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Electronic Supplementary Material

for the
Communication

(Oligo)aromatic species with one or two conjugated Si=Si bonds: near-IR emission of anthracenyl-bridged tetrasiladiene

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1. Plots of NMR spectra

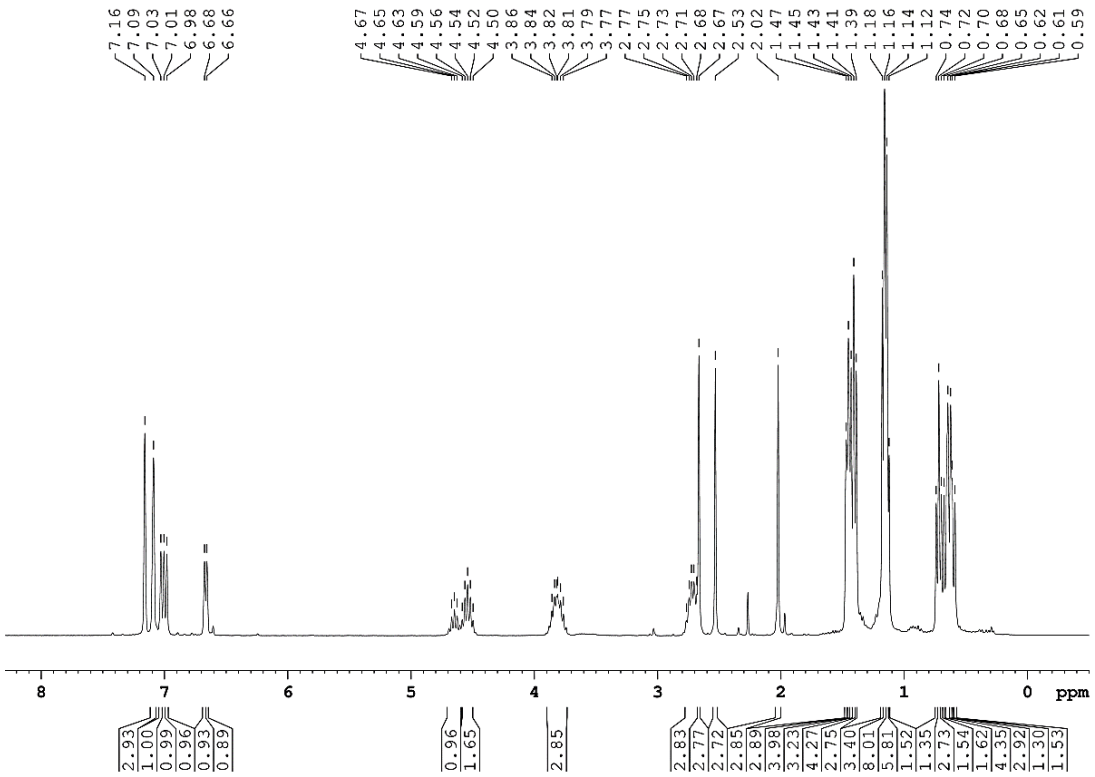

Figure S1: ^{1}H NMR of **2a** in C_6D_6 at 300 K.

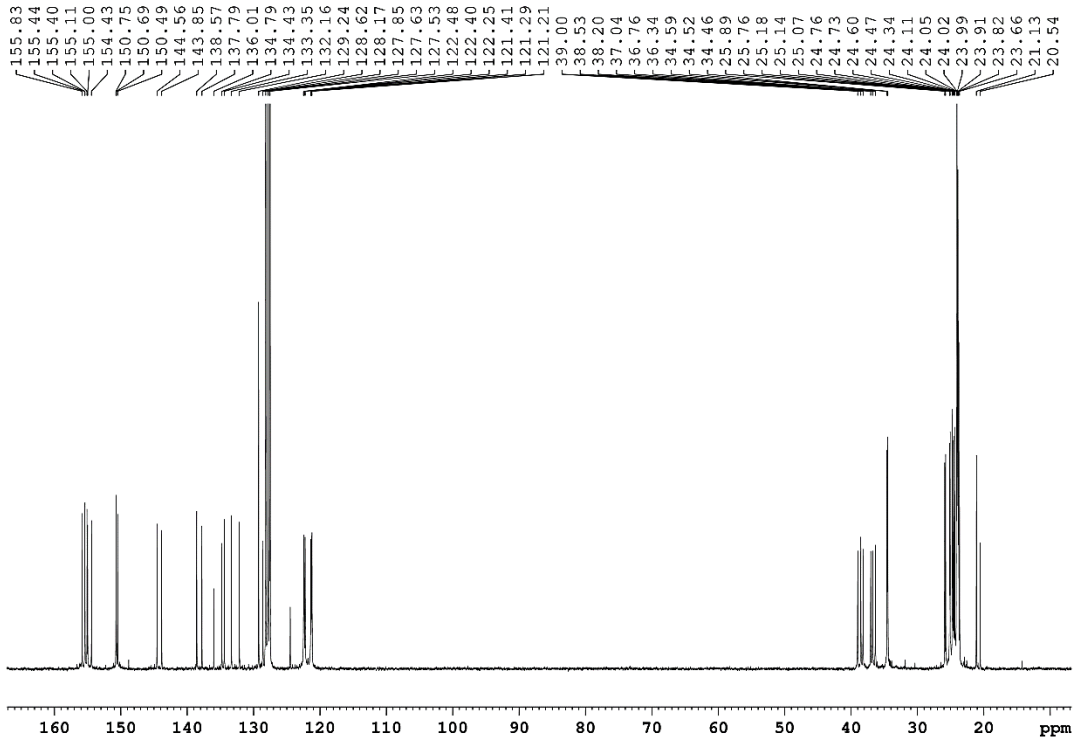

Figure S2: ^{13}C NMR of **2a** in C_6D_6 at 300 K.

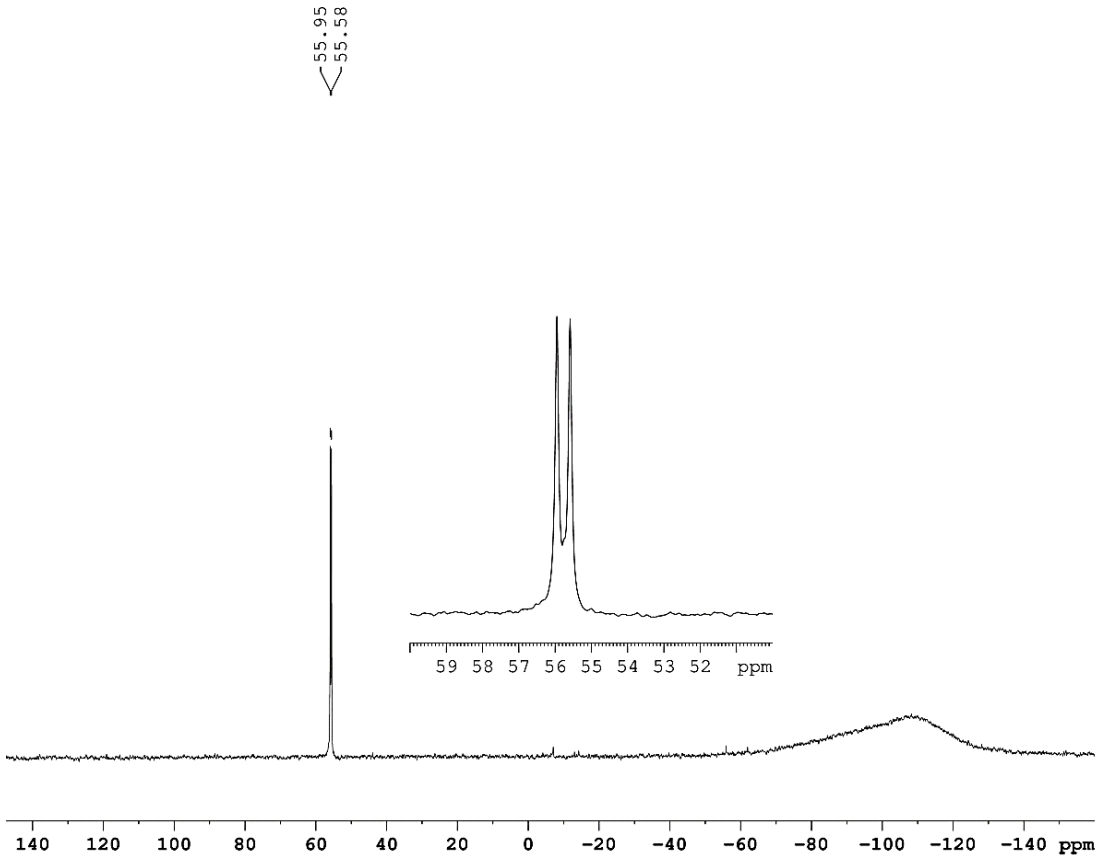

Figure S3: ^{29}Si NMR **2a** in C_6D_6 at 300 K.

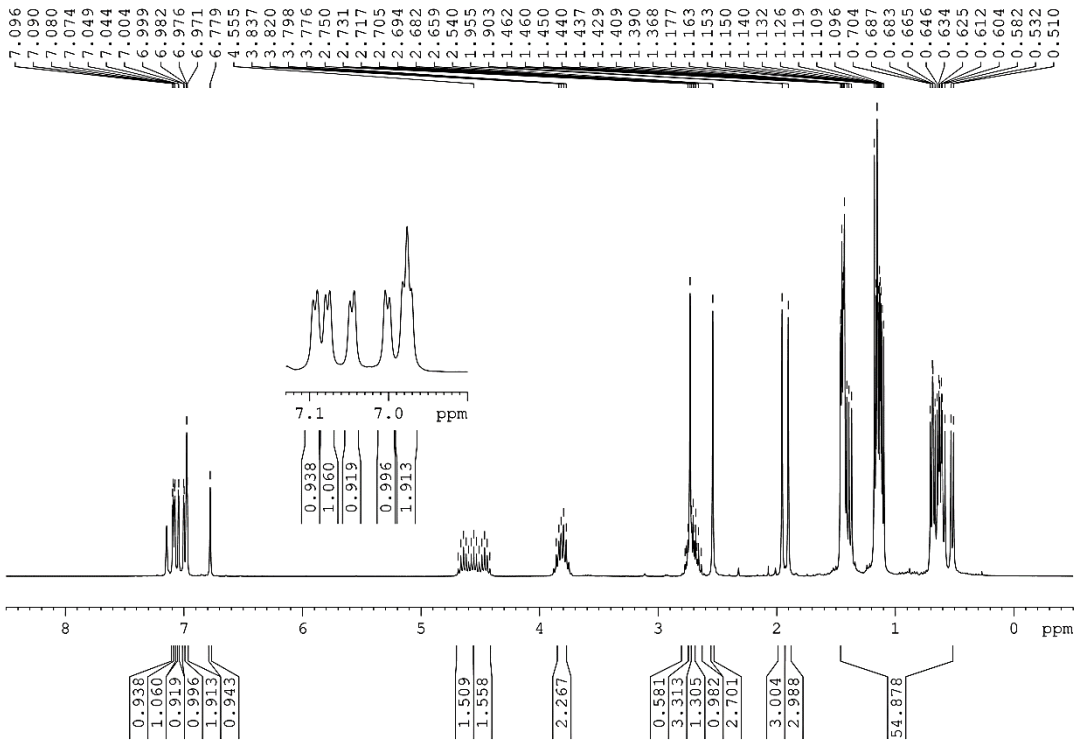

Figure S4: ^{1}H NMR of **2b** in C_6D_6 at 300 K.

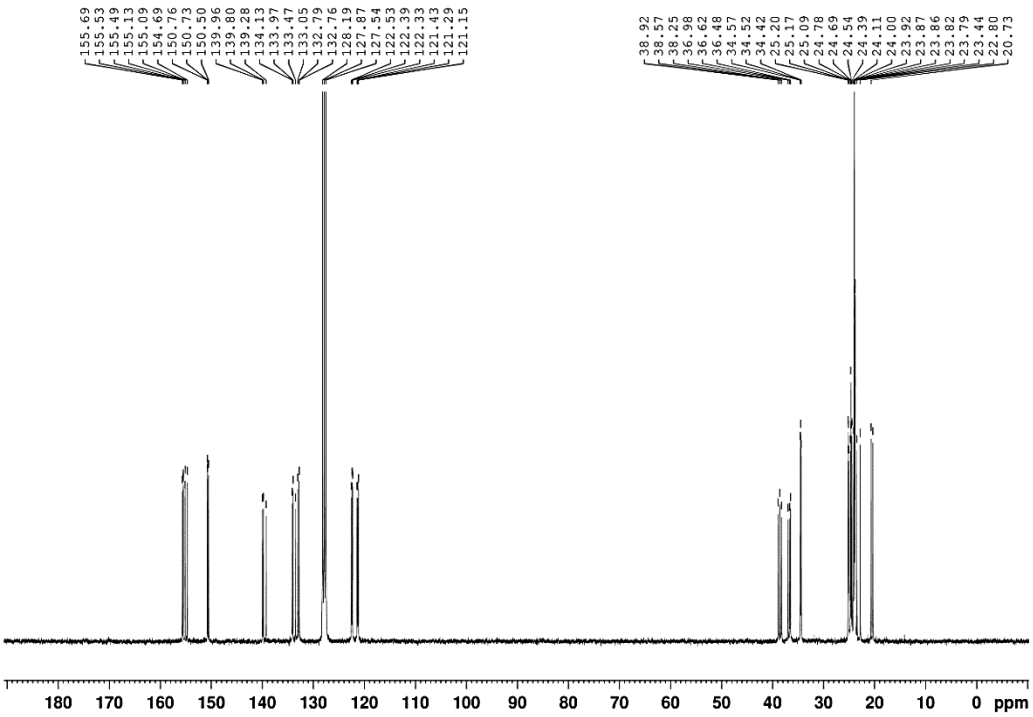

Figure S5: ^{13}C NMR of **2b** in C_6D_6 at 300 K.

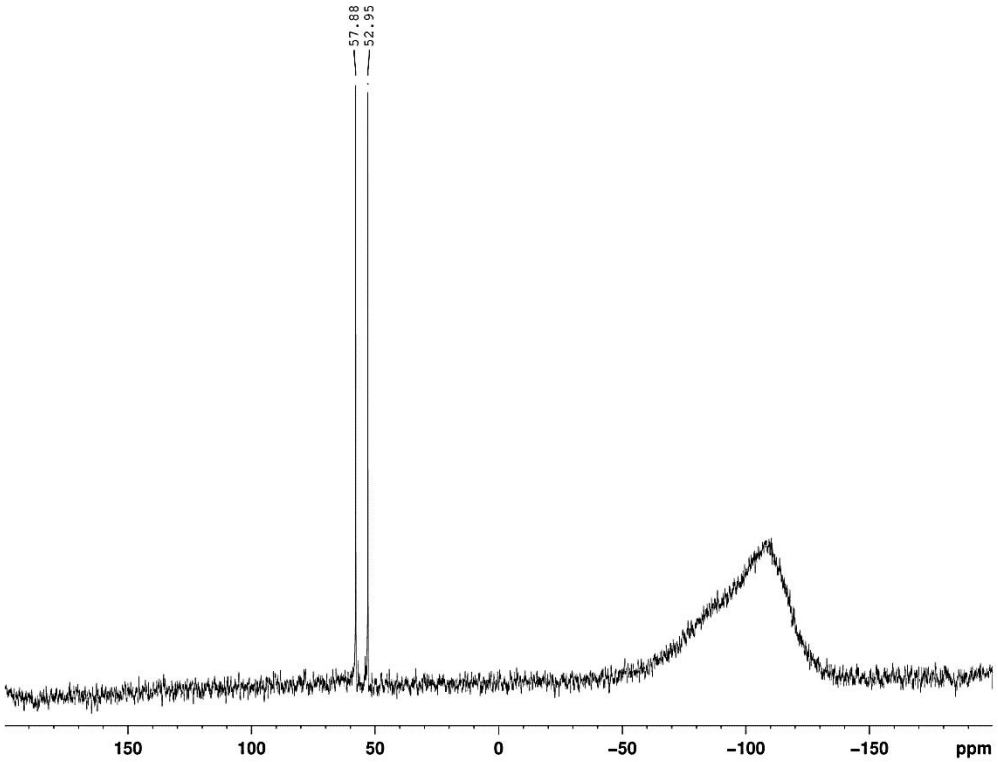

Figure S6: ^{29}Si NMR **2b** in C_6D_6 at 300 K.

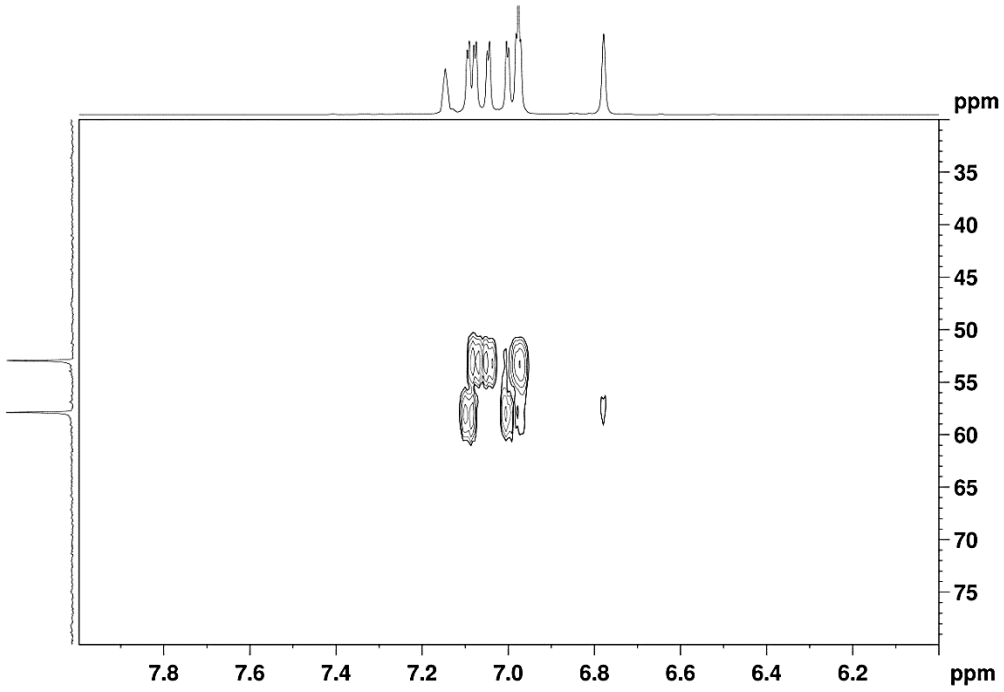

Figure S7: ^{29}Si-^{1}H NMR of **2b** in C_6D_6 at 300 K.

