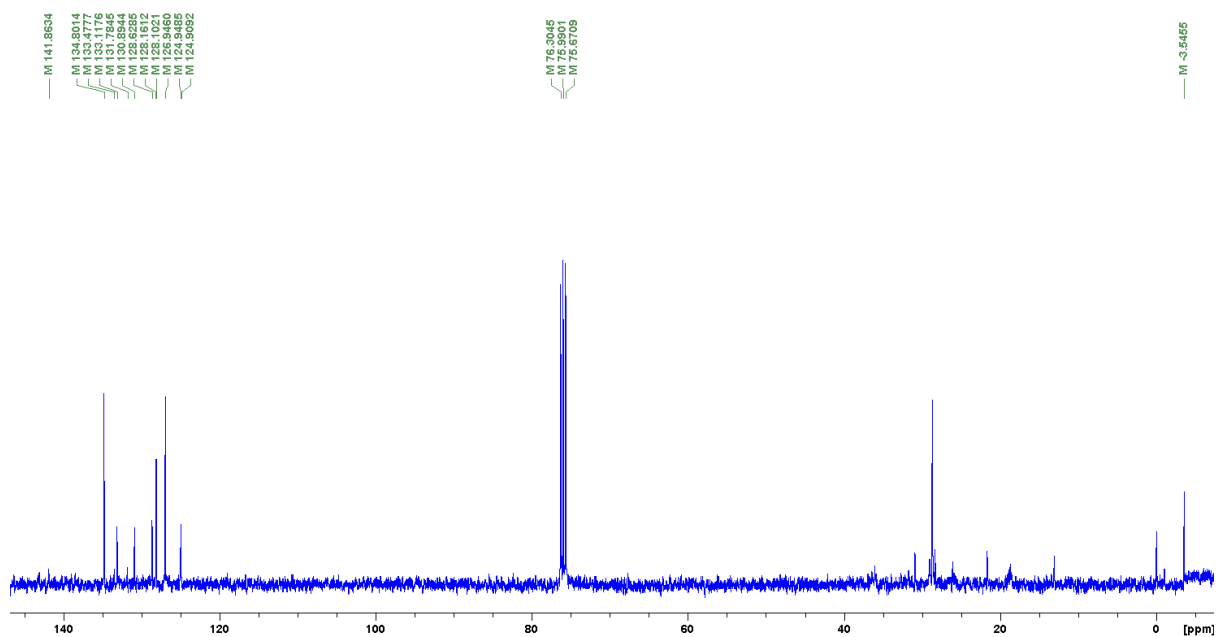


Figure S9 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1b**, in CDCl_3

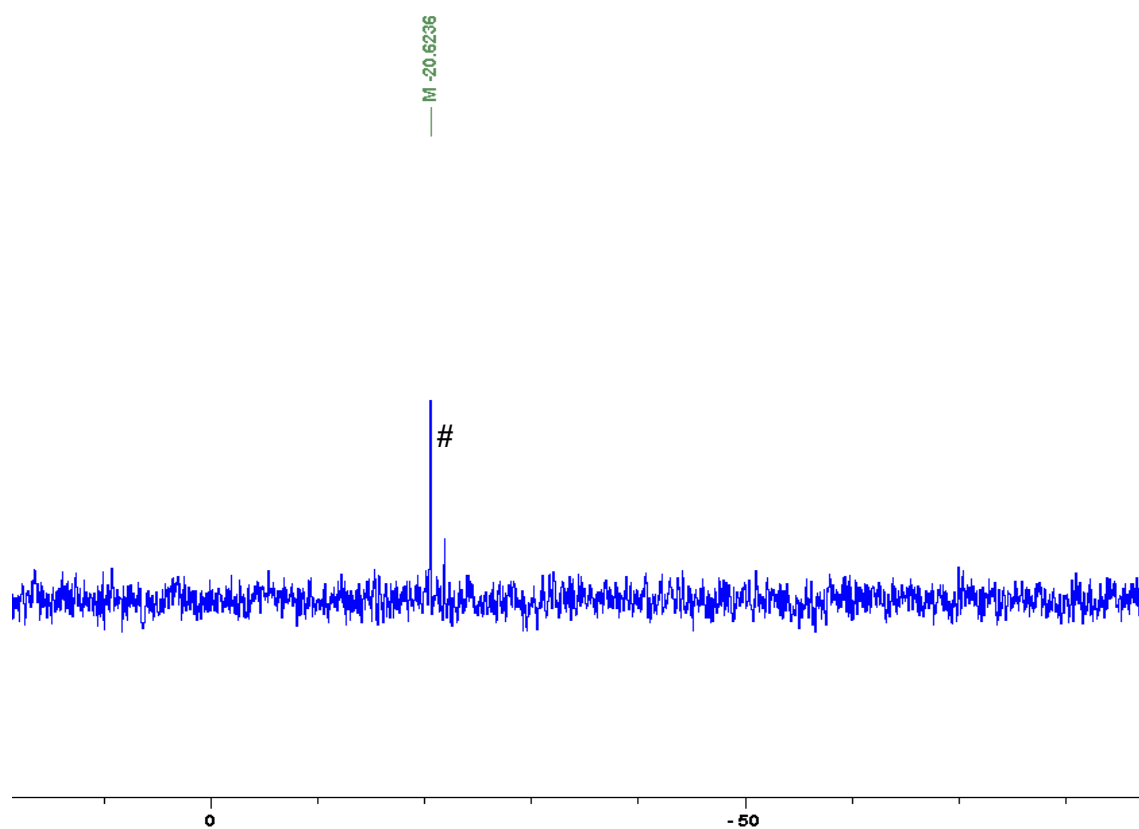


Figure S10 $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **1b**, in CDCl_3 (# grease).