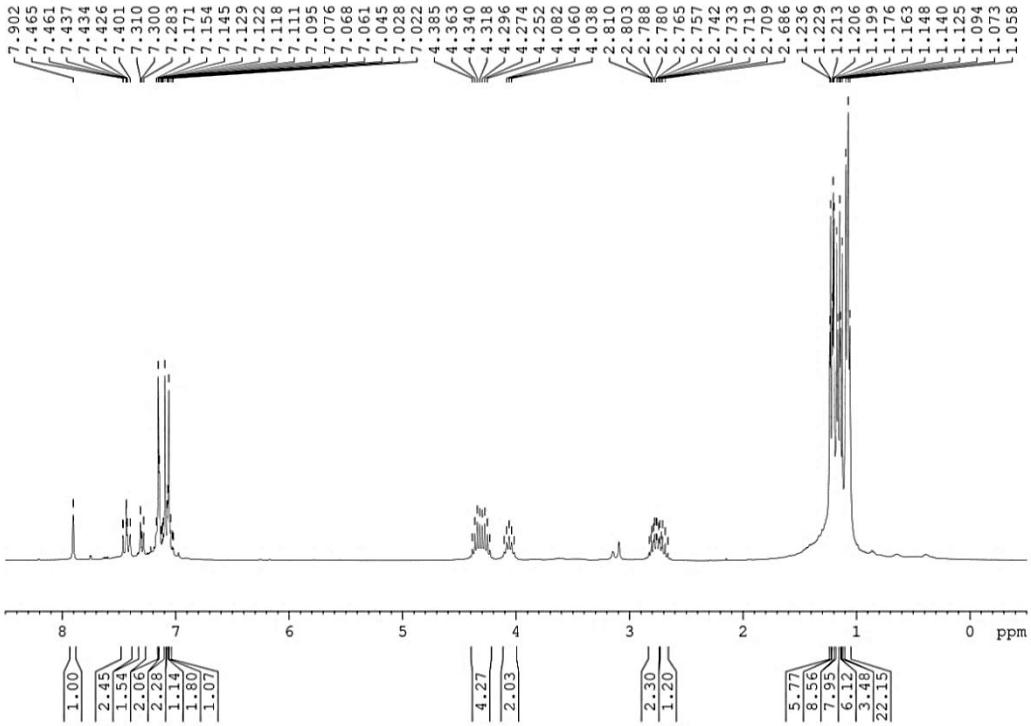

Figure S8: ^{1}H NMR of **2c** in C_6D_6 at 300 K.

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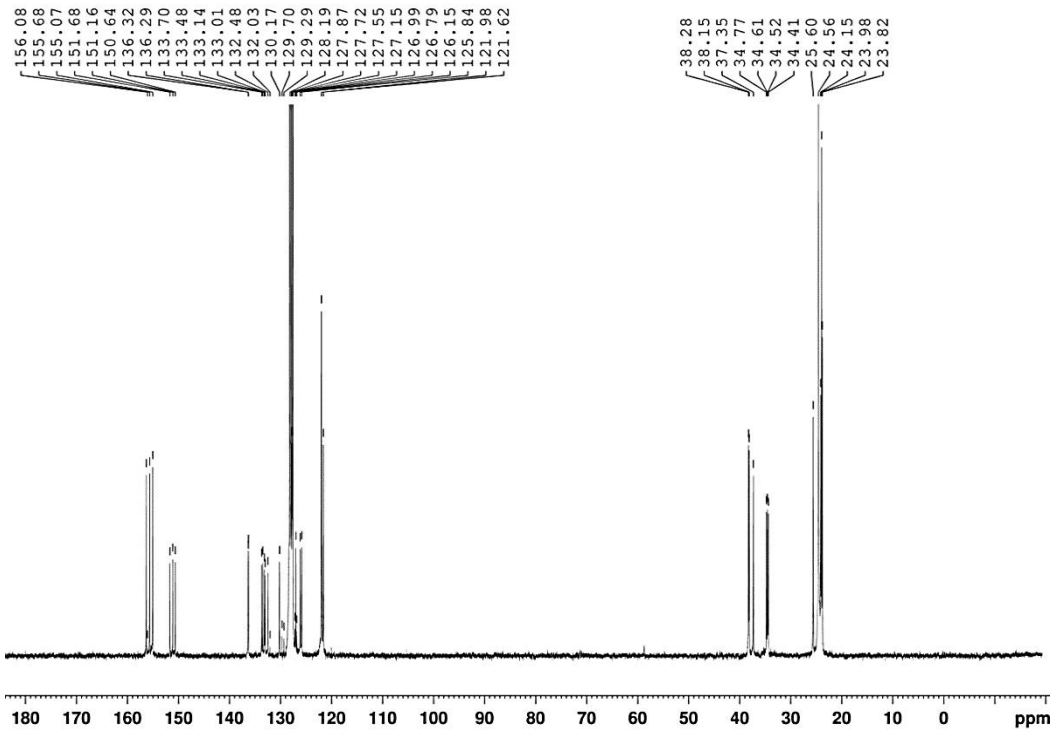


Figure S9: ^{13}C NMR of **2c** in C_6D_6 at 300 K.

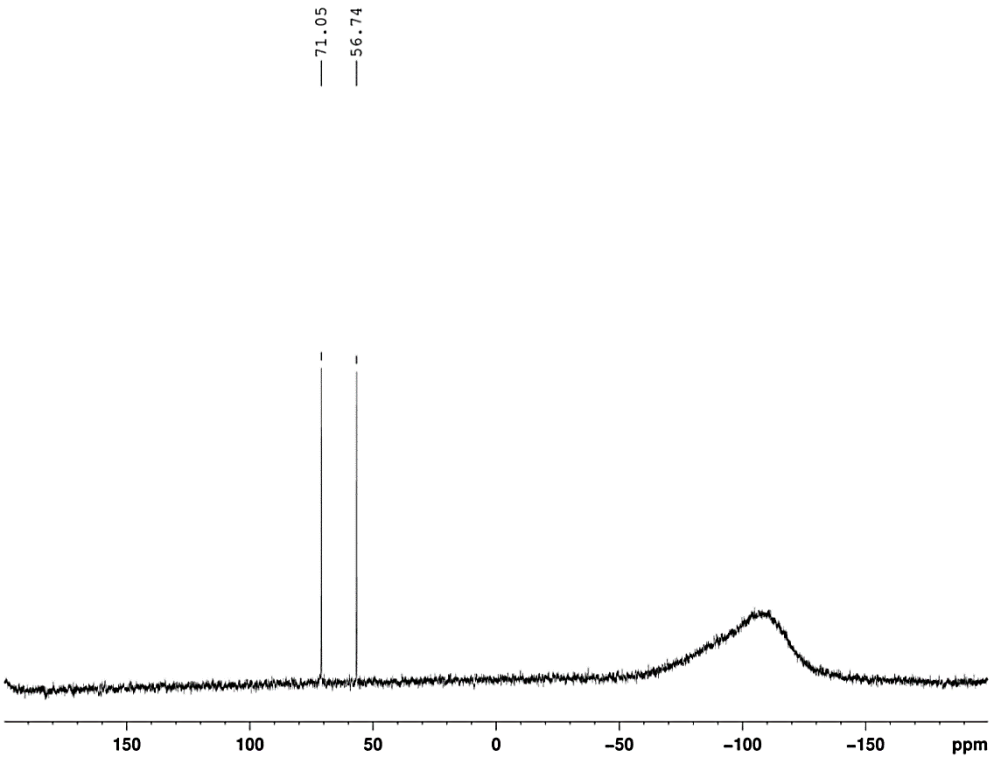


Figure S10: ^{29}Si NMR of **2c** in C_6D_6 at 300 K.

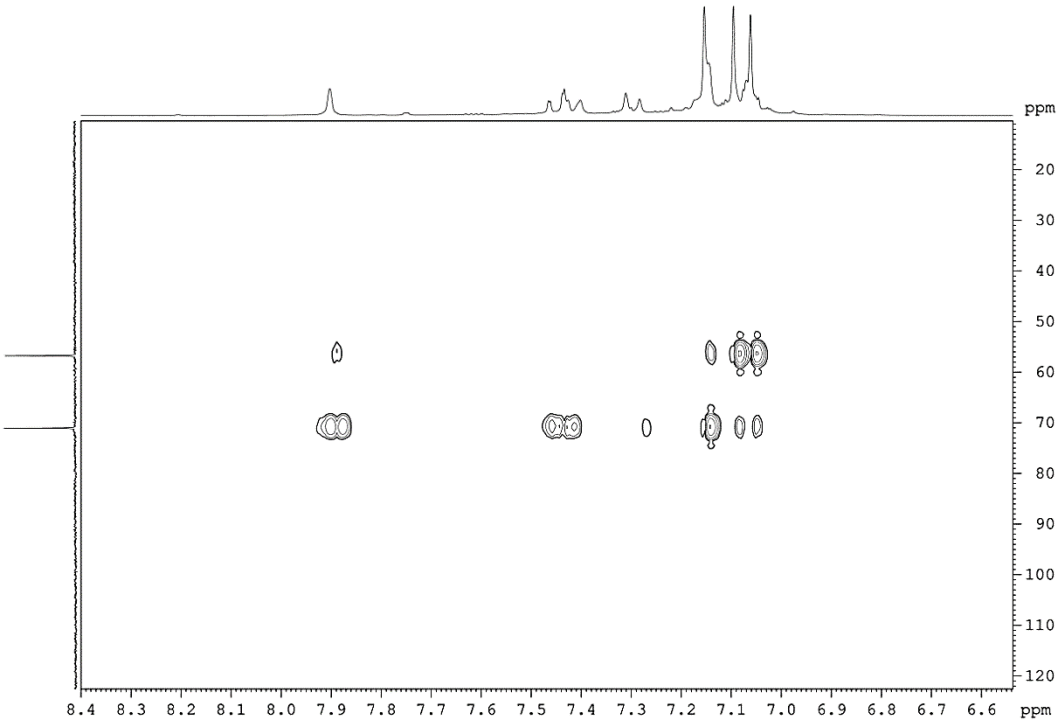


Figure S11: ^{29}Si-^{1}H NMR of **2c** in C_6D_6 at 300 K.

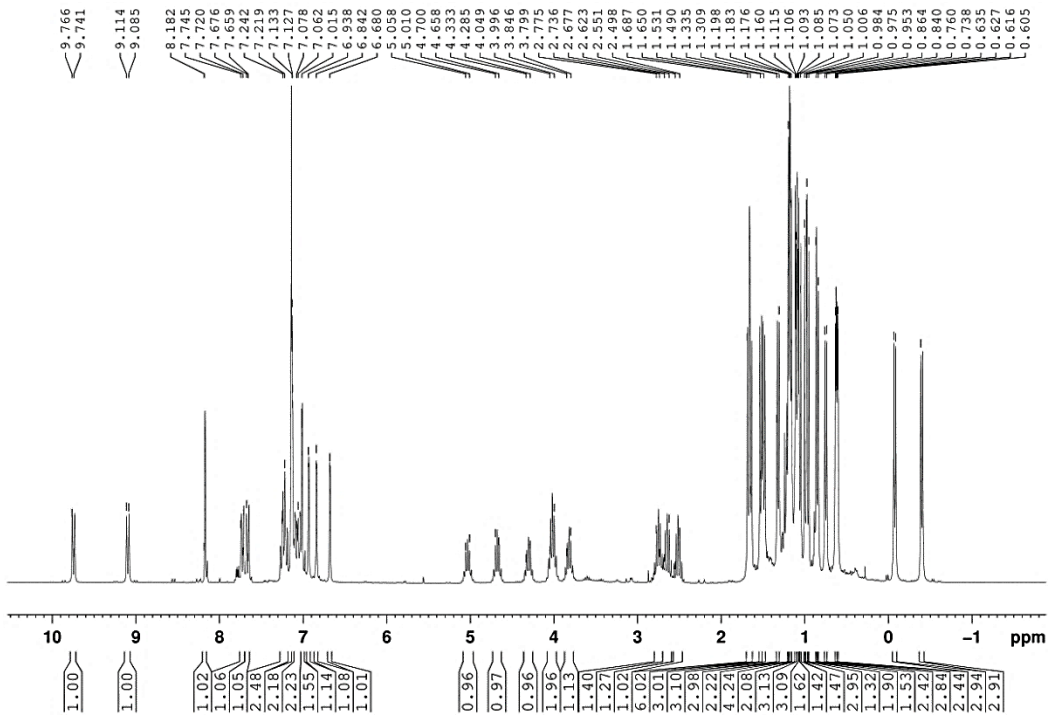


Figure S12: ^{1}H NMR of **2d** in C_6D_6 at 300 K.

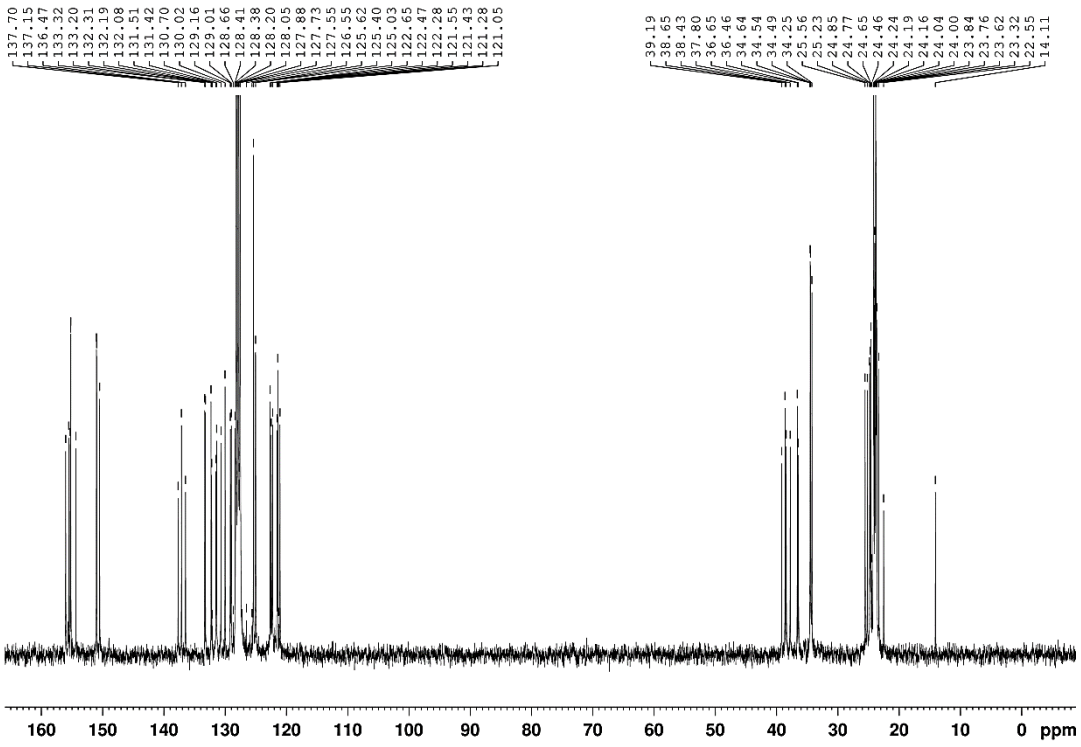


Figure S13: ^{13}C NMR of **2d** in C_6D_6 at 300 K.

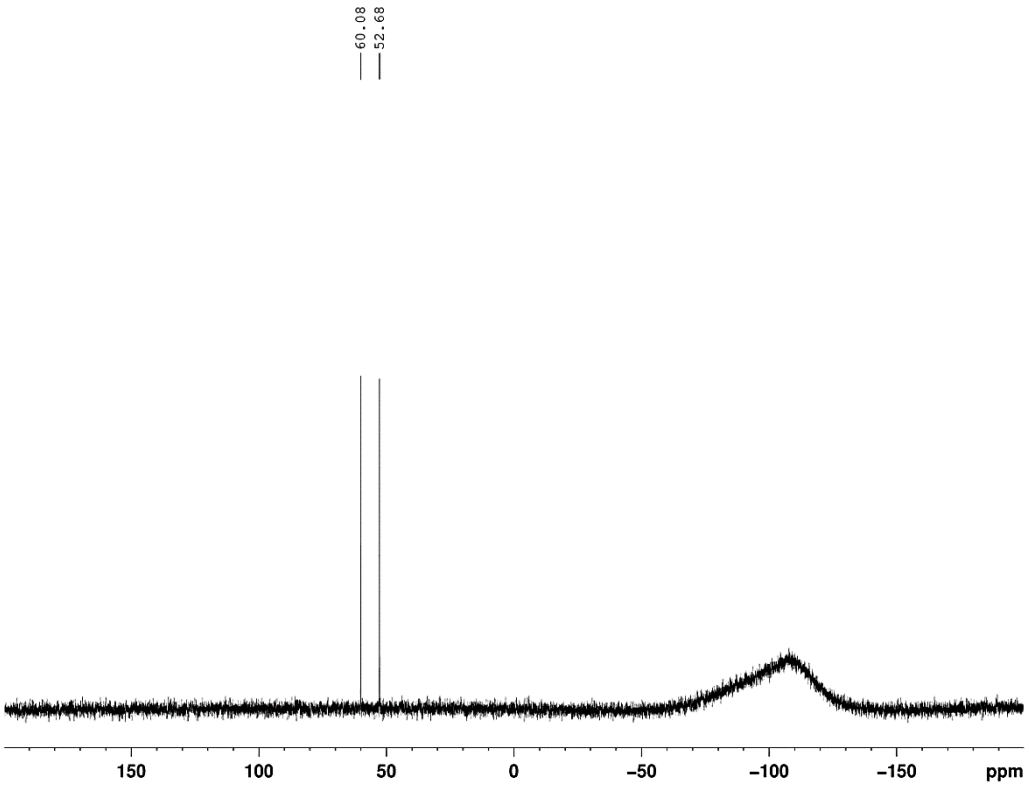


Figure S14: ^{29}Si NMR of **2d** in C_6D_6 at 300 K.

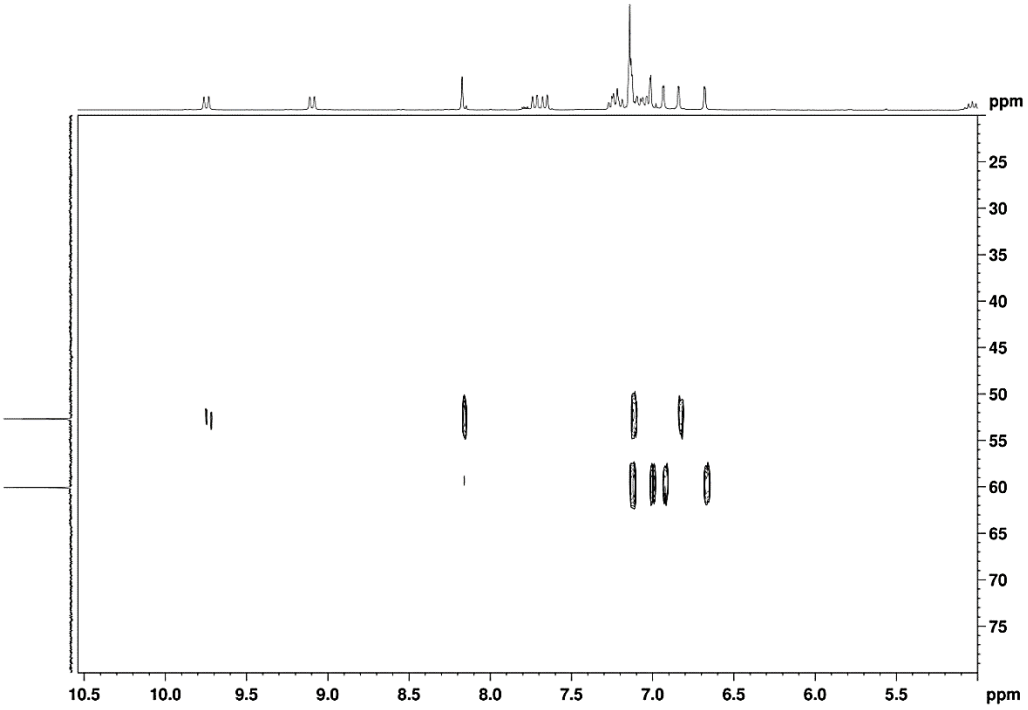


Figure S15: ^{29}Si-^{1}H NMR of **2d** in C_6D_6 at 300 K.

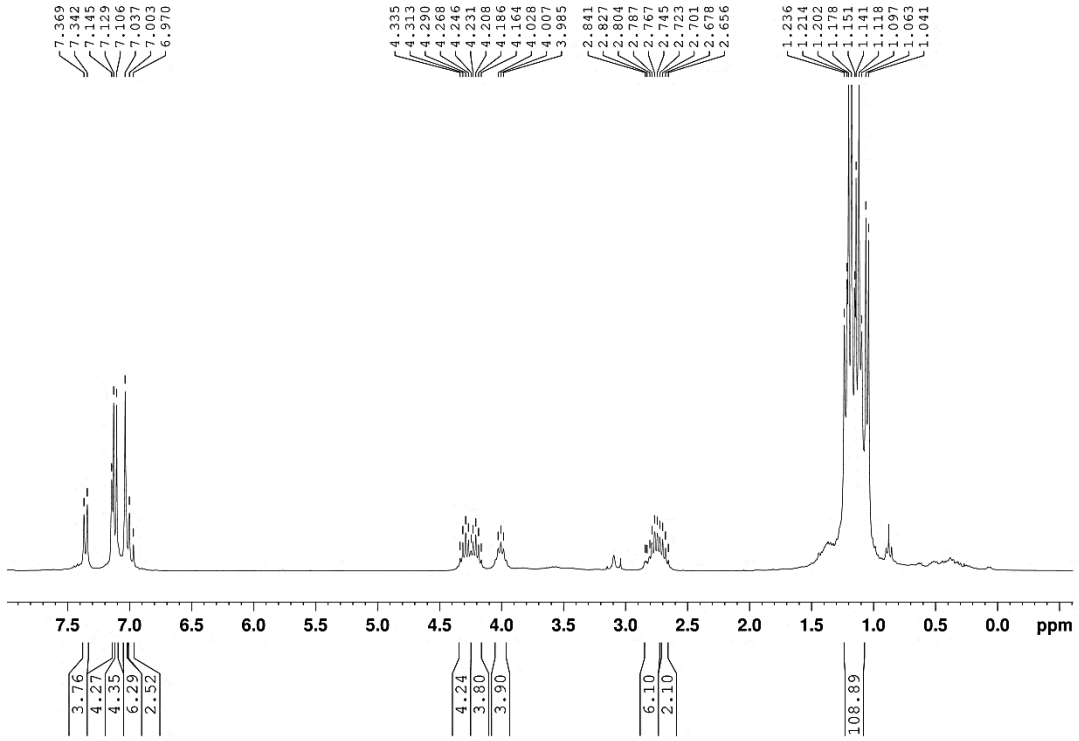


Figure S16: ^{1}H NMR of **3a** in C_6D_6 at 300 K.

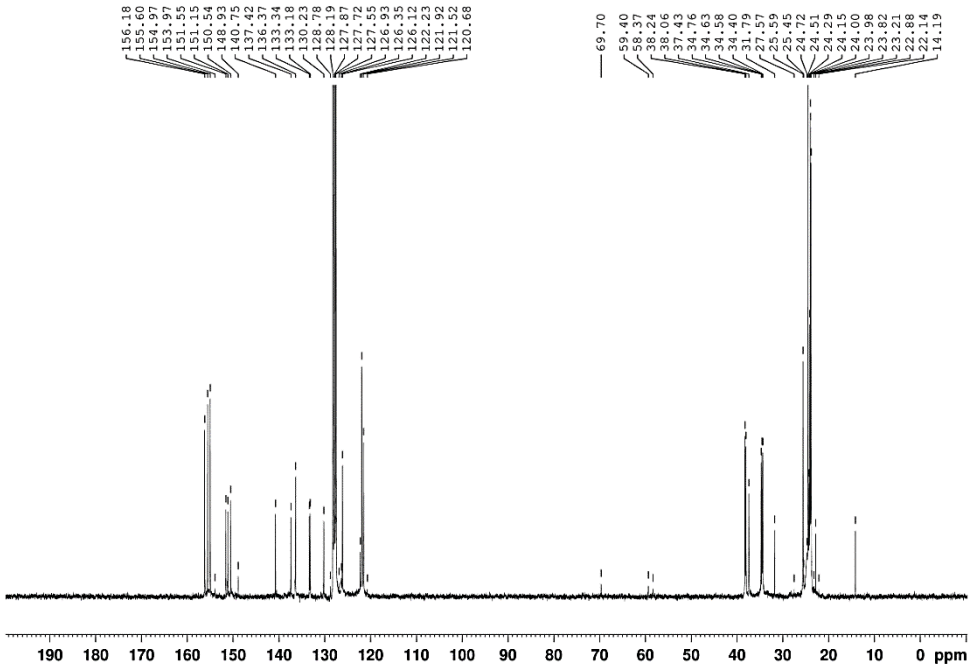


Figure S17: ^{13}C NMR of **3a** in C_6D_6 at 300 K.

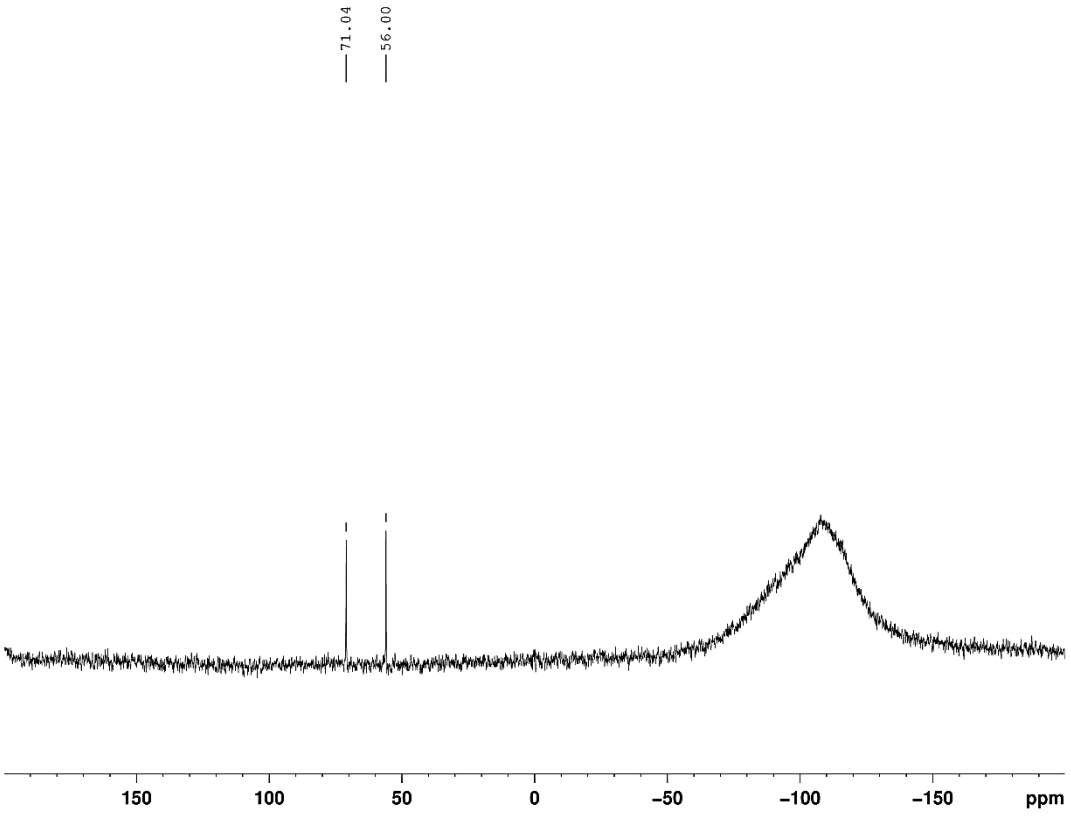


Figure S18: ^{29}Si NMR of **3a** in C_6D_6 at 300 K.

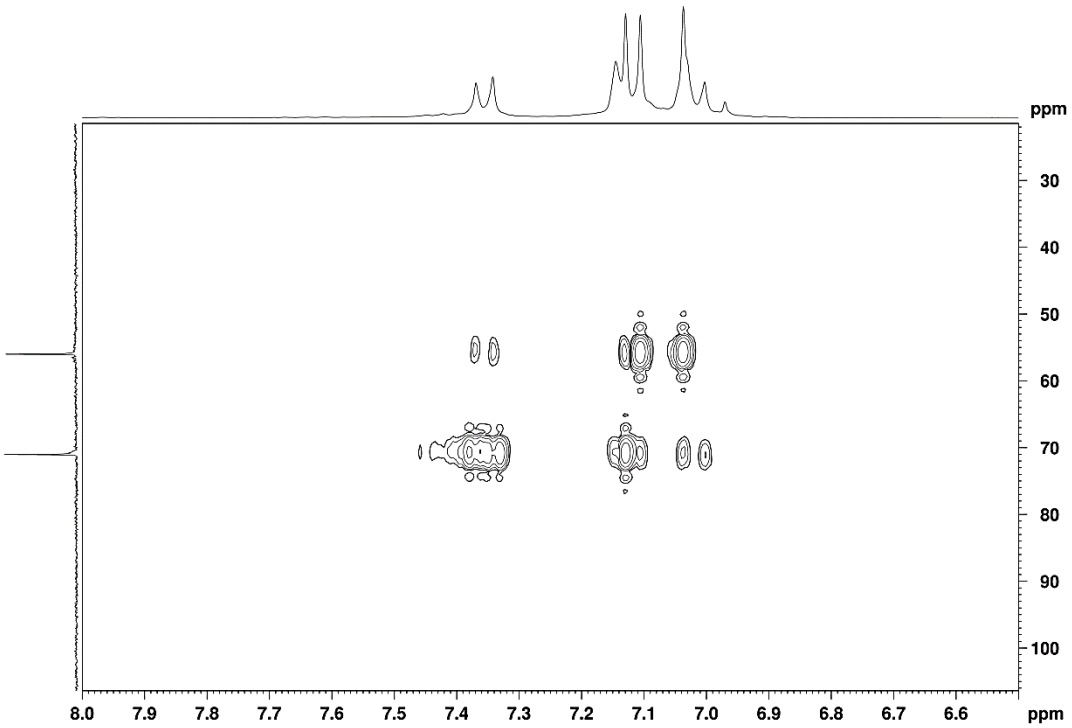


Figure S19: ^{29}Si-^{1}H NMR of **3a** in C_6D_6 at 300 K.

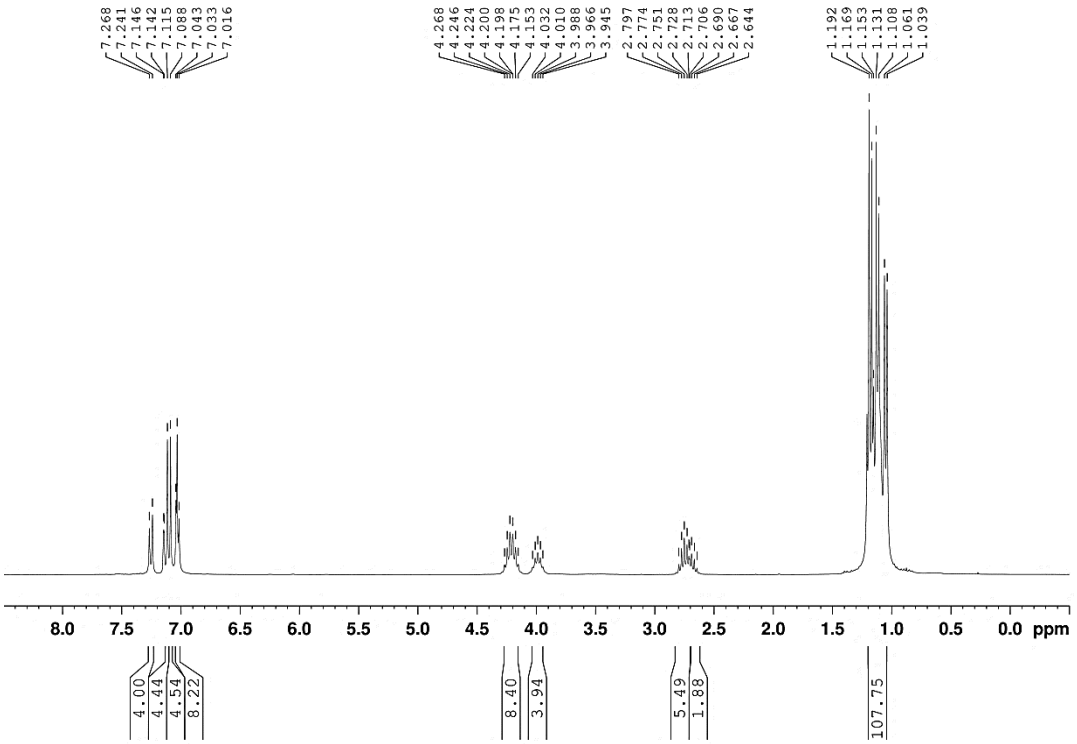


Figure S20: ^{1}H NMR of **3b** in C_6D_6 at 300 K.

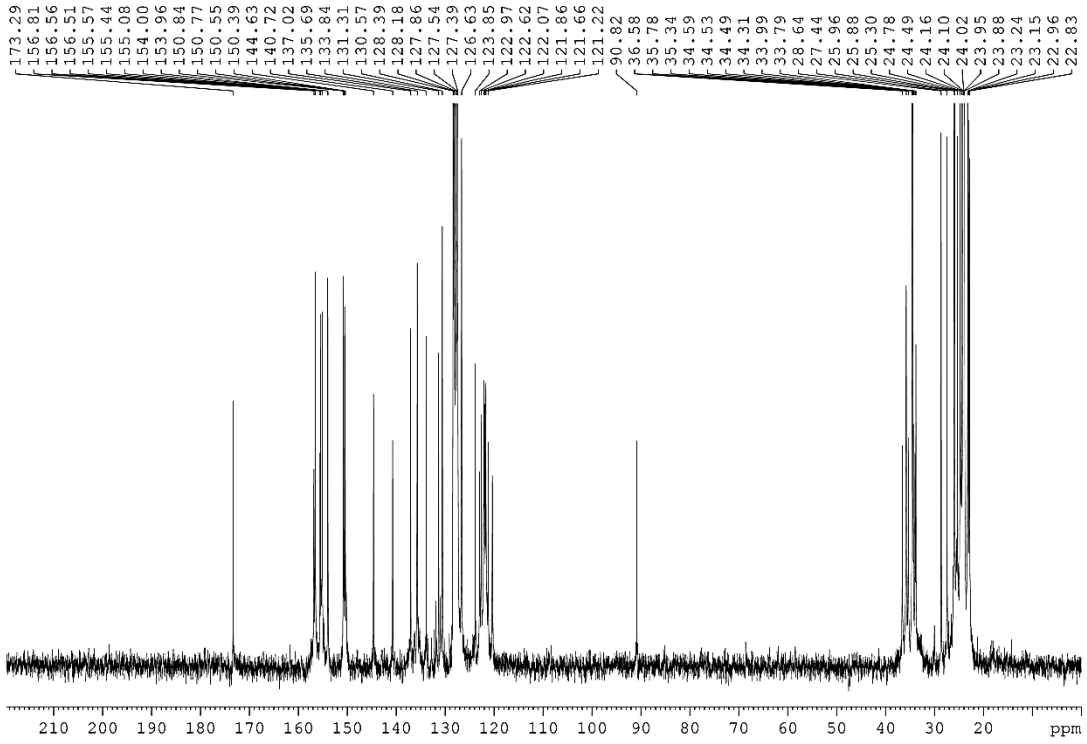


Figure S21: ^{13}C NMR of **3b** in C_6D_6 at 300 K.

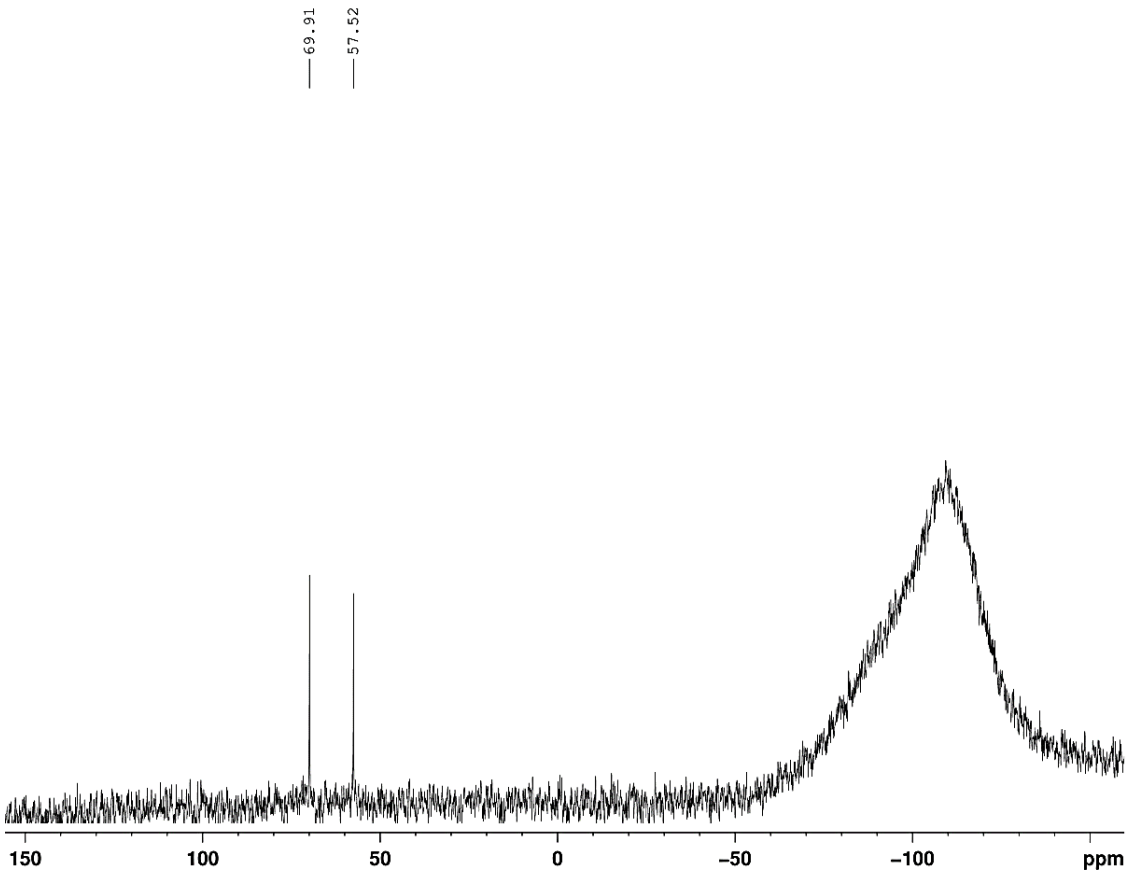


Figure S22: ^{29}Si NMR of **3b** in C_6D_6 at 300 K.