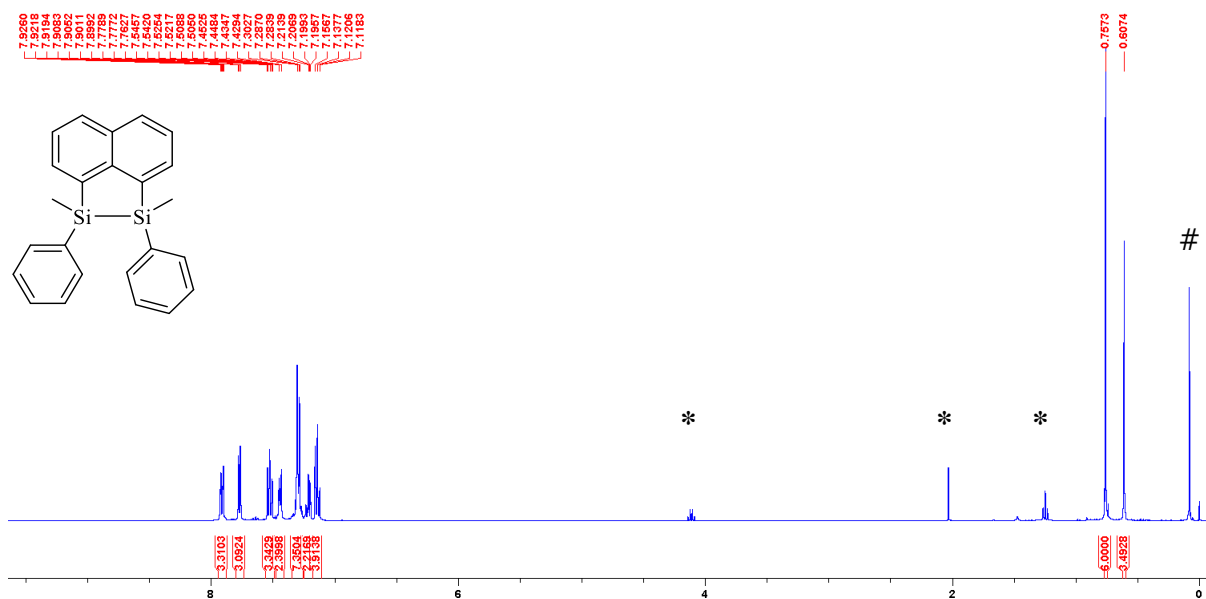


Figure S11 ¹H NMR spectrum of **2b**, in CDCl₃ (*diethyl ether and acetone, and # grease)