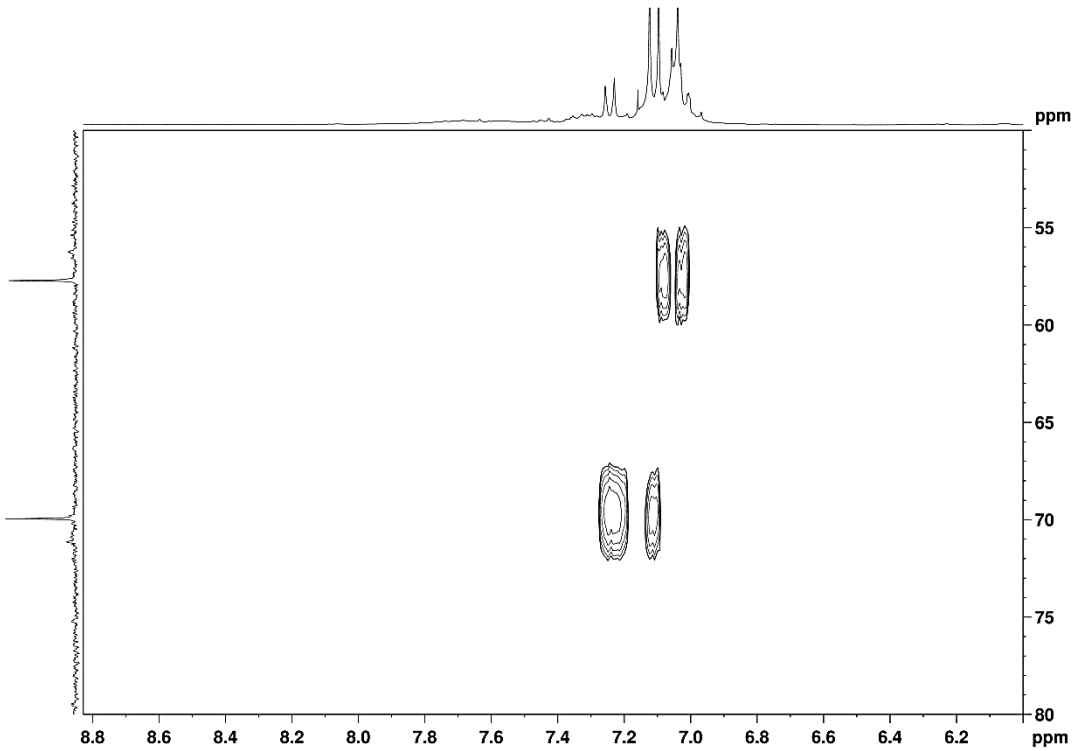


Figure S23: ^{29}Si-^{1}H NMR of **3b** in C_6D_6 at 300 K.

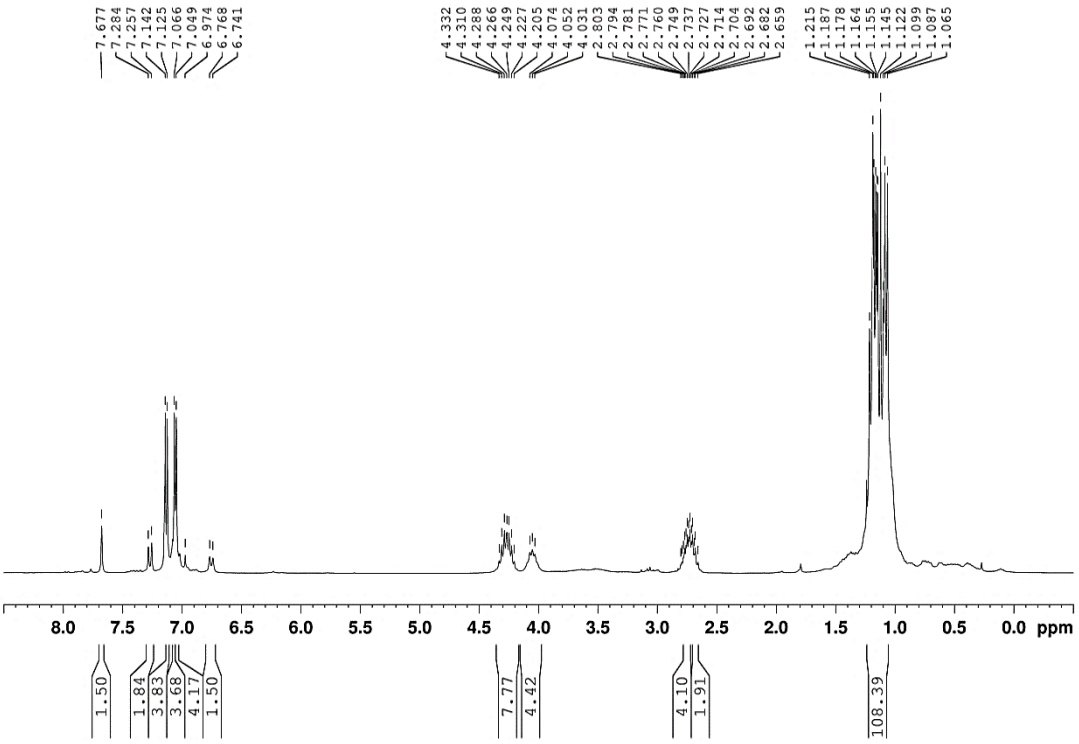


Figure S24: ^{1}H NMR of **3c** in C_6D_6 at 300 K.

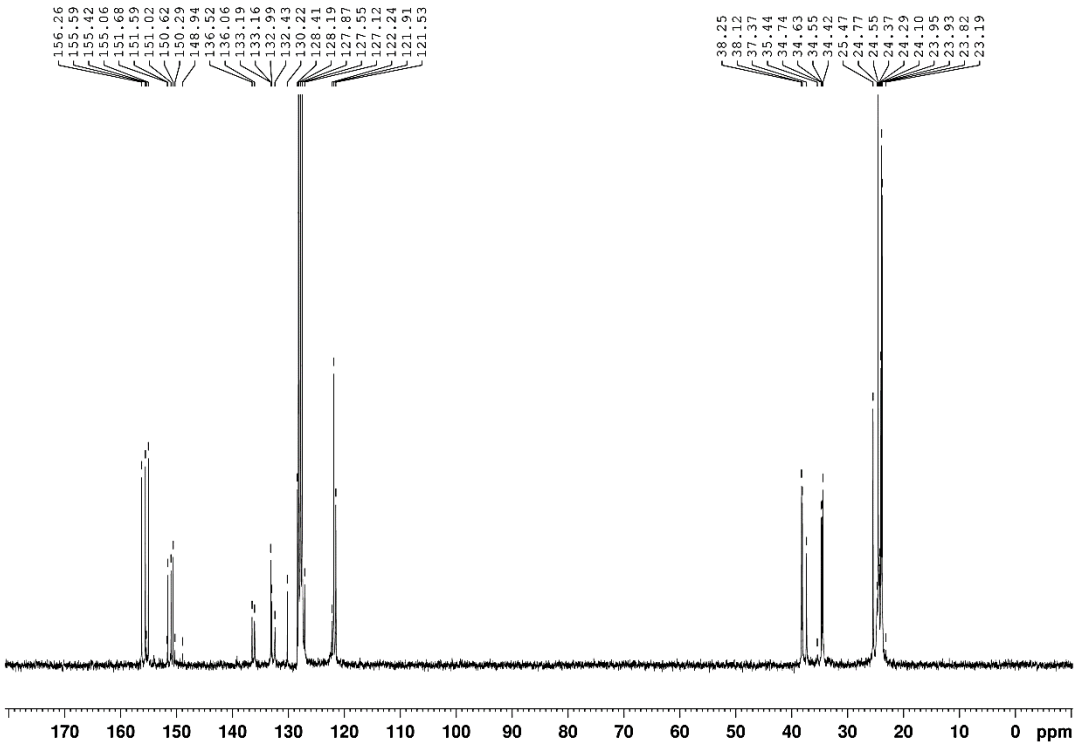


Figure S25: ^{13}C NMR of **3c** in C_6D_6 at 300 K.

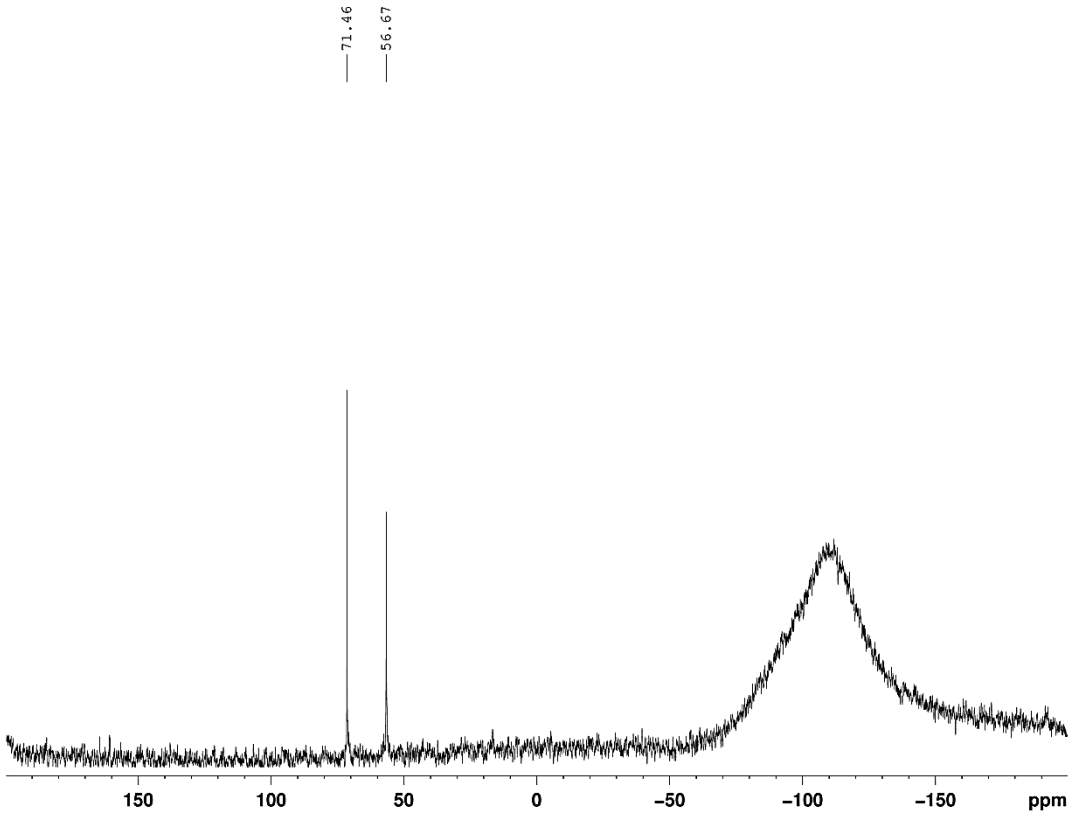


Figure S26: ^{29}Si NMR of **3c** in C_6D_6 at 300 K.

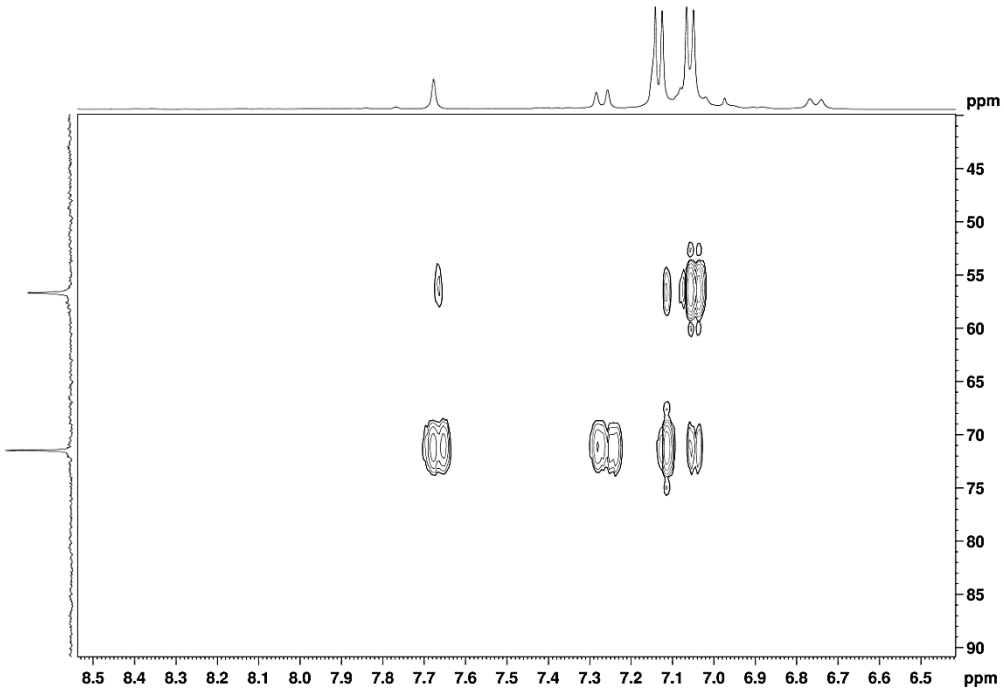


Figure S27: ^{29}Si-^{1}H NMR of **3c** in C_6D_6 at 300 K.

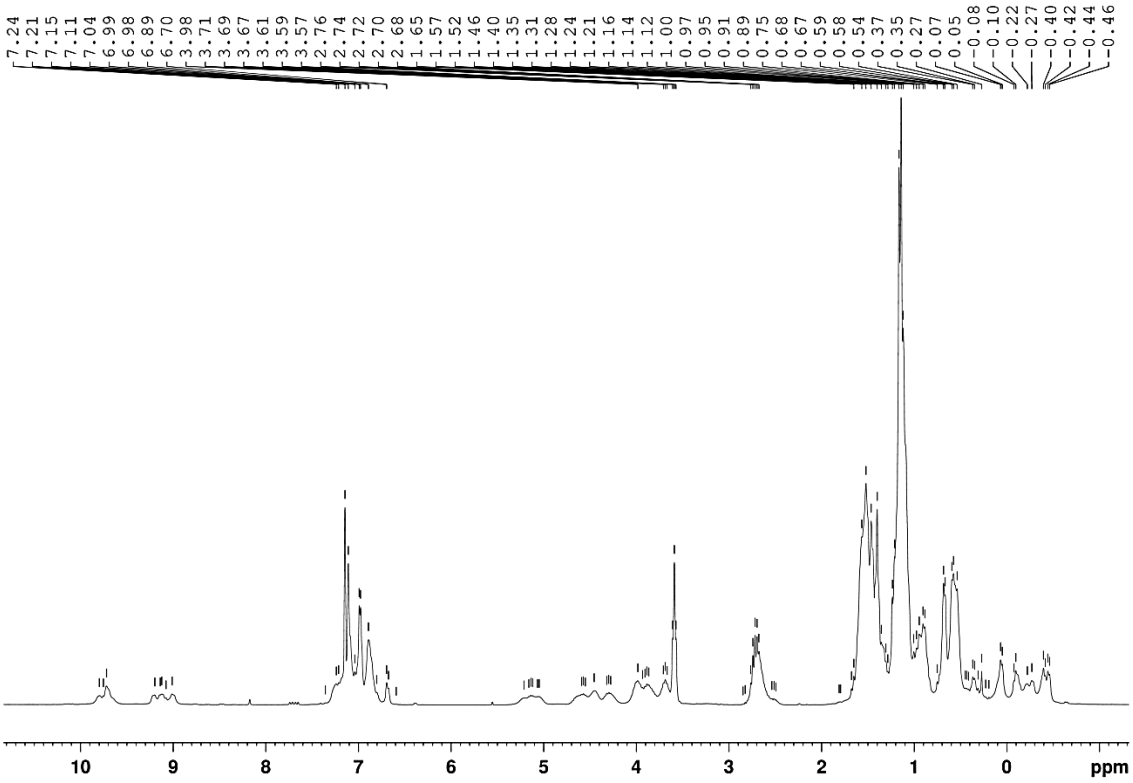


Figure S28: ^{1}H NMR of **3d** in C_6D_6 at 300 K.

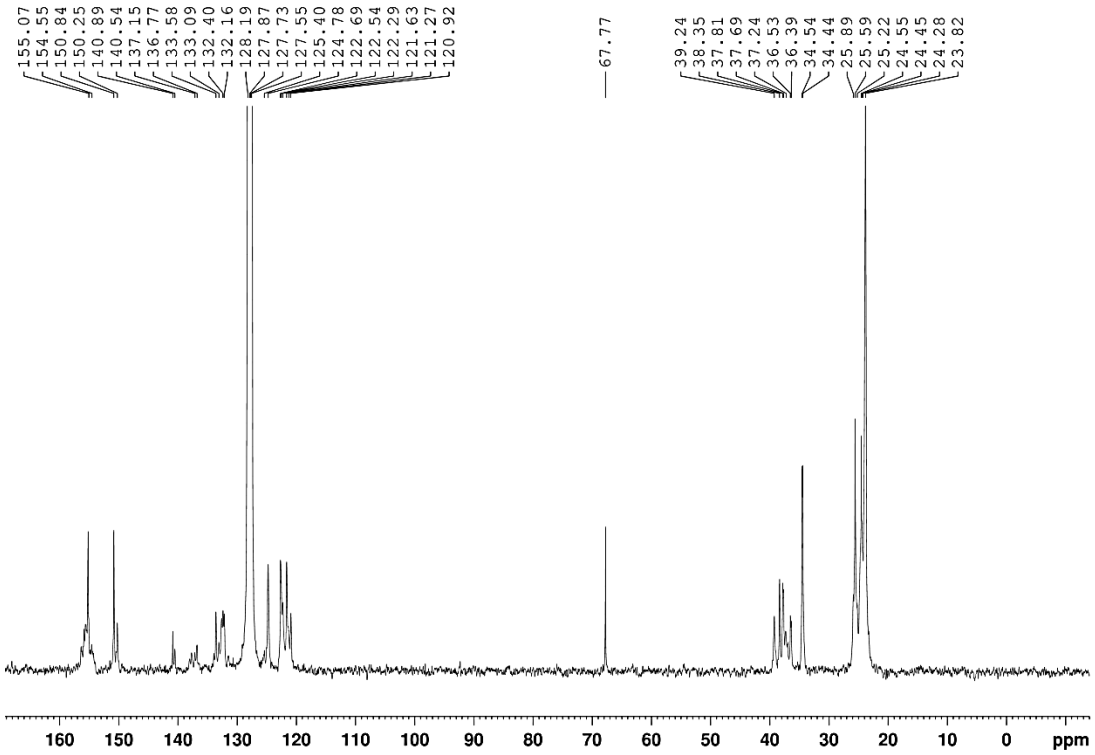


Figure S29: ^{13}C NMR of **3d** in C_6D_6 at 300 K.

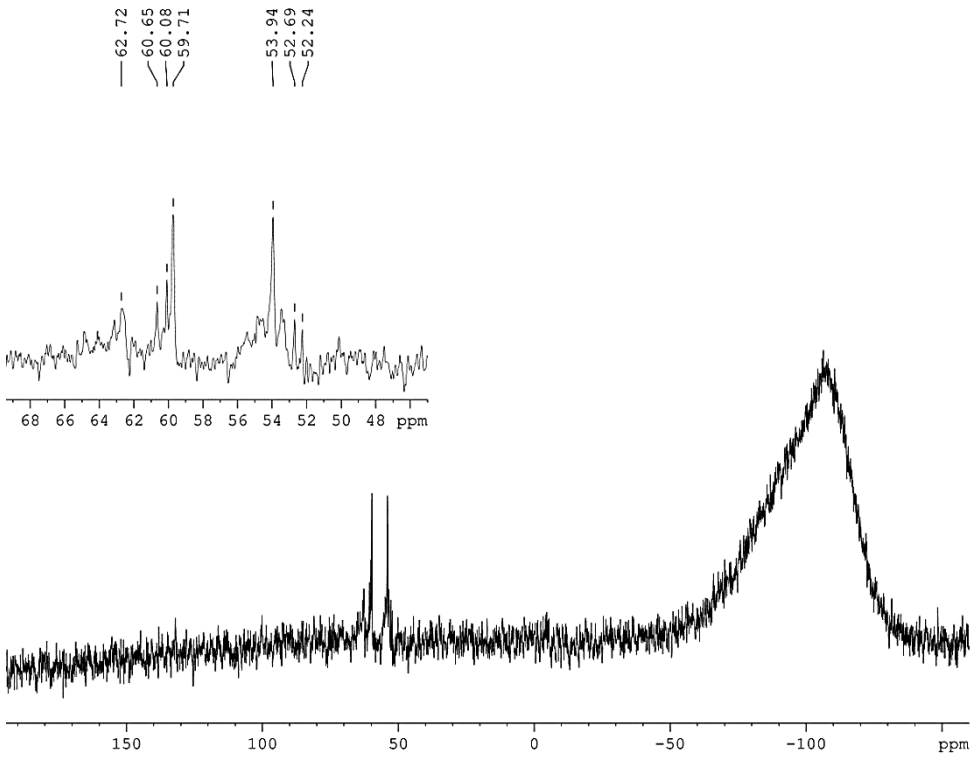


Figure S30: ^{29}Si NMR of **3d** in C_6D_6 at 300 K.

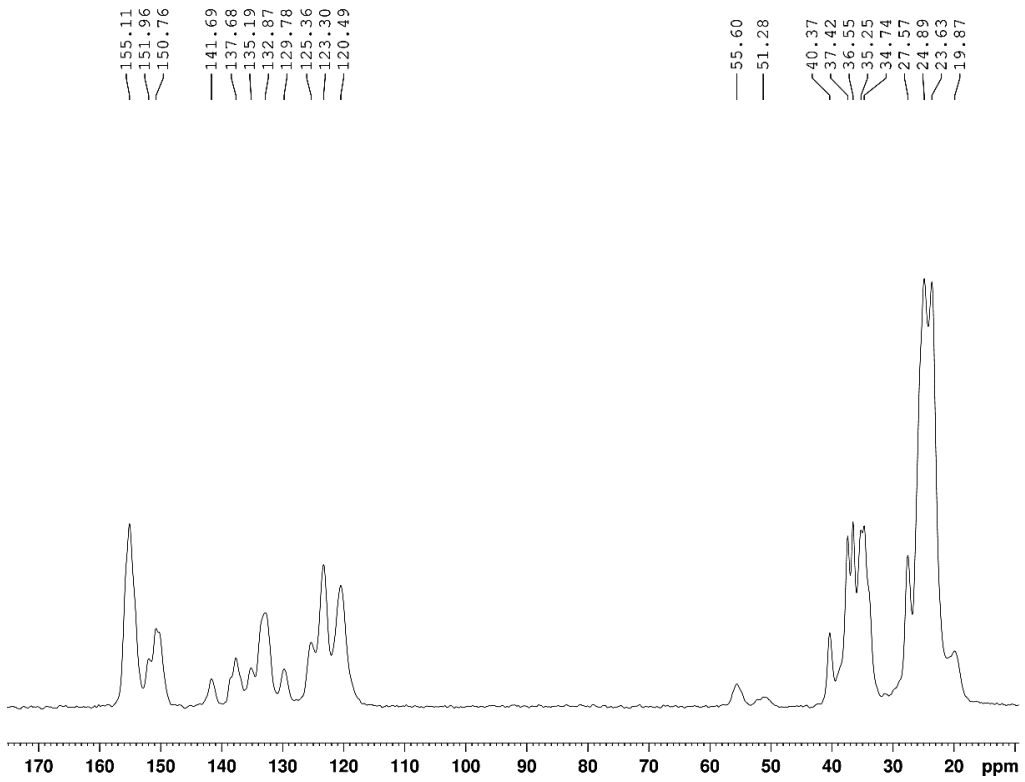


Figure S31: CP-MAS ^{13}C NMR of **3d** in solid state at 300 K.

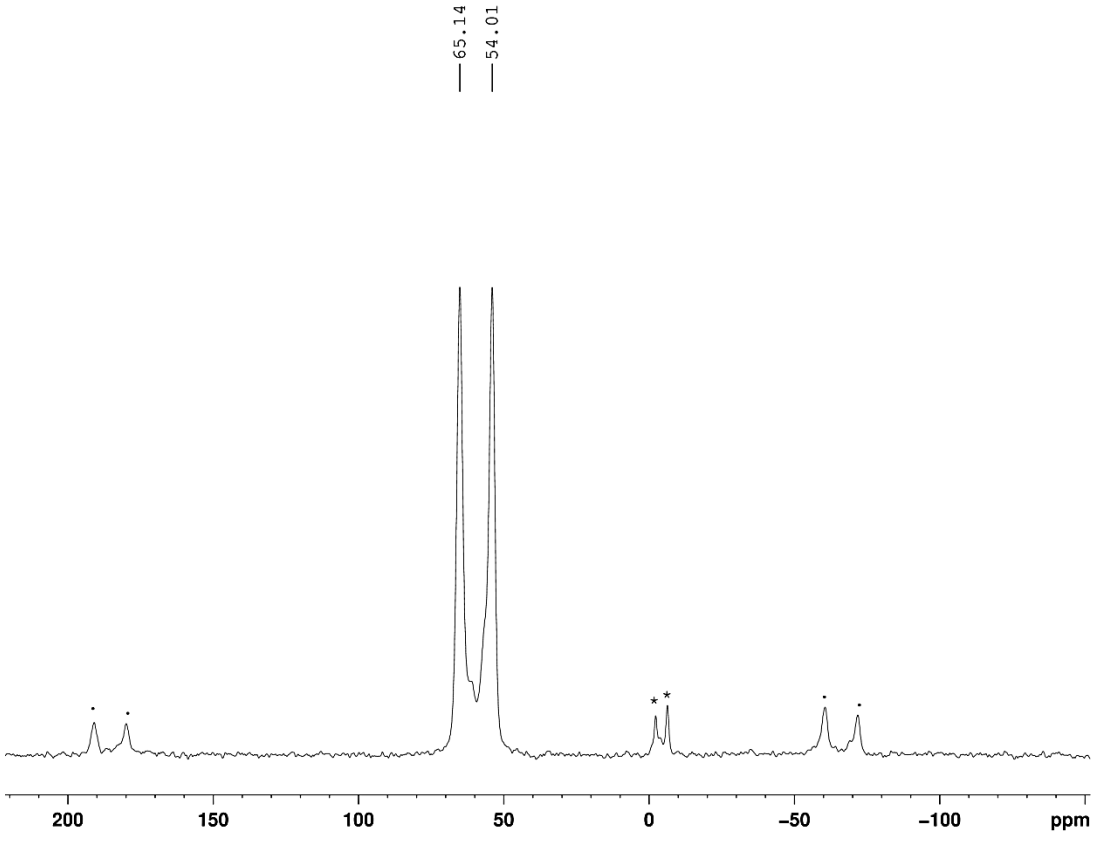


Figure S32: CP-MAS ^{29}Si NMR of **3d** in solid state at 300 K, ***** = minor signals for unknown impurities, • = rotational side band with sample rotation frequency = 10000 Hz.

2. Absorption spectra

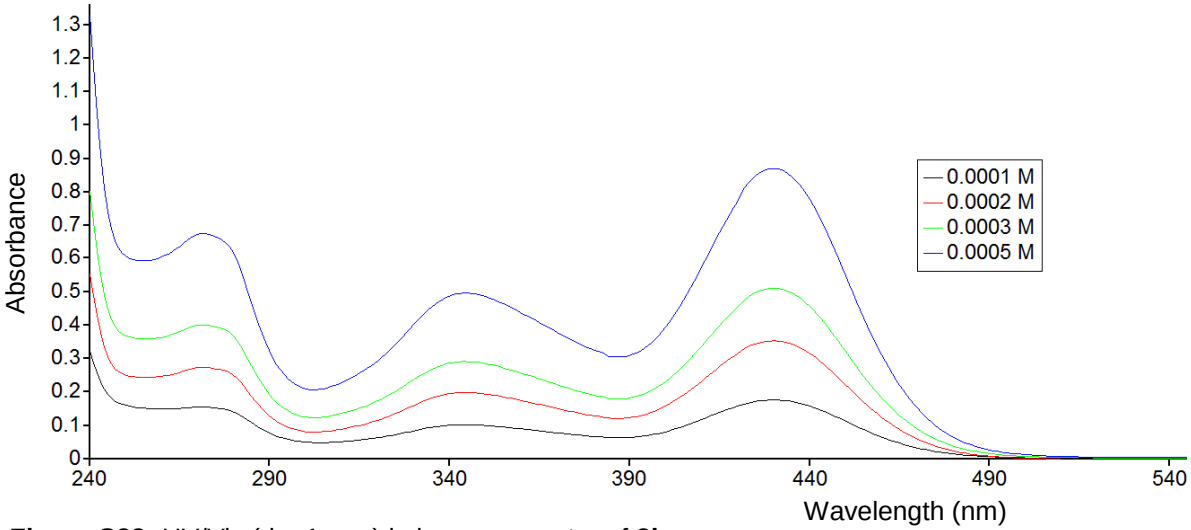


Figure S33: UV/Vis (d = 1 mm) in hexane spectra of **2b.**

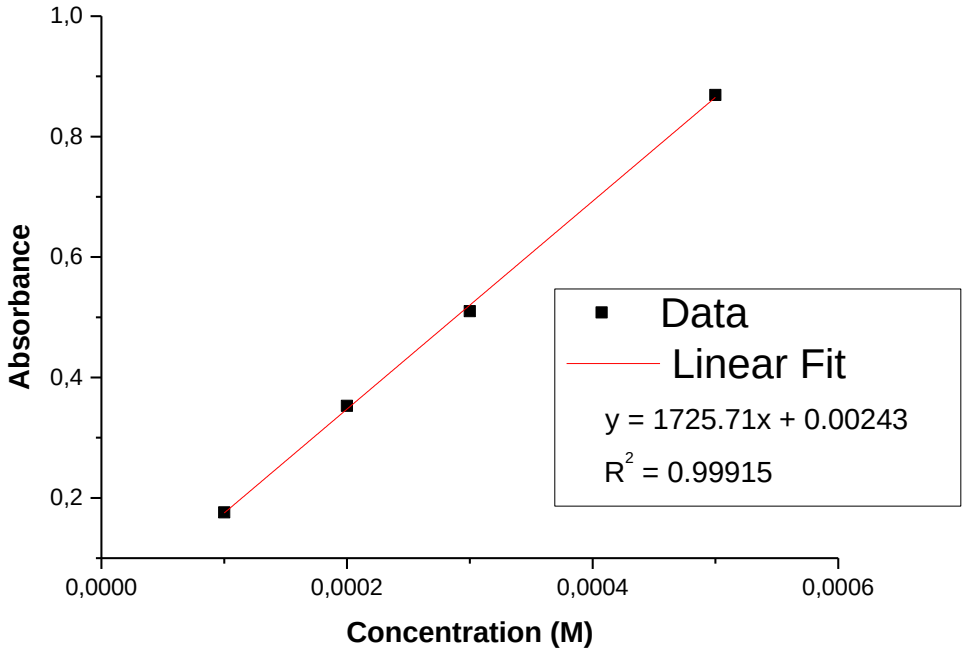


Figure S34: Linear fit for UV/Vis data of **2b** for (λ = 430 nm).

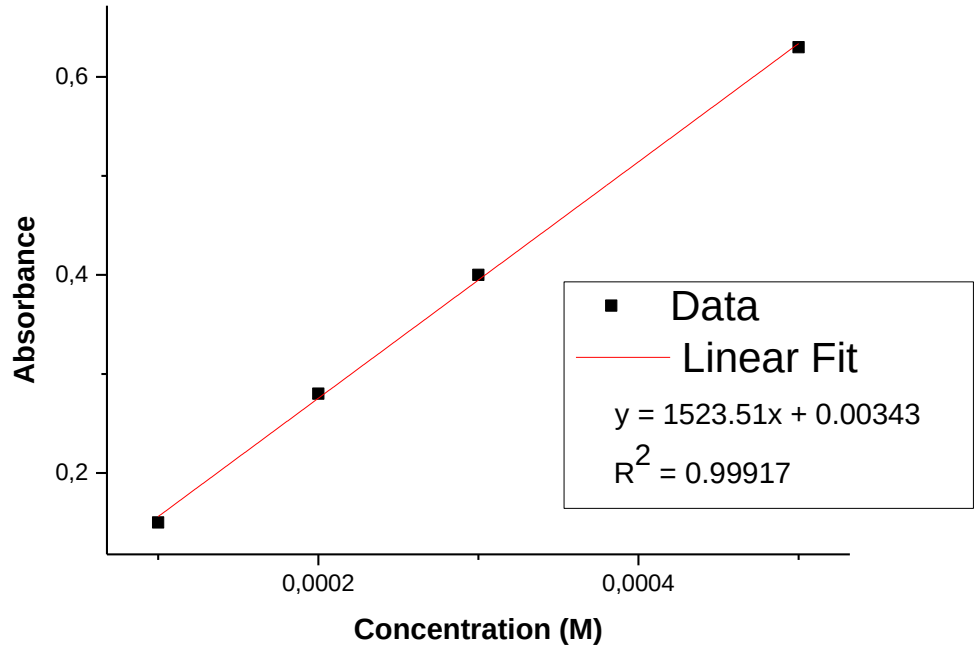


Figure S35: Linear fit for UV/Vis data of **2b** for (λ = 335 nm).