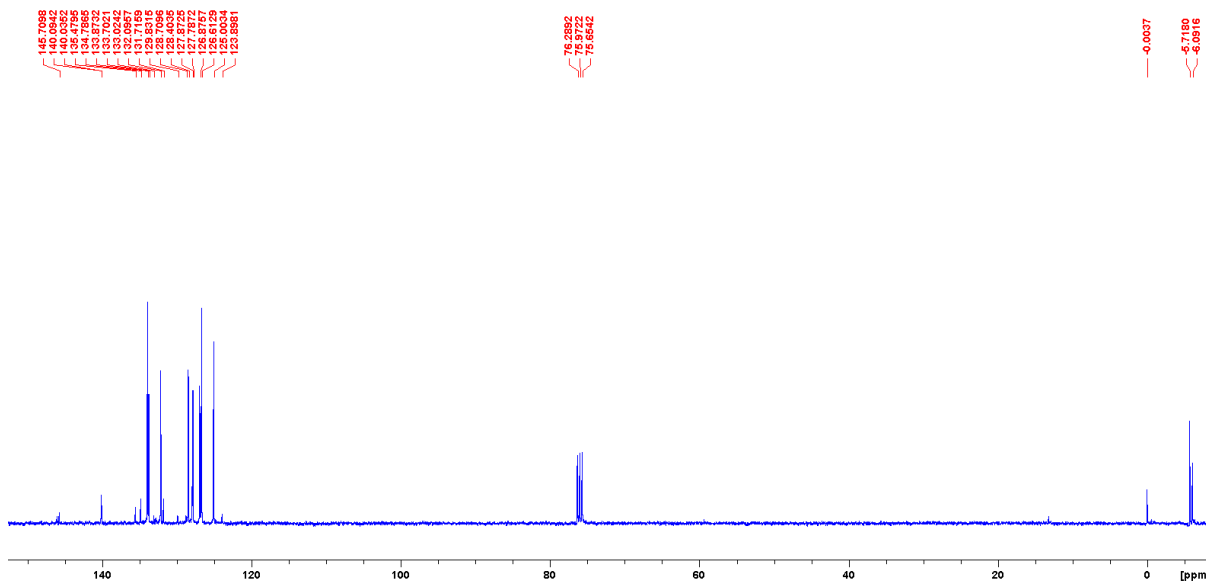


Figure S12 ¹³C {¹H} NMR spectrum of **2b**, in CDCl₃

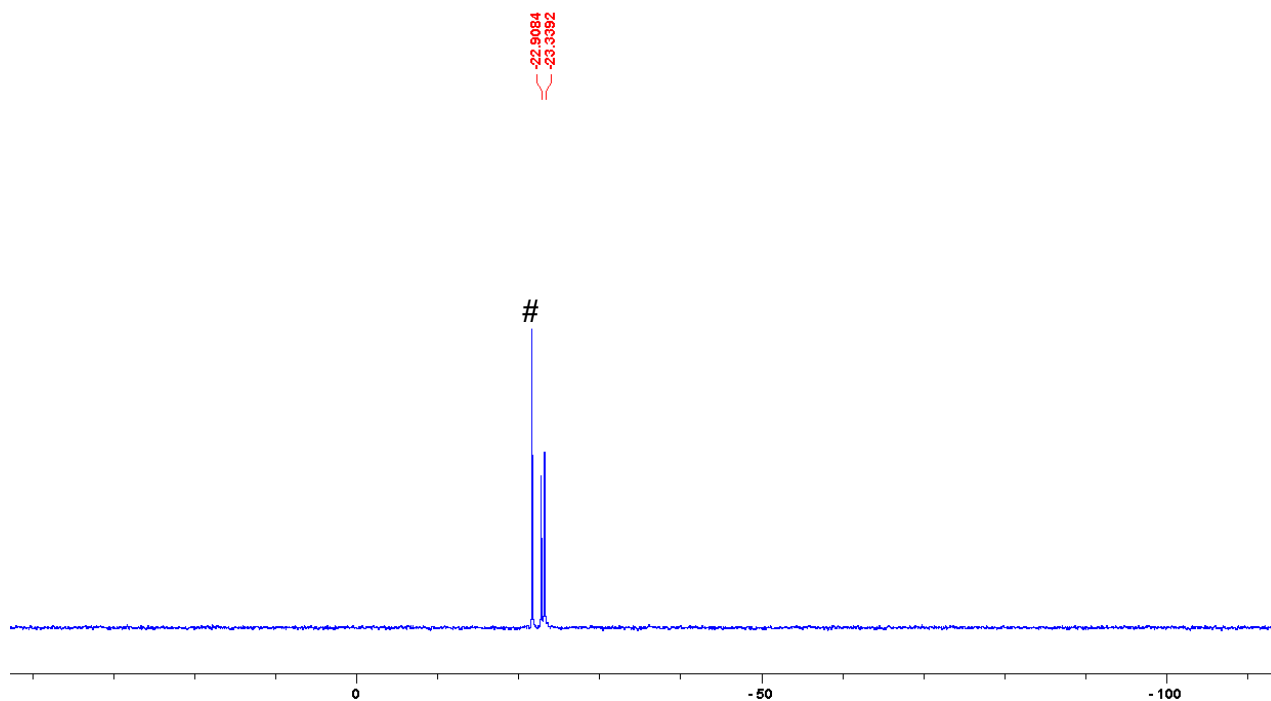


Figure S13 $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **2b**, in CDCl_3 (# grease). Two peaks in the spectrum correspond to the two isomeric products of **2b**

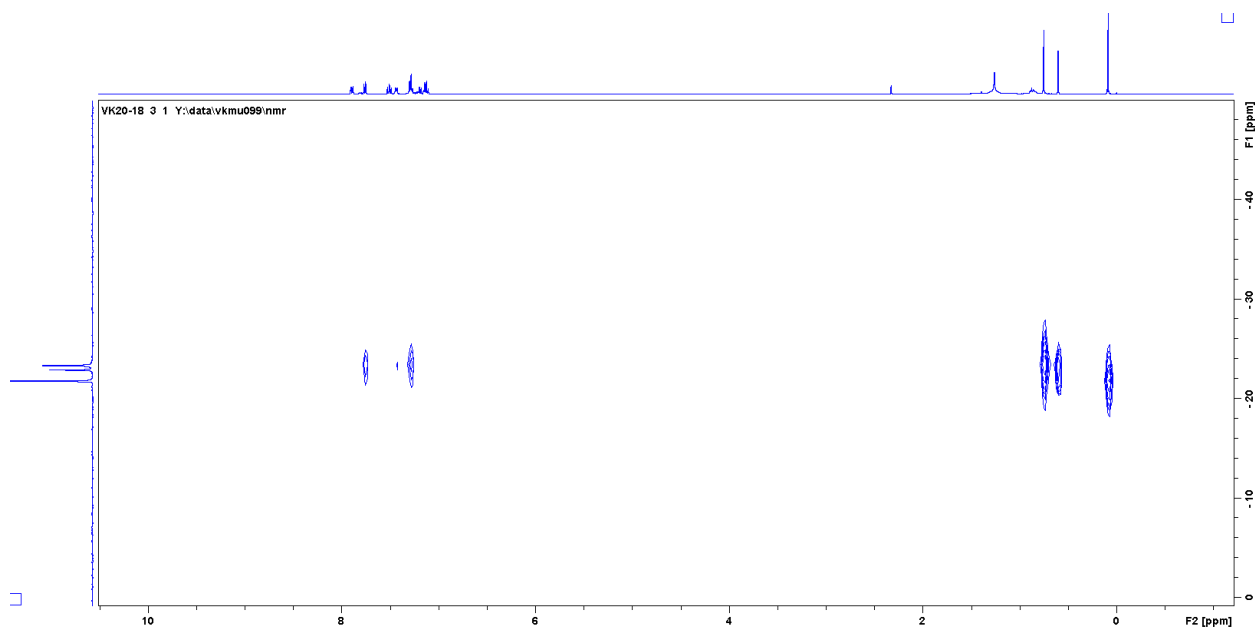
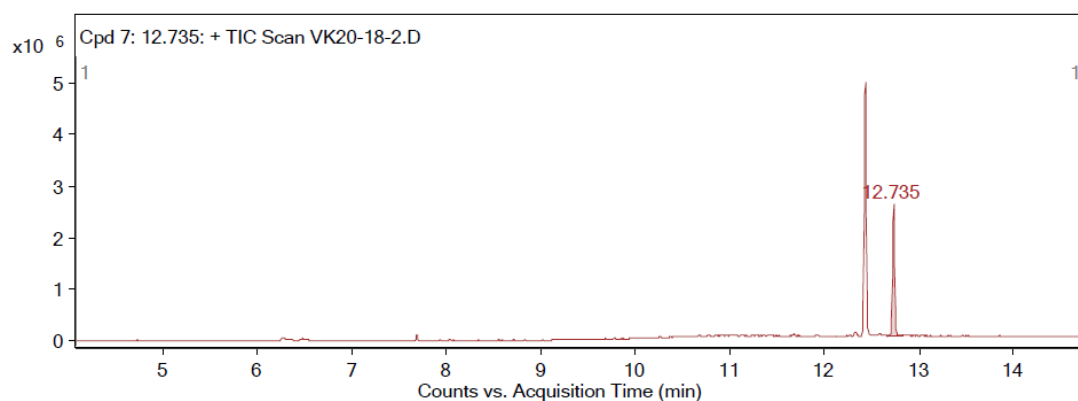
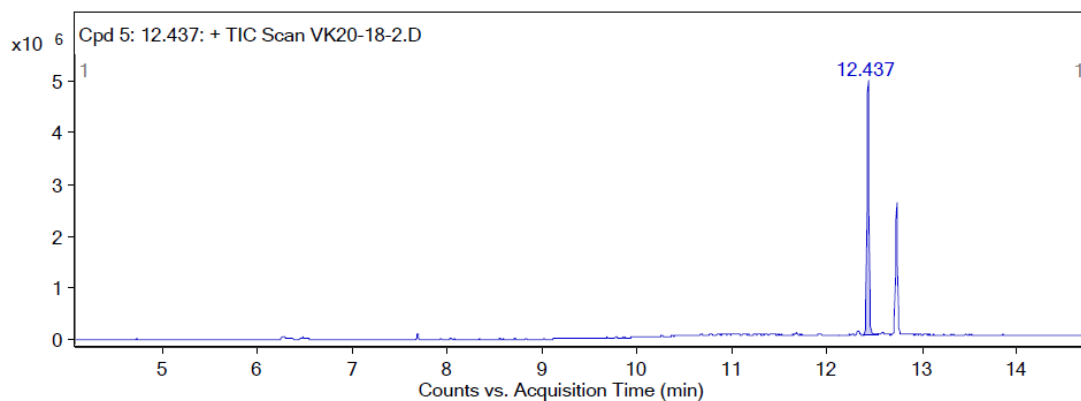