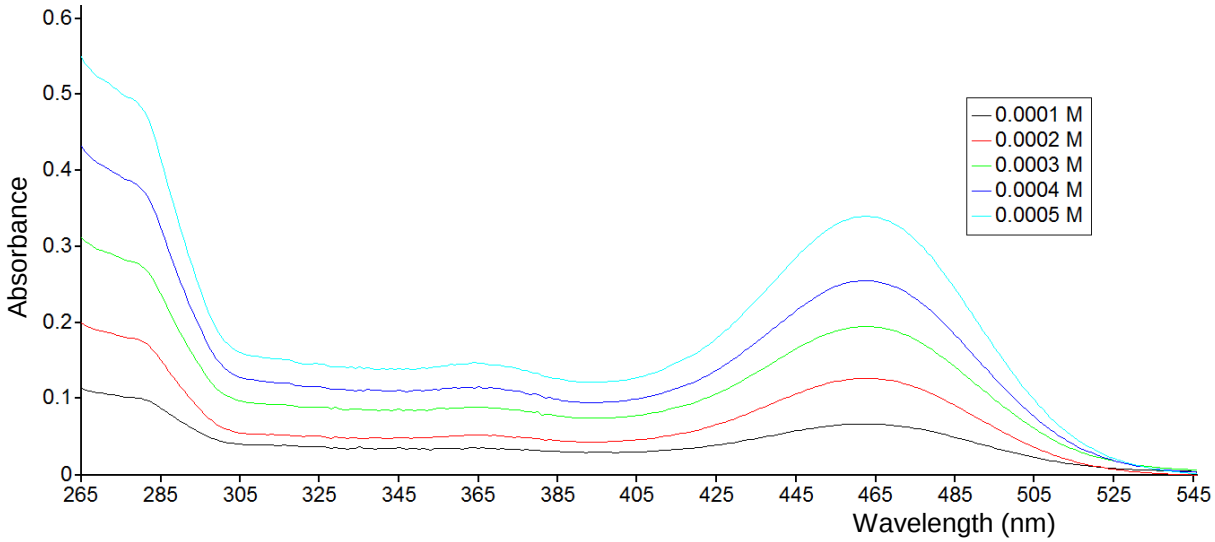


Figure S36: UV/Vis (d = 1 mm) in hexane spectra of **2c.**

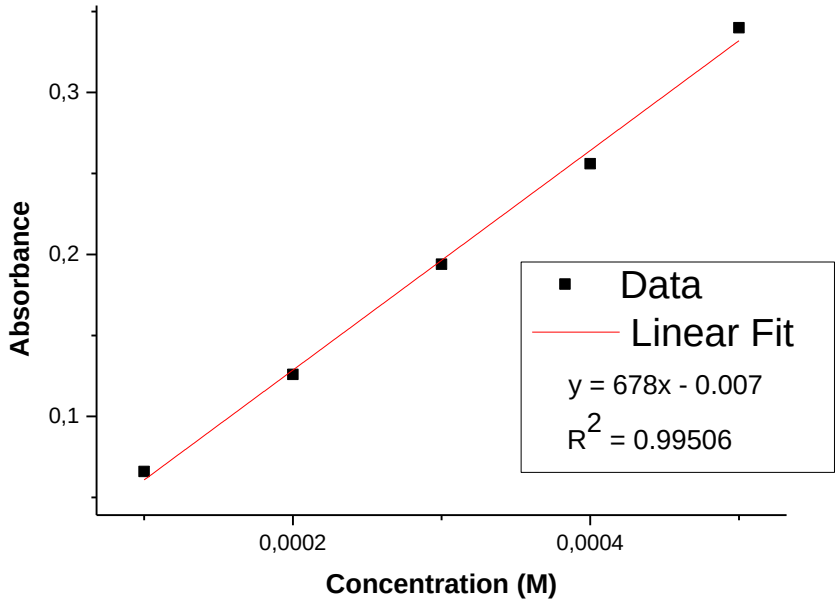


Figure S37: Linear fit for UV/Vis data of **2c.**

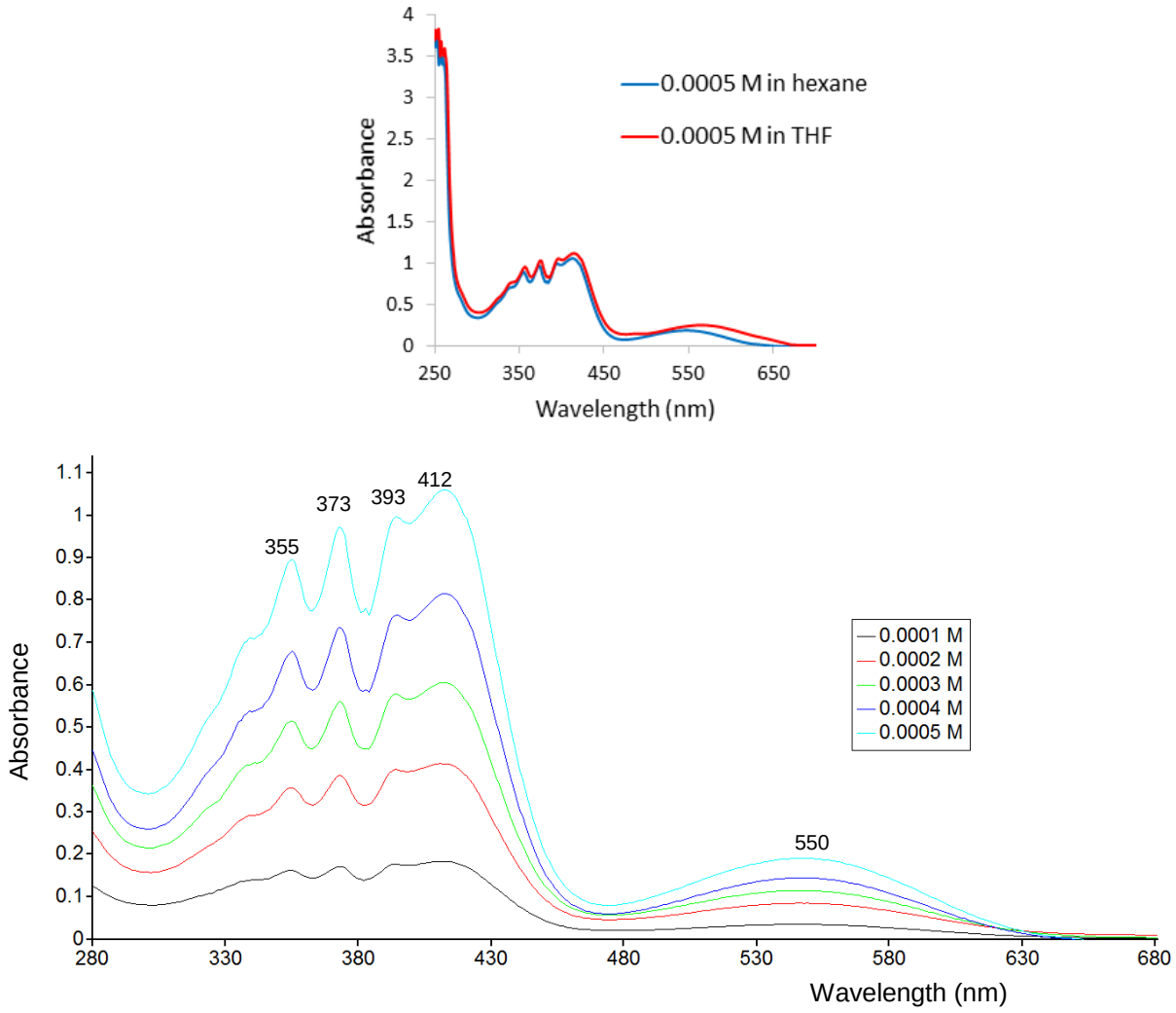


Figure S38: UV/Vis (d = 1 mm) of **2d** recorded in hexane and THF (0.0005 M) at room temperature (Top) and in hexane at different Concentrations spectra (Bottom).

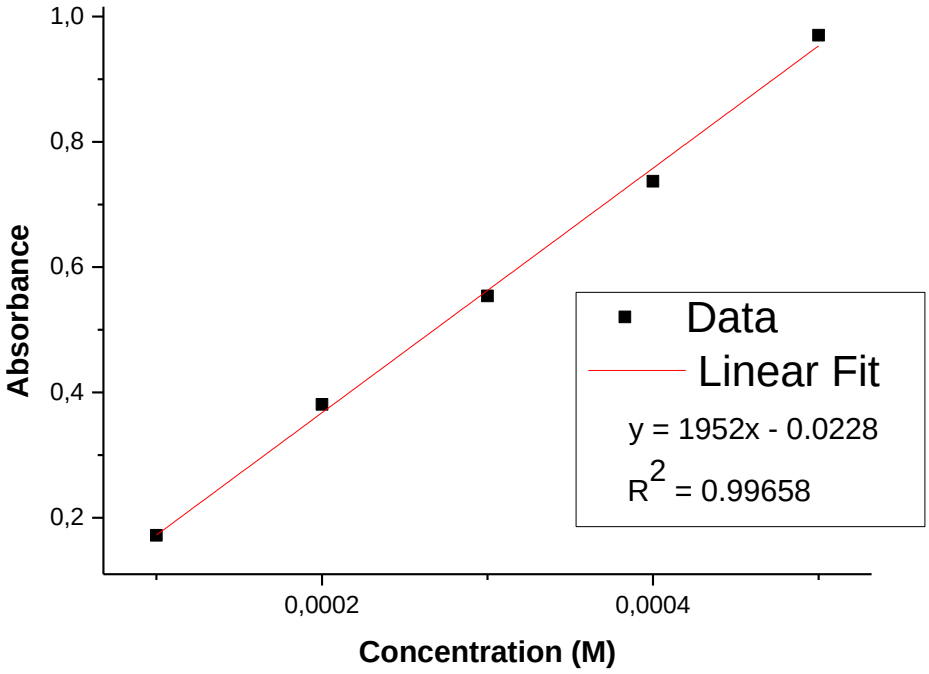


Figure S39: Linear fit for UV/Vis data of **2d** (λ = 373 nm).

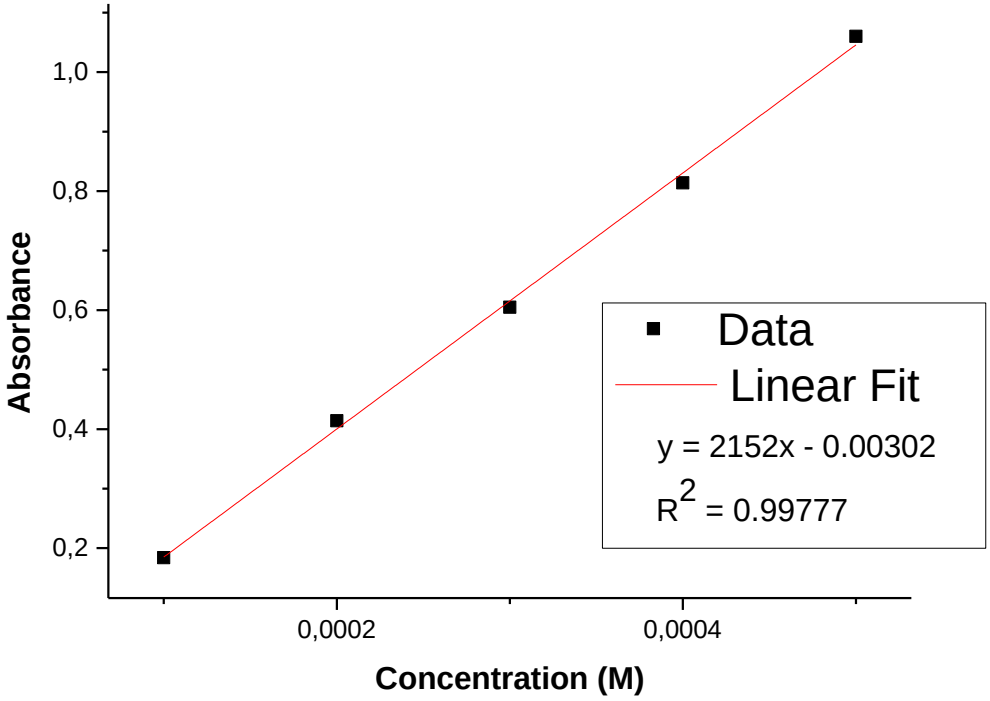


Figure S40: Linear fit for UV/Vis data of **2d** (λ = 412 nm).

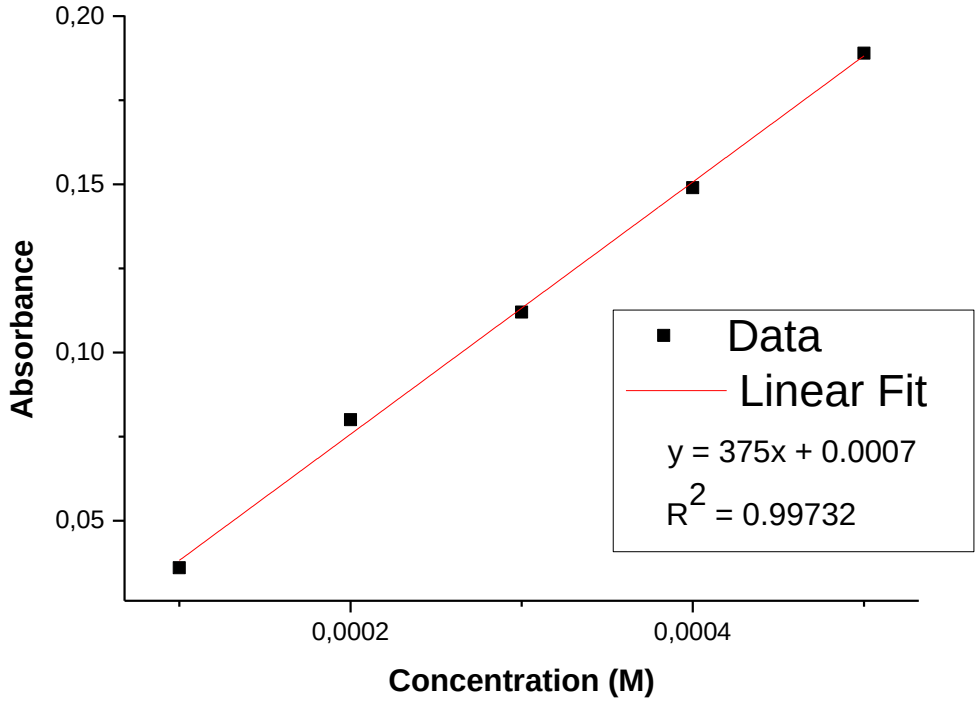


Figure S41: Linear fit for UV/Vis data of **2d** (λ = 550 nm).

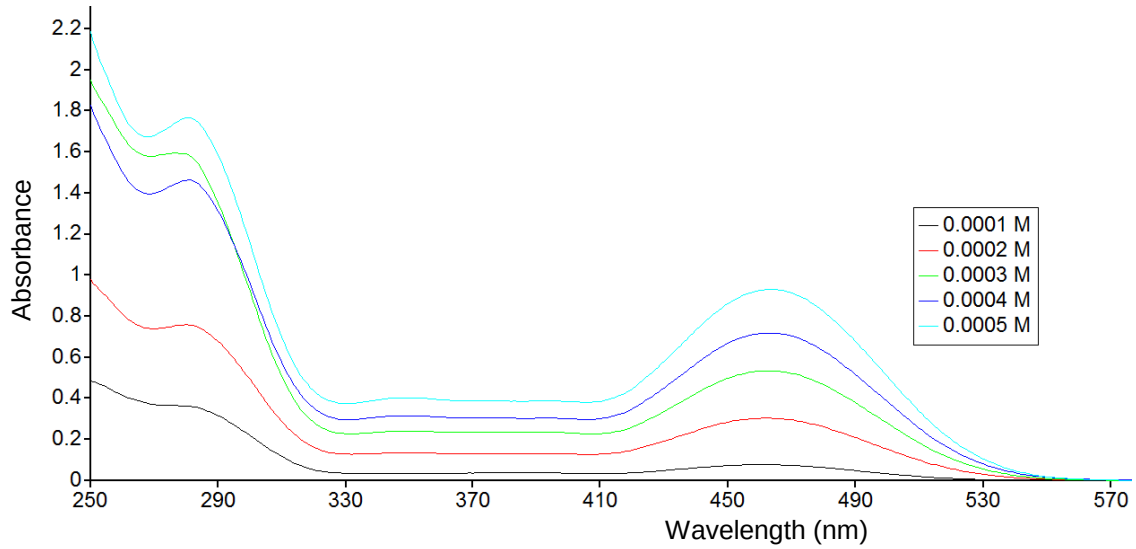


Figure S42: UV/Vis (d = 1 mm) in hexane spectra of **3a.**

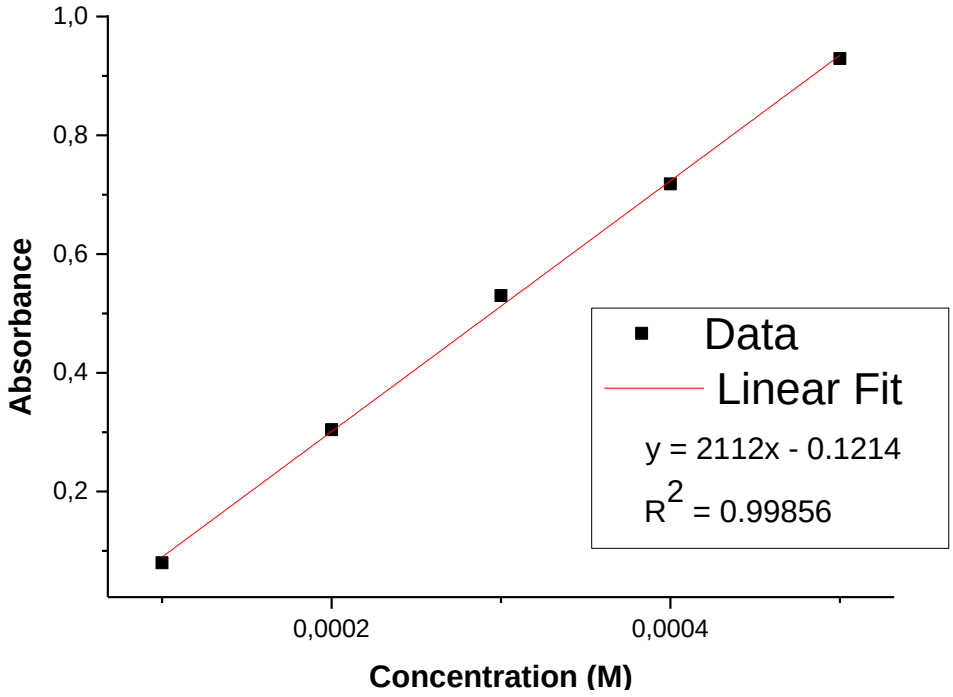


Figure S43: Linear fit for UV/ Vis data of **3a** above for (λ = 463 nm).

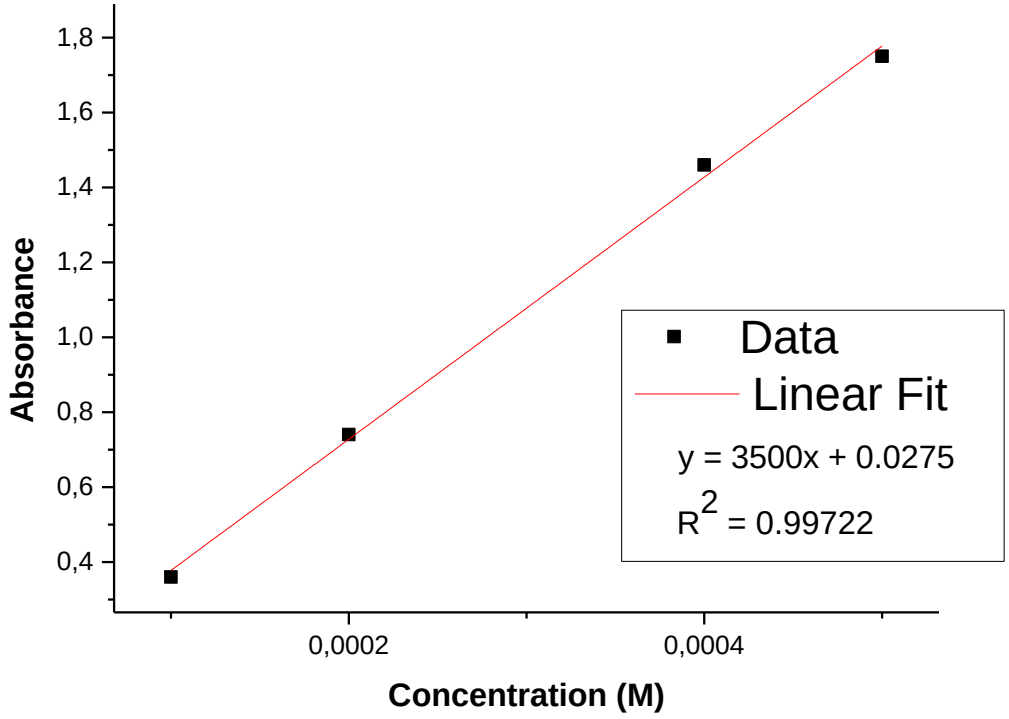


Figure S44: Linear fit for UV/ Vis data of **3a** for (λ = 227 nm).

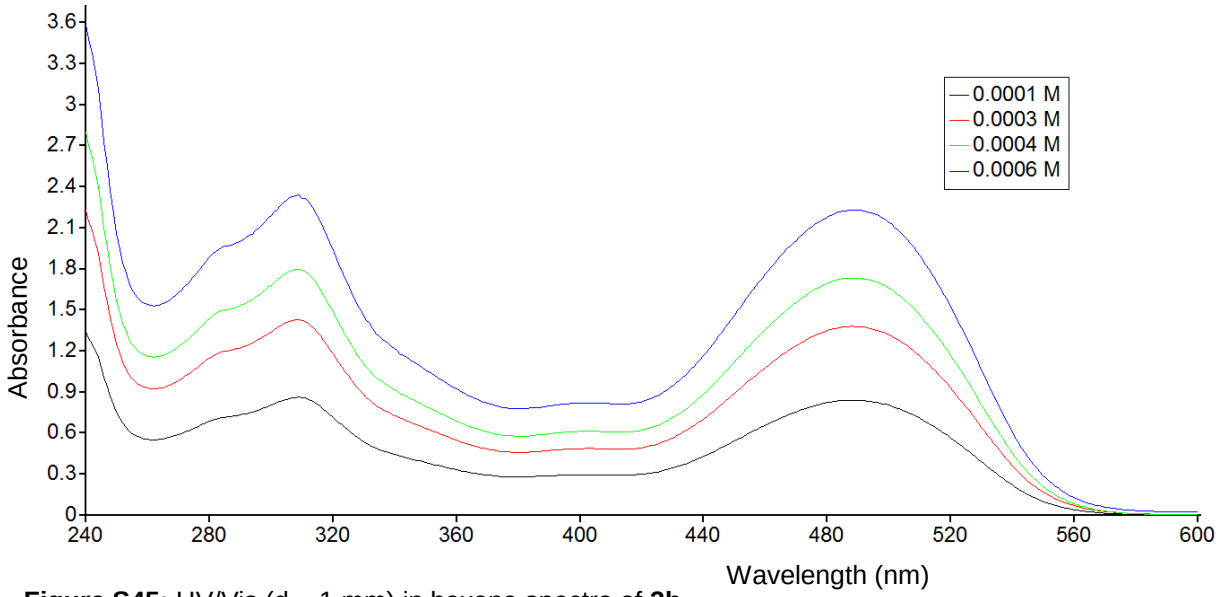


Figure S45: UV/Vis (d = 1 mm) in hexane spectra of **3b.**

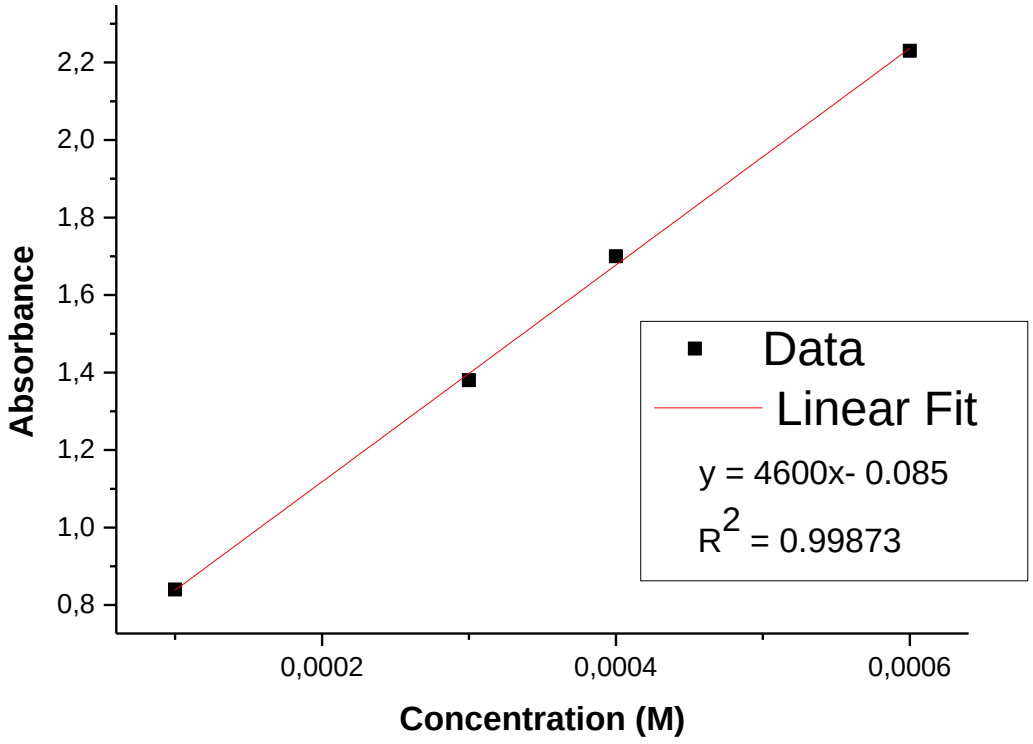


Figure S46: Linear fit for UV/Vis data of **3b** for (λ = 488 nm).