Figure S14 $^{29}\text{Si}\{^1\text{H}\}$ -HMBC NMR spectrum of **2b**, in CDCl_3 .



MS Spectrum

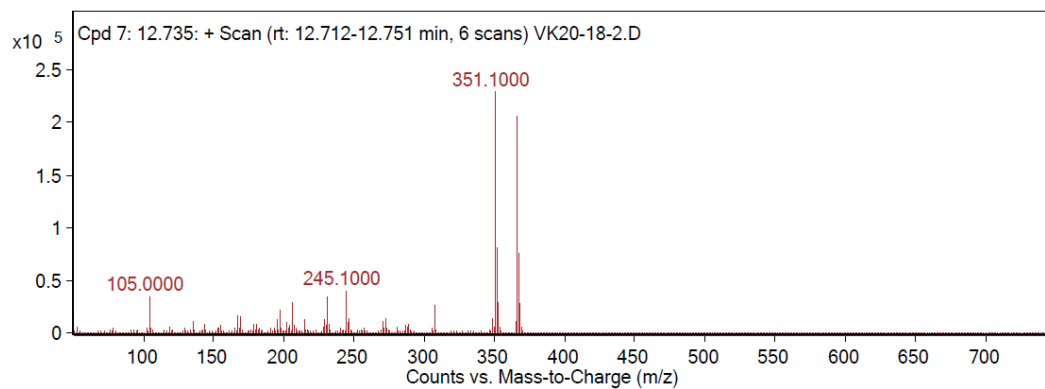
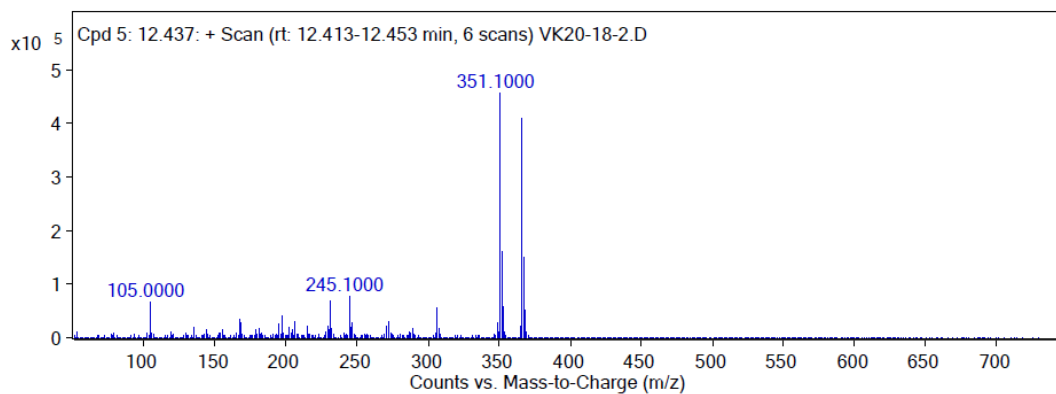


Figure S15 GC-MS spectra of **2b** confirming the presence of two isomers.

(ii) XRD data and calculated LUMOs

Table S1. Crystallographic data for compounds **1a** and **1b**.

Compound	1a	1b
CCDC deposition number	2060937	2060939
Chemical Formula	C ₂₄ H ₂₄ Si ₂	C ₂₄ H ₂₂ Si ₂
<i>M</i> /g mol ⁻¹	368.63	366.59
Temperature /K	174(30)	100(1)
Crystal system	Monoclinic	Orthorhombic
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> /Å	9.2512(2)	7.7979(2)
<i>b</i> /Å	18.1877(6)	36.7369(6)
<i>c</i> /Å	12.5609(3)	14.1416(2)
α /°	90	90
β /°	104.094(2)	90
γ /°	90	90
Volume /Å ³	2049.85(10)	4051.15(14)
<i>Z</i>	4	8
ρ_{calc} /cm ³	1.194	1.202
μ /mm ⁻¹	1.583	1.602
<i>F</i> (000)	784	1552
Crystal size/mm ³	0.15 x 0.12 x 0.11	0.050 x 0.050 x 0.010
Radiation (wavelength/Å)	CuK α (λ =1.54184)	CuK α (λ =1.54184)
2 θ range /°	11.782 to 135.462	11.488 to 136.486
Index ranges	-8 \leq <i>h</i> \leq 11, -21 \leq <i>k</i> \leq 21, -15 \leq <i>l</i> \leq 15	-9 \leq <i>h</i> \leq 9, -36 \leq <i>k</i> \leq 44, -10 \leq <i>l</i> \leq 17
Reflections collected	24447	26139
Independent reflections	3691(0.0700)	7418(0.0557)
Date/restraints/parameters	3691/0/245	7418/0/473
Goodness-of-Fit on <i>F</i> ²	1.103	1.032
Final <i>R</i> indexes [<i>I</i> \geq 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0422, <i>wR</i> ₂ = 0.1035	<i>R</i> ₁ = 0.0341, <i>wR</i> ₂ = 0.0795
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0521, <i>wR</i> ₂ =0.1138	<i>R</i> ₁ = 0.0414, <i>wR</i> ₂ = 0.0824
Largest diff. peak/hole / e Å ⁻³	0.32/-0.44	0.27/-0.21
Flack parameter	-	0.036(17)

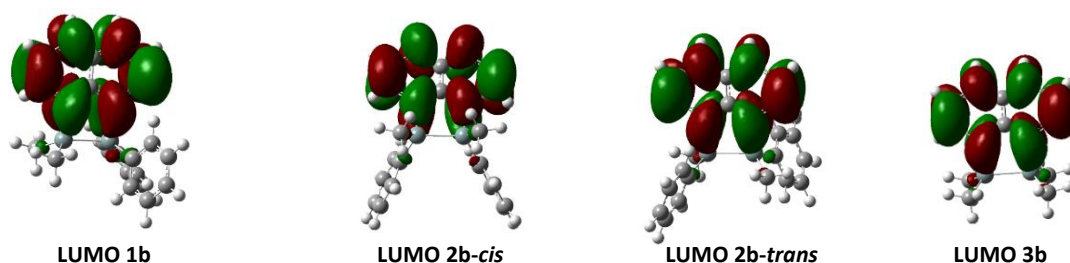


Figure S16 Calculated LUMOs from the optimised structures of **1b**, **2b** (*cis/trans*) and **3b**

(iii) UV-Vis and fluorescence spectra

The experimental set-up consisted of a quartz cuvette for spectroscopic measurements. HPLC grade and dry solvents were used to prepare the samples.

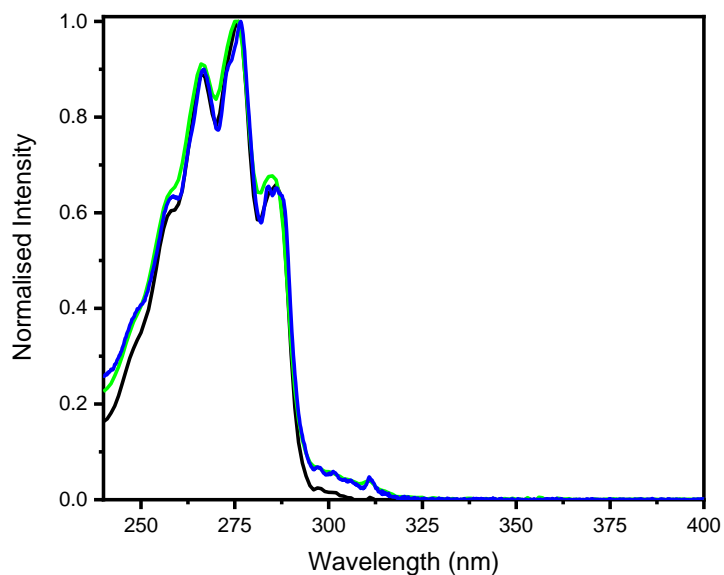


Figure S17 Absorption spectra of **naphthalene** in cyclohexane (*black*), THF (*blue*), acetonitrile (*green*).

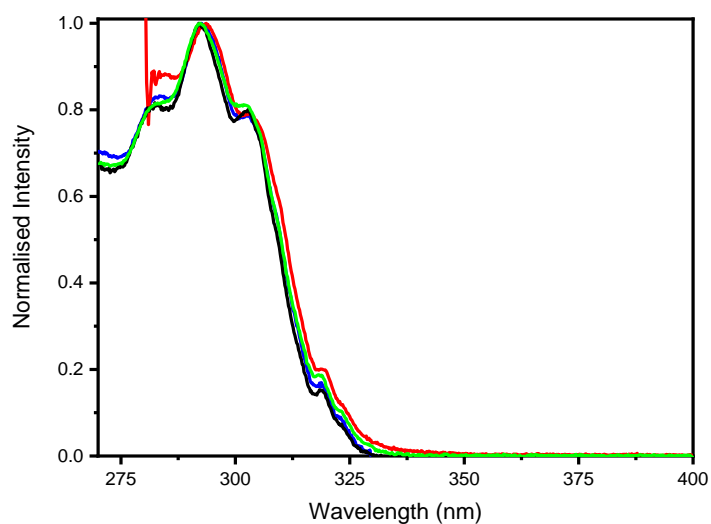


Figure S18 Absorption spectra of **1b** in cyclohexane (*black*), toluene (*red*), THF (*blue*), acetonitrile (*green*).

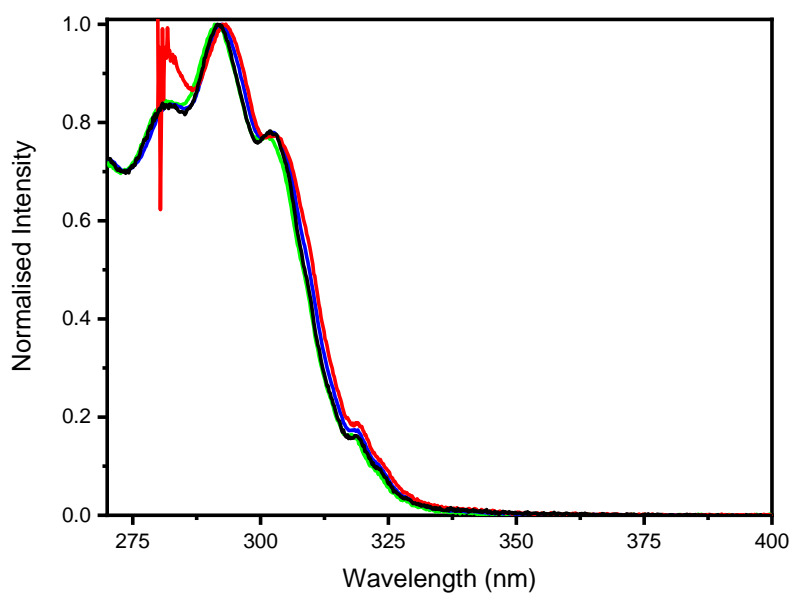


Figure S19 Absorption spectra of **2b** in cyclohexane (*black*), toluene (*red*), THF (*blue*), acetonitrile (*green*).