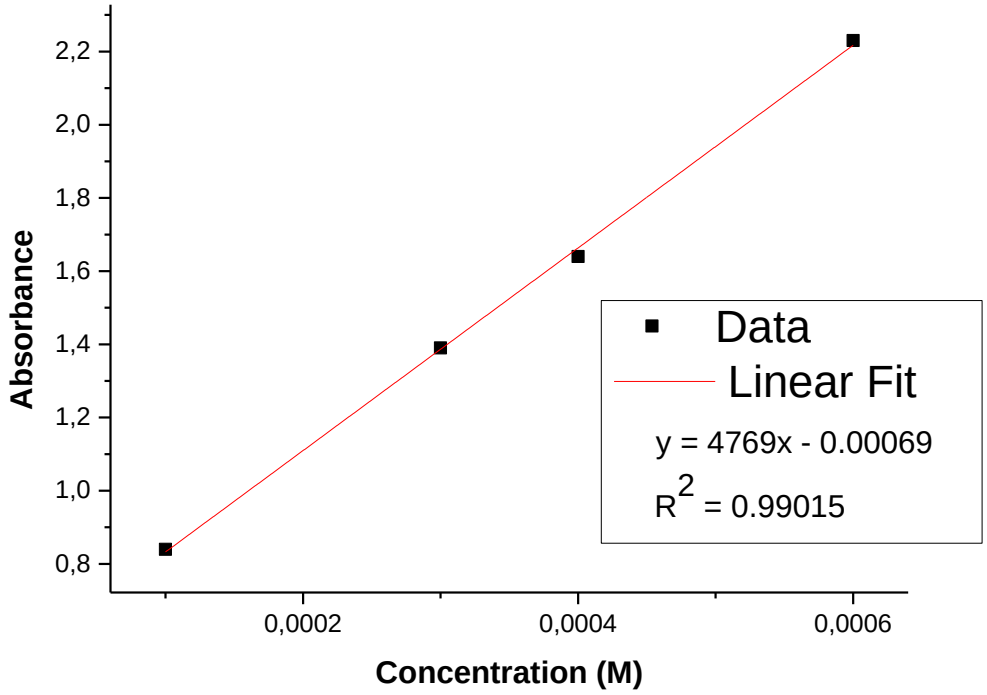


Figure S47: Linear fit for UV/Vis data of **3b** for (λ = 309 nm).

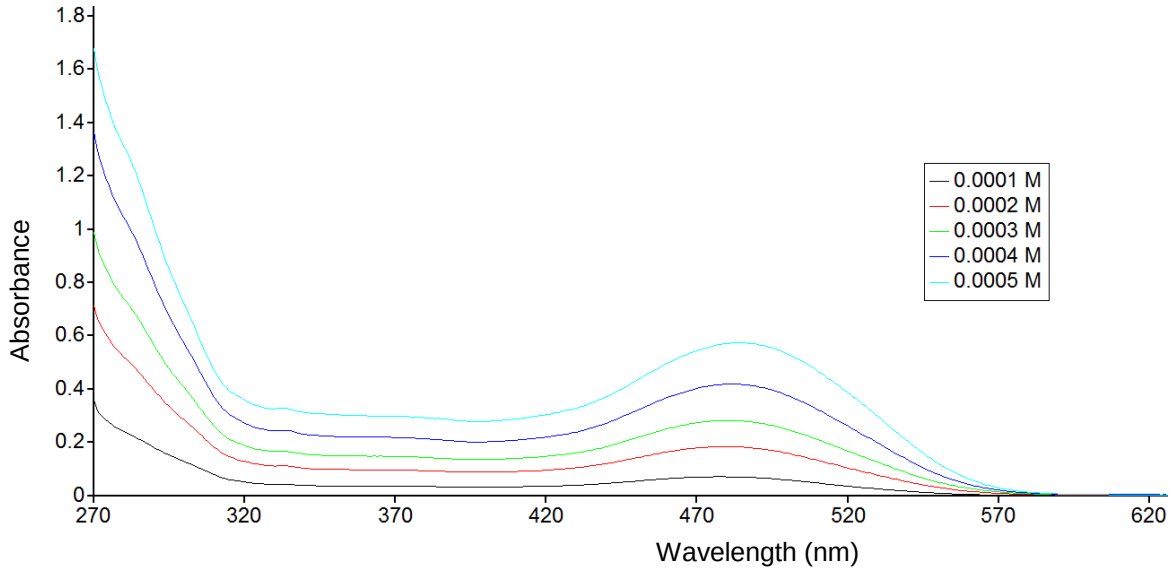


Figure S48: UV/Vis (d = 1 mm) in hexane spectra of **3c.**

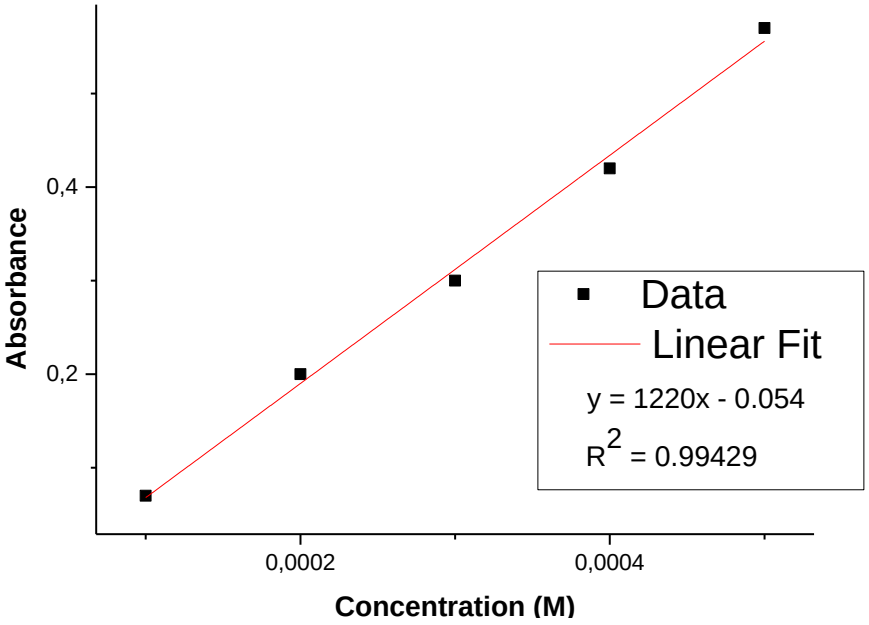


Figure S49: Linear fit for UV/ Vis data of **3c.**

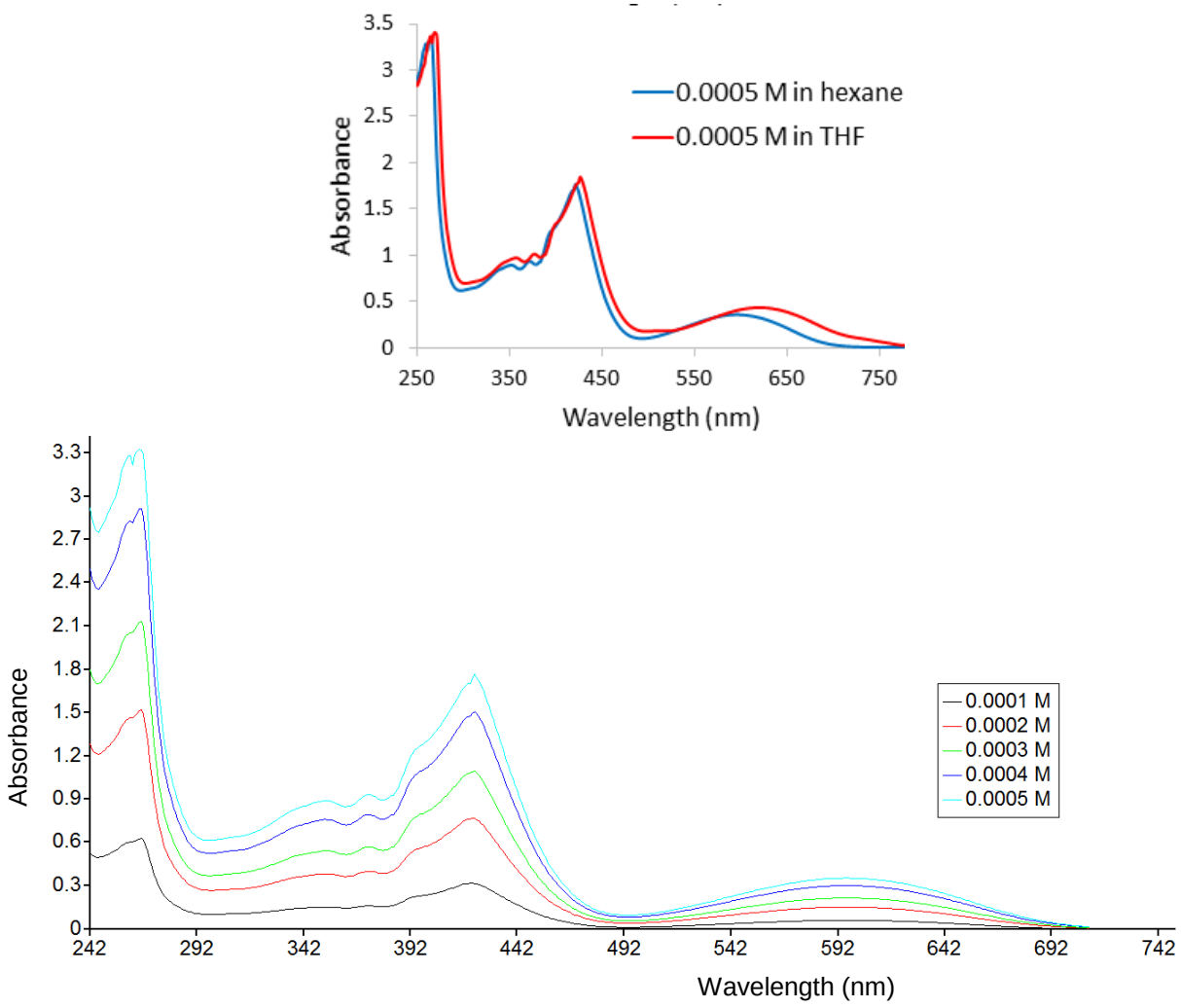


Figure S50: UV/Vis (d = 1 mm) of **3d** recorded in hexane and THF (0.0005 M) at room temperature (Top) and in hexane at different Concentrations spectra (Bottom).

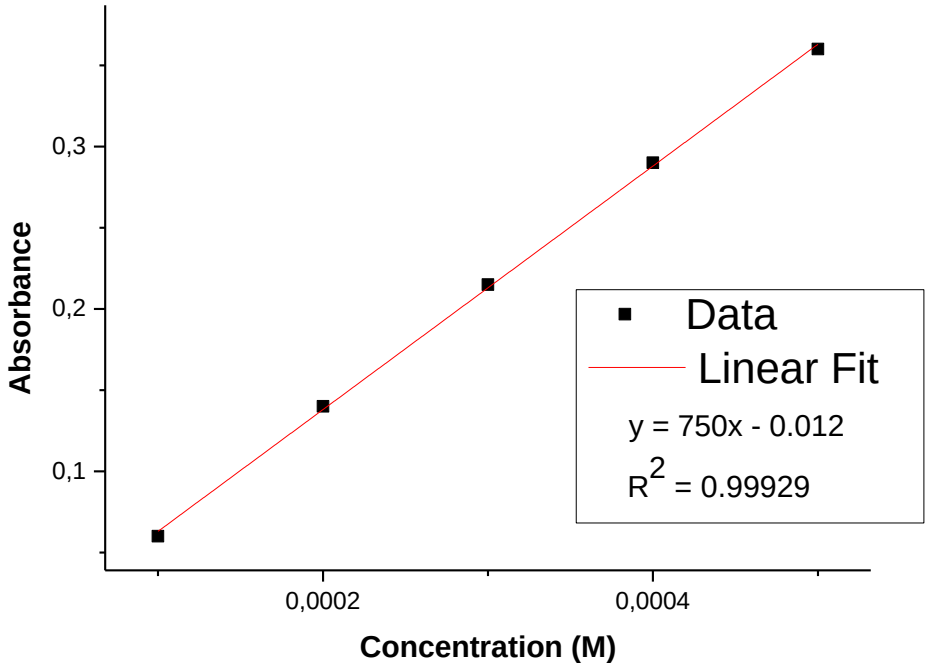


Figure S51: Linear fit for UV/Vis data of **3d** (λ = 597 nm).

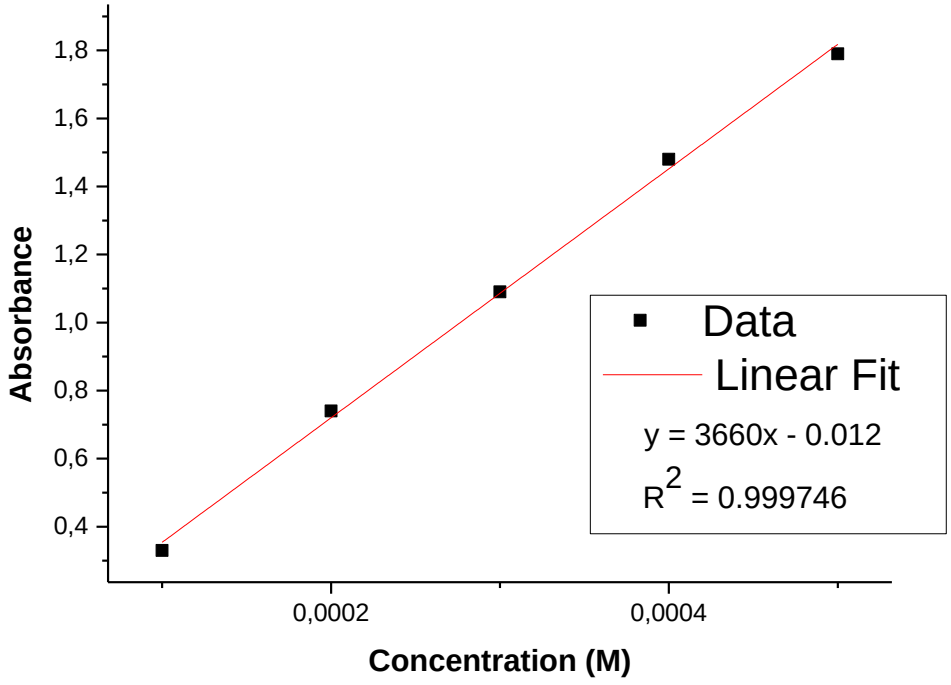


Figure S52: Linear fit for UV/Vis data of **3d** (λ = 422 nm).

3. Fluorescence spectra

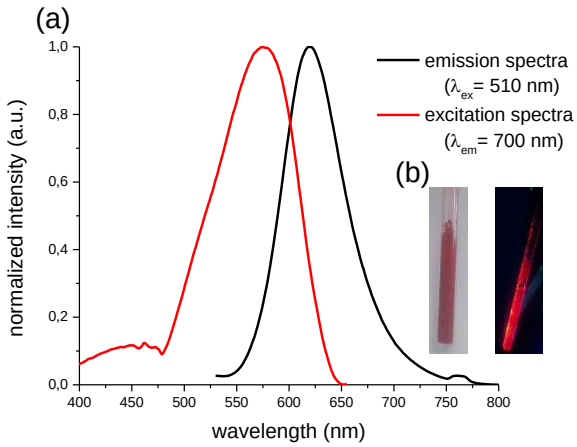


Figure S53: (a) Excitation and emission spectra of **3b** in solid state at room temperature, (b) Solid-state color under room light and under 360 nm UV light of **3b** at room temperature.

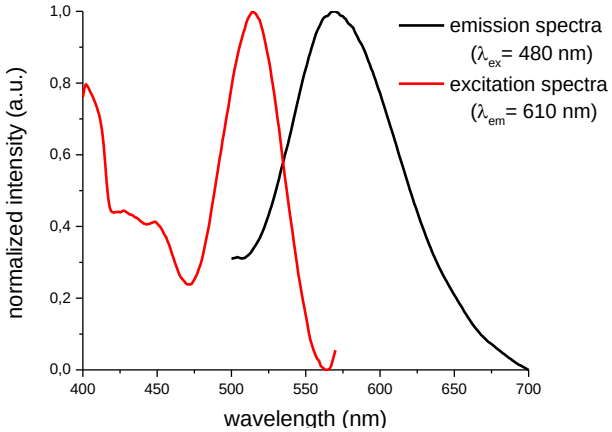


Figure S54: Excitation and emission spectra of **3b** in hexane at room temperature.