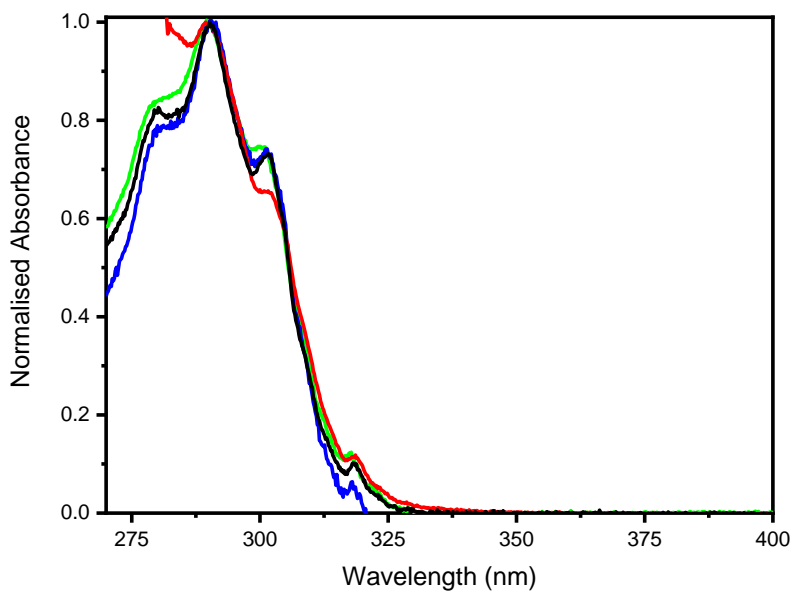


Figure S20 Absorption spectra of **3b** in cyclohexane (*black*), toluene (*red*), THF (*blue*), acetonitrile (*green*).

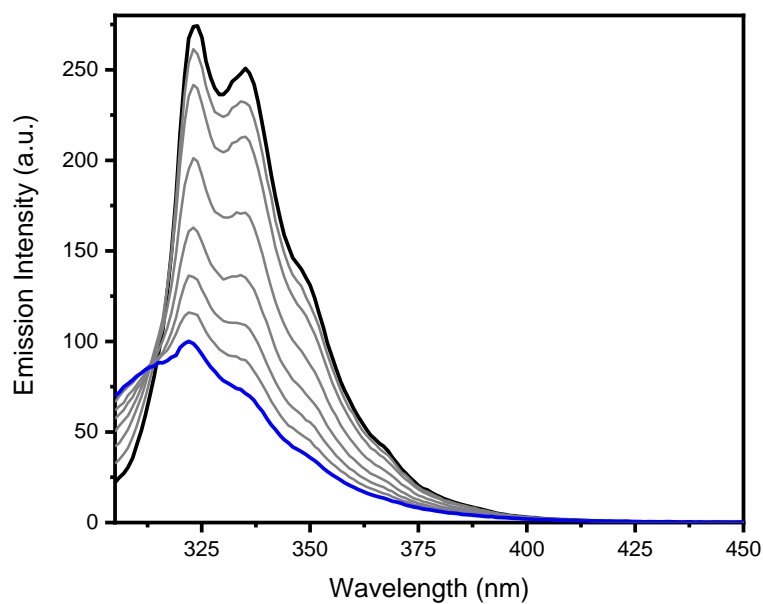


Figure S21 Concentration dependent emission of compound **naphthalene** in THF upon excitation at 288 nm. Concentration range of compound **naphthalene**: 1.76×10^{-4} M (*black*) \rightarrow 3.49×10^{-5} M (*blue*).

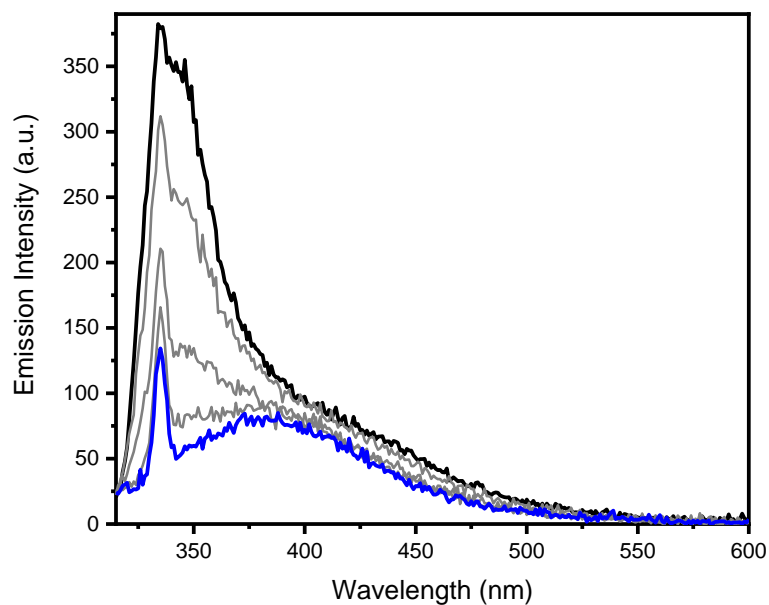


Figure S22 Concentration dependent emission of compound **1b** in THF upon excitation at 305 nm. Concentration range of compound **1b**: 1.26×10^{-4} M (*black*) \rightarrow 1.50×10^{-6} M (*blue*).

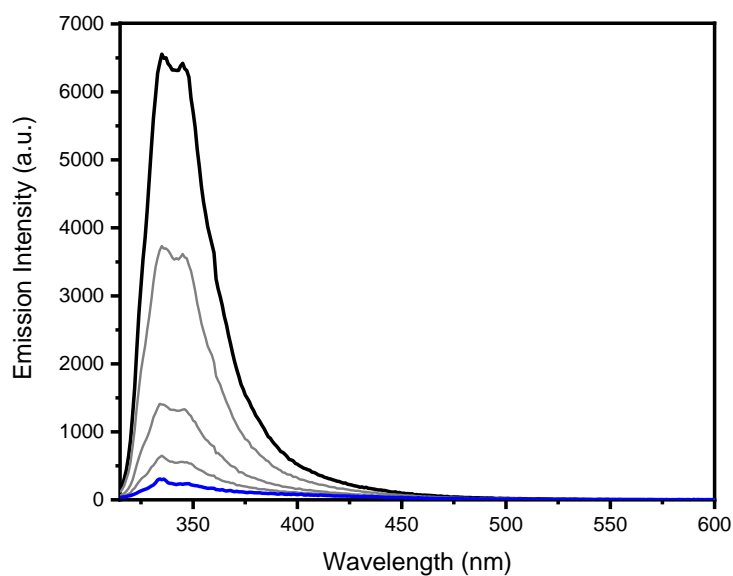


Figure S23 Concentration dependent emission of compound **2b** in THF upon excitation at 305 nm. Concentration range of compound **2b**: 1.36×10^{-4} M (*black*) \rightarrow 1.61×10^{-6} M (*blue*).

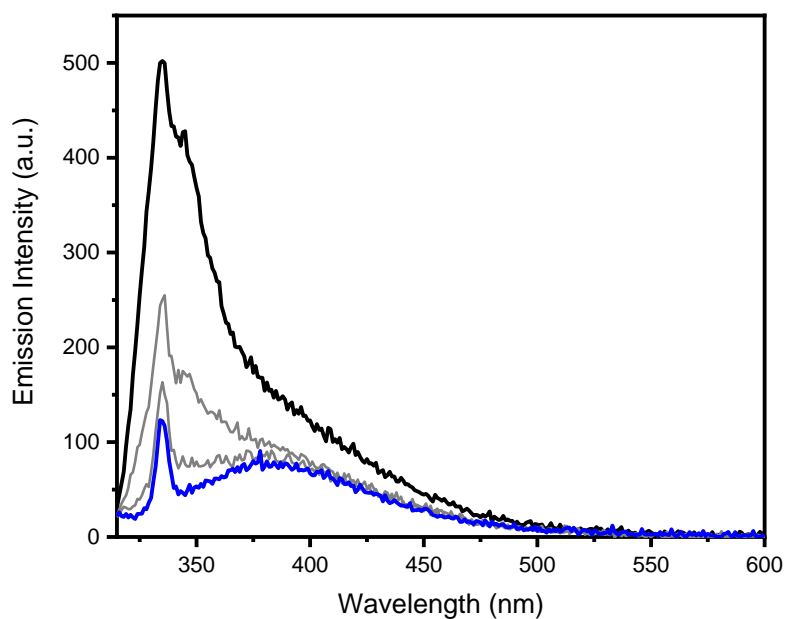


Figure S24 Concentration dependent emission of compound **3b** in THF upon excitation at 305 nm. Concentration range of compound **3b**: 1.82×10^{-4} M (*black*) \rightarrow 1.40×10^{-6} M (*blue*).

(iv) Cyclic Voltammetry measurements

Cyclic voltammetry of the bridged disilanes (**1b**, **2b** and **3b**) were performed at room temperature utilizing a BAS CGME Controlled Mercury Electrode cell stand at scan rates of 0.1 Vs^{-1} , with glassy carbon as the working electrode, a platinum auxiliary electrode and silver wire as a quasi-reference electrode. The glassy electrode was polished with Al_2O_3 fine particles and washed with water and acetone prior to use. The auxiliary electrode and the reference electrode were washed with acetone prior to use. The measurements were performed in dry acetonitrile in presence of $n\text{-Bu}_4\text{NPF}_6$ (0.2 mol/L) as the electrolyte and ferrocene/ferrocenium couple acting as the internal standard. The concentration of the bridged disilanes used was 1 mmol/L and the samples were degassed with nitrogen prior to the measurements which were also maintained under a nitrogen blanket.

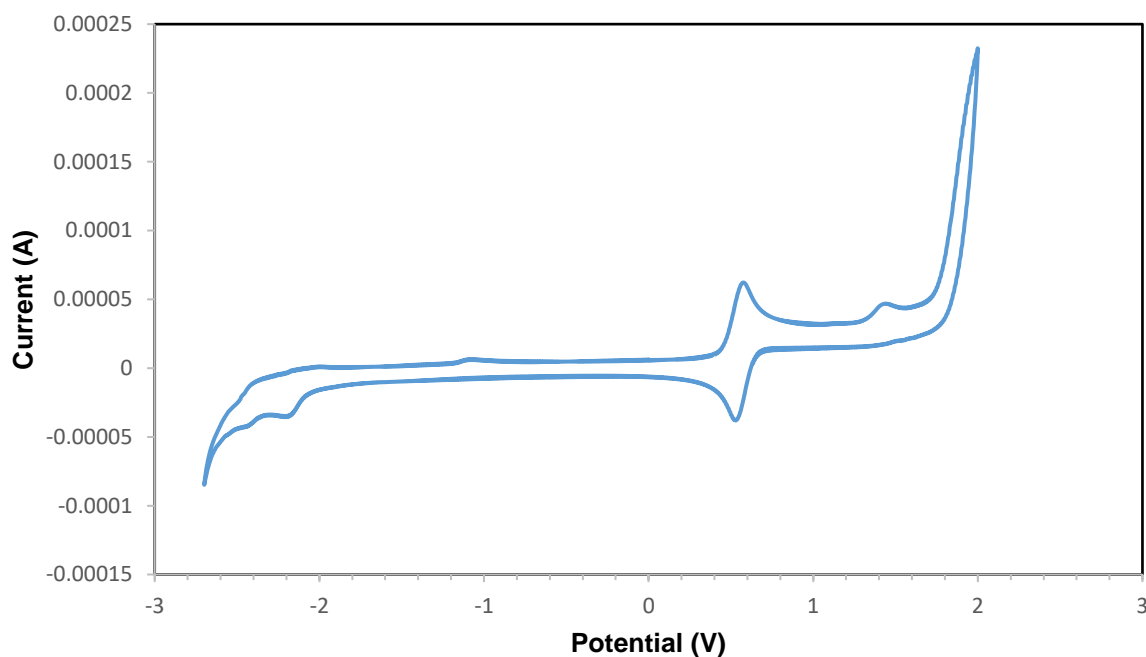


Figure S25 Cyclic voltammogram of **1b**.

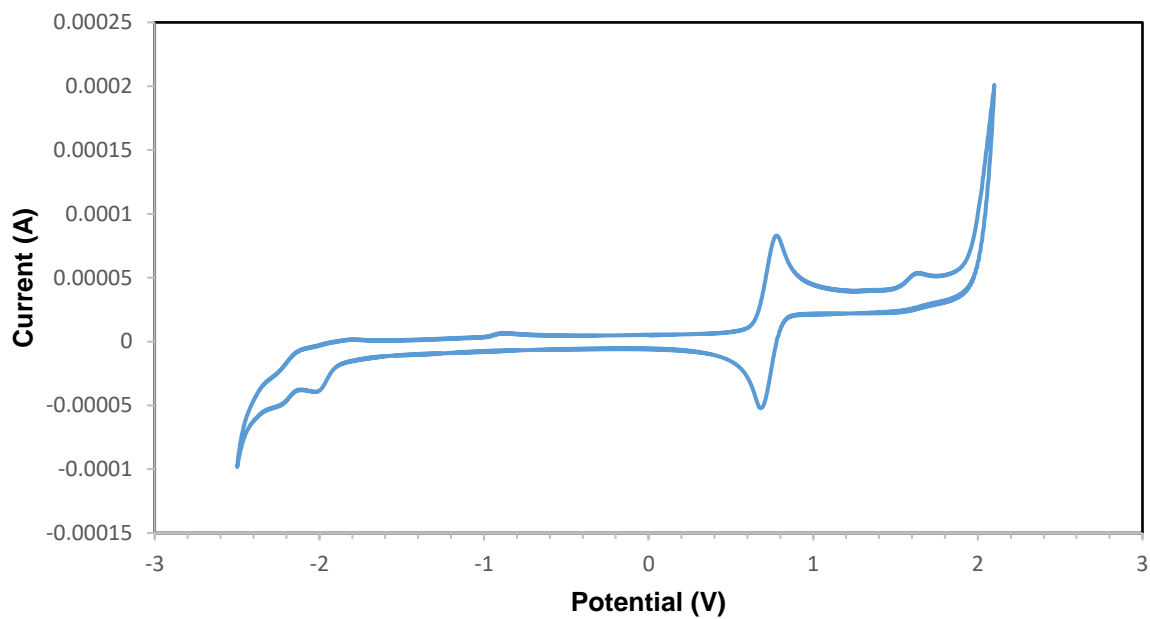


Figure S26 Cyclic voltammogram of **2b**.

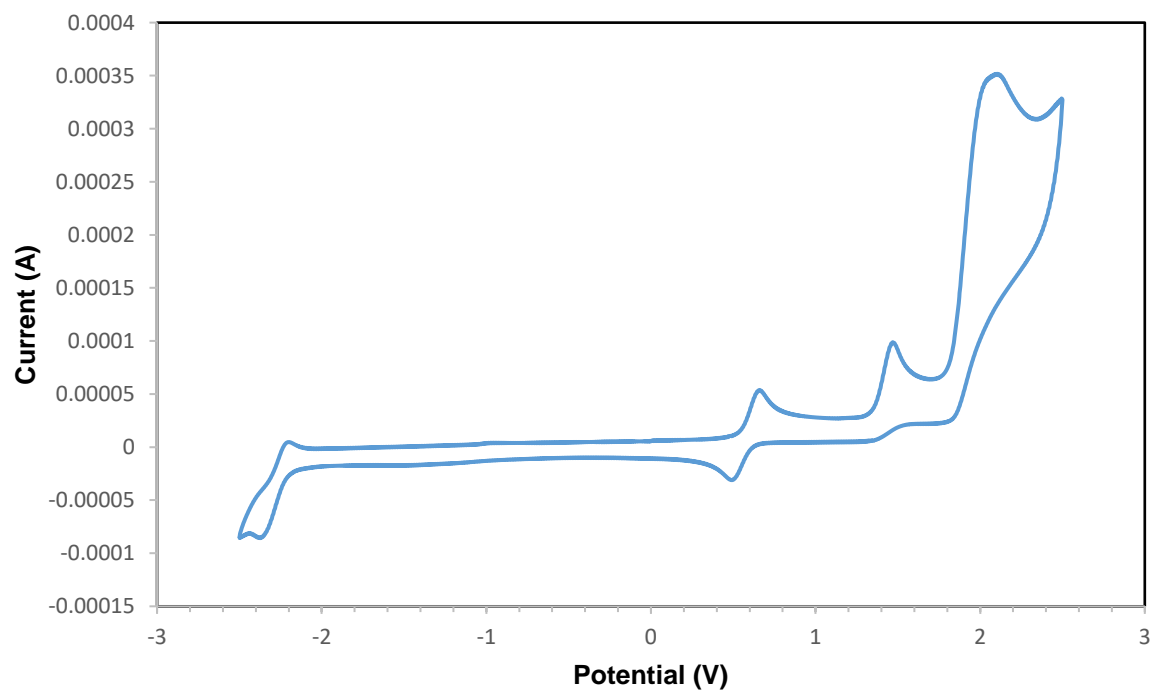


Figure S27 Cyclic voltammogram of **3b**.

Table S2. Electrochemical data of **1b**, **2b** and **3b**.

Compound	E_{ox} (V)	HOMO (eV)^a	E_{red} (V)	LUMO (eV)^a	HOMO-LUMO gap (eV)
1b	1.44	- 5.65	-2.18	- 2.03	3.62
2b	1.60	- 5.69	-2.07	- 2.02	3.67
3b	1.48	- 5.71	-2.37	- 1.86	3.85

^a The energy levels were calculated from the oxidation and reduction peaks as referenced to Fc/Fc⁺ (4.8 eV) below vacuum level.