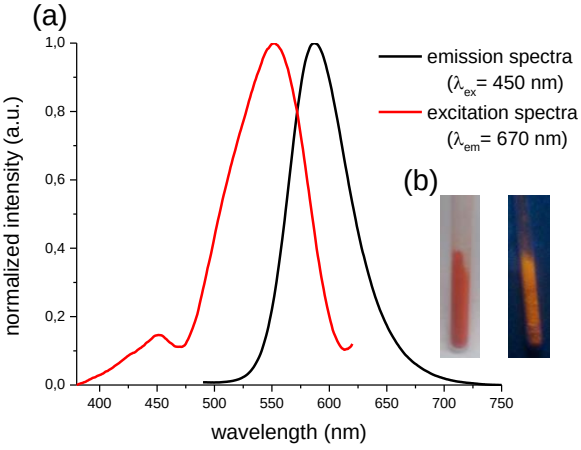


Figure S55: (a) Excitation and emission spectra of **3c** in solid state at room temperature, (b) Solid-state color under room light and under 360 nm UV light of **3c** at room temperature.

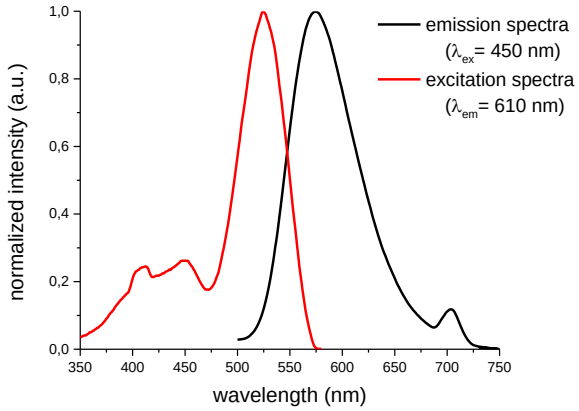


Figure S56: Excitation and emission spectra of **3b** in hexane at room temperature.

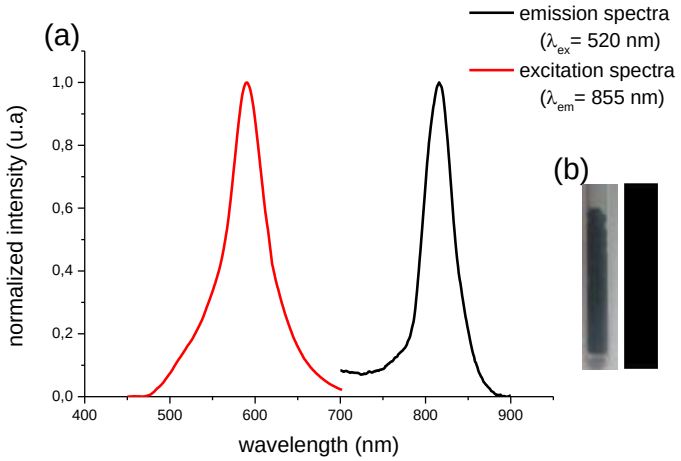


Figure S57: (a) Excitation and emission spectra of **3d** in solid state at room temperature, (b) Solid-state color under room light and under 360 nm UV light of **3d** at room temperature.

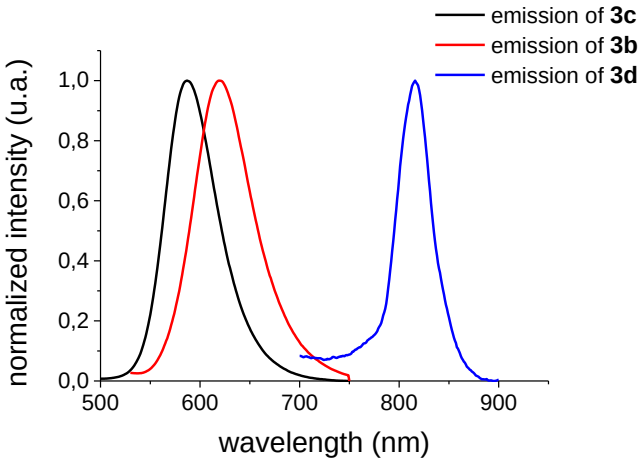


Figure S58: Emission spectra of **3b, 3c,** and **3d** in solid state at room temperature.

4. X-ray data

The X-ray crystal structure of 2a

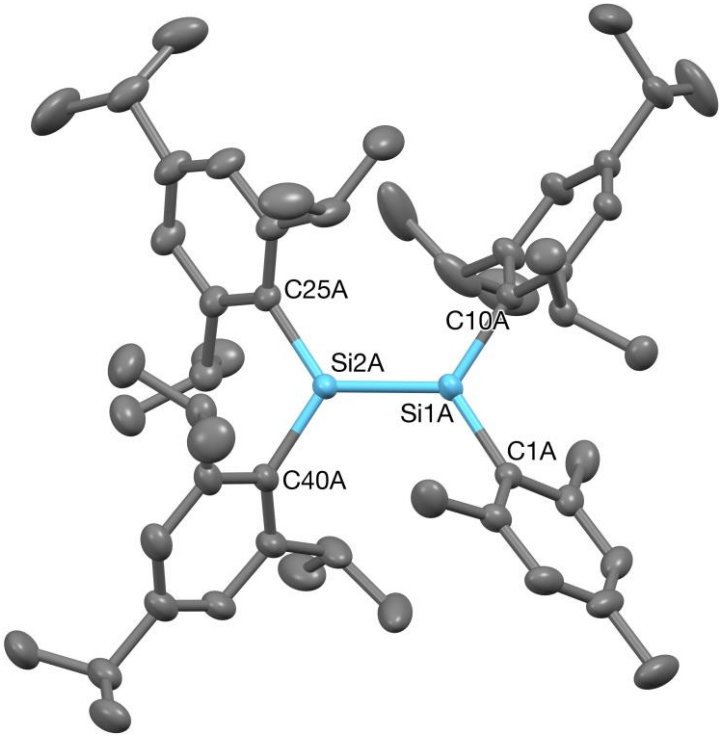


Figure S59: The crystal structure of one (**1-A**) of the two independent molecules present in the crystal of **2a** (50% probability ellipsoids).

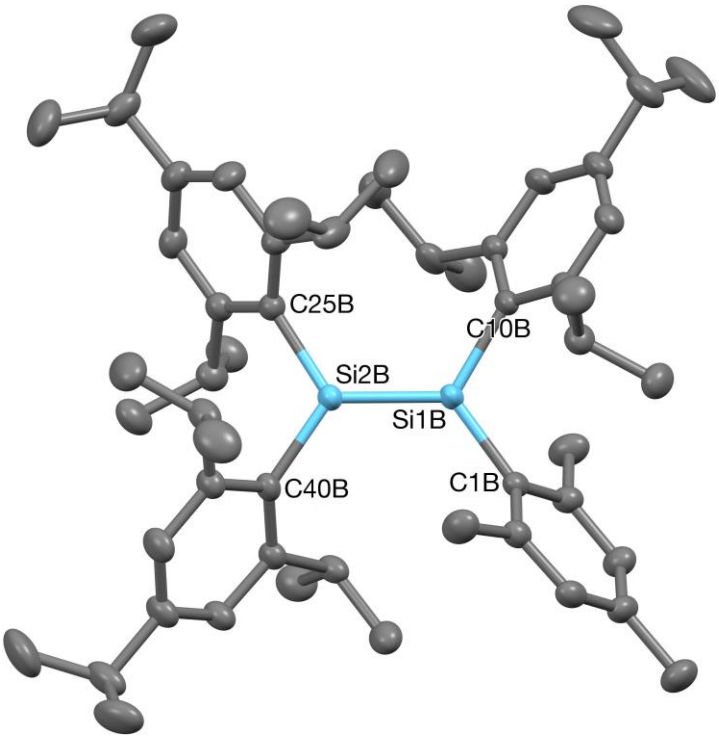


Figure S60: The crystal structure of one (**1-B**) of the two independent molecules present in the crystal of **2a** (50% probability ellipsoids).

Crystal data for **2a**: $C_{54}H_{80}Si_2$, M = 785.36, triclinic, P-1 (no. 2), a = 14.5604(3), b = 18.2609(4), c = 19.9406(4) Å, α = 98.3330(17), β = 102.4825(18), γ = 91.8560(17)°, V = 5110.79(19) Å^3, Z = 4 (2 independent molecules), D_c = 1.021 g cm^{-3}, μ(Mo-Kα) = 0.101 mm^{-1}, T = 173 K, yellow blocks, Oxford Diffraction Xcalibur 3 diffractometer; 33378 independent measured reflections (R_{int} = 0.0179), F^2 refinement,[X1] R_1(obs) = 0.0658, wR_2(all) = 0.1874, 23950 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{max}$ = 66°], 1028 parameters. CCDC 976704.

Reciprocal space analysis of the data set for the structure of **1** clearly showed the crystal to be twinned. Despite numerous attempts, modelling this twinning at the data processing stage gave unsatisfactory results, and so the data was processed without any twin modelling. However, signs of the unresolved twinning are evident in the final ΔF map, with one residual electron density peak (Q1) significantly larger than the rest at 2.24 eÅ^{-3} (the next four are 1.20, 0.84, 0.80 and 0.73 eÅ^{-3}). This peak sits in relatively empty space, its closest approach being *ca*. 1.84 Å to the methine hydrogen of the C37-based isopropyl group. This site is *ca*. 2.69 Å away from Si2B, and the Si2B···Q1 vector is almost orthogonal to the Si1B–Si2B bond, the Si1B–Si2B···Q1 angle being *ca*. 88.7°. Since there seems no sensible chemical explanation for this peak, it is most likely that it is an artefact of the unresolved twinning.

The structure was found to contain two crystallographically independent molecules, **1-A** and **1-B**. The C34-based isopropyl unit in molecule **1-A** was found to be disordered. Two orientations were identified of *ca*. 81 and 19% occupancy, their geometries were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically).

The X-ray crystal structure of 2b

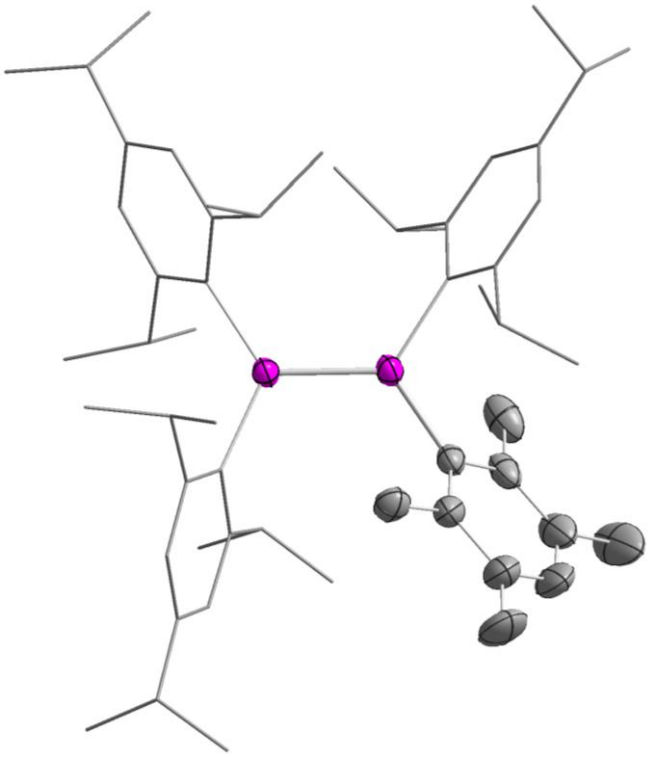


Figure S61: Solid state molecular structure of **2b** (50% probability ellipsoids), H atoms and disordered *i*Pr groups are omitted for clarity). Selected bond lengths [Å]: Si1-Si2 2.1516(7), Si1-C1 1.8825(19).

Table S1: Crystal data and structure refinement for **2b.**

CCDC	1529968	
Empirical formula	C_{55} H_{82} Si_2 x 0.5 C_6 H_{14}	
Formula weight	842.47	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.8482(9) Å	α= 109.835(4)°.
	b = 13.2841(12) Å	β= 101.906(4)°.
	c = 17.9857(14) Å	γ = 97.497(4)°.
Volume	2757.7(4) $Å^3$	
Z	2	
Density (calculated)	1.015 Mg/m^3	
Absorption coefficient	0.097 mm^{-1}	
F(000)	930	
Crystal size	0.489 x 0.308 x 0.128 mm^3	
Theta range for data collection	1.250 to 28.122°.	
Index ranges	-16<=h<=16, -17<=k<=17, -23<=l<=23	
Reflections collected	50119	
Independent reflections	13225 [R(int) = 0.0382]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7087	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13225 / 163 / 594	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0553, wR2 = 0.1364	
R indices (all data)	R1 = 0.0888, wR2 = 0.1545	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.427 and -0.340 e.$Å^{-3}$	

The X-ray crystal structure of 2c

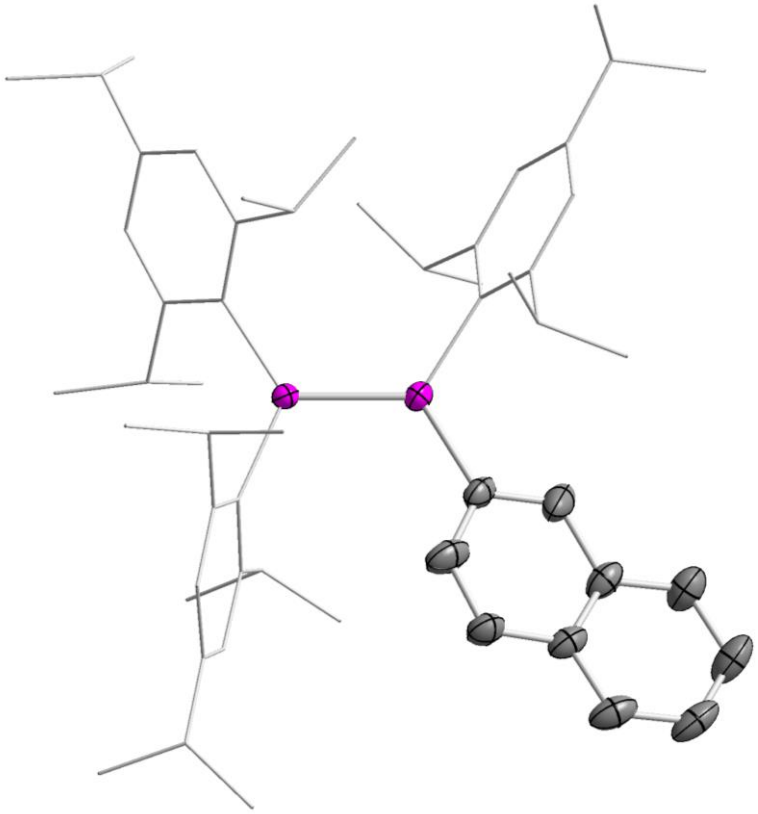


Figure S62: Solid state molecular structure of **2c** (50% probability ellipsoids) H atoms and disordered *i*Pr groups are omitted for clarity). Selected bond lengths [Å]: Si1-Si2 2.1525(6), Si1-C1 1.8700(18).

Table S2: Crystal data and structure refinement for **2c.**

CCDC	1529974	
Empirical formula	C_{55} H_{76} S_{i2}	
Formula weight	793.33	
Temperature	152(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.7724(7) Å	α= 88.036(3)°.
	b = 13.4029(8) Å	β= 89.589(3)°.
	c = 16.1636(10) Å	γ = 76.942(3)°.
Volume	2483.0(3) $Å^3$	
Z	2	
Density (calculated)	1.061 Mg/m^3	
Absorption coefficient	0.105 mm^{-1}	
F(000)	868	
Crystal size	0.253 x 0.203 x 0.203 mm^3	
Theta range for data collection	1.261 to 27.582°.	
Index ranges	-15<=h<=15, -17<=k<=17, -21<=l<=19	
Reflections collected	42683	
Independent reflections	11462 [R(int) = 0.0217]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7006	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11462 / 204 / 572	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.1392	
R indices (all data)	R1 = 0.0670, wR2 = 0.1506	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.086 and -0.287 $e.Å^{-3}$	

The X-ray crystal structure of 2d

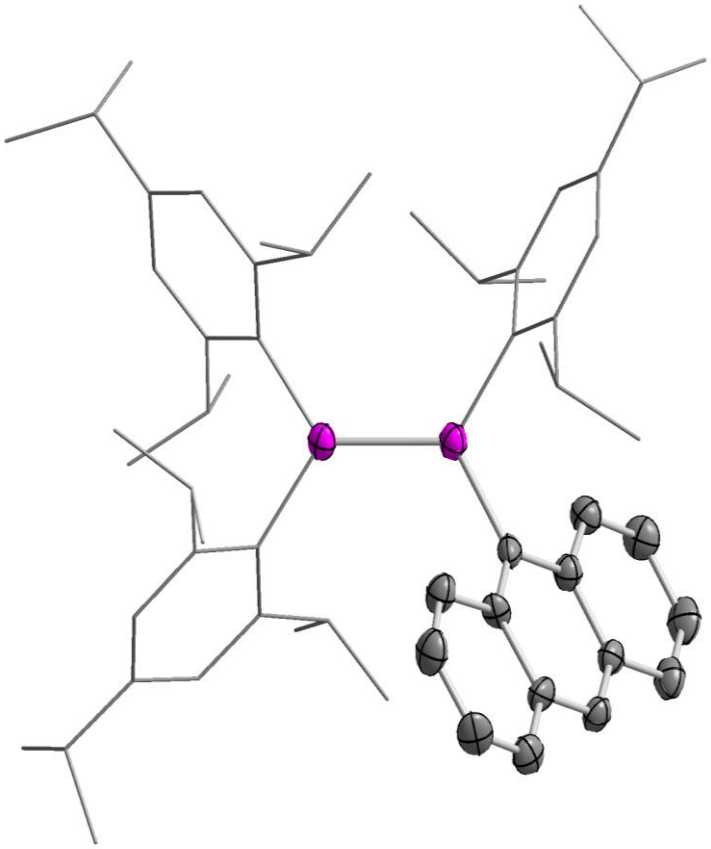


Figure S63: Solid state molecular structure of **2d** (50% probability ellipsoids).

Table S3: Crystal data and structure refinement for **2d.**

CCDC	1529972	
Empirical formula	C_{59} H_{78} Si_2 x 0.5(C_5 H_{12}) x 0.25(C_6 H_6)	
Formula weight	898.99 g/mol	
Temperature	122(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.5999(9) Å	α= 95.878(3)°.
	b = 19.1502(11) Å	β= 101.103(3)°.
	c = 20.8629(13) Å	γ = 96.251(3)°.
Volume	5644.2(6) $Å^3$	
Z	4	
Density (calculated)	1.058 Mg/m^3	
Absorption coefficient	0.099 mm^{-1}	
F(000)	1966	
Crystal size	0.539 x 0.220 x 0.092 mm^3	
Theta range for data collection	1.003 to 26.555°.	
Index ranges	-18<=h<=18, -23<=k<=23, -24<=l<=26	
Reflections collected	66625	
Independent reflections	21894 [R(int) = 0.1047]	
Completeness to theta = 25.242°	95.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6219	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	21894 / 976 / 1183	
Goodness-of-fit on F^2	1.606	
Final R indices [I>2sigma(I)]	R1 = 0.2122, wR2 = 0.2552	
R indices (all data)	R1 = 0.2892, wR2 = 0.2733	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.129 and -0.770 e.$Å^{-3}$	

The X-ray crystal structure of 3a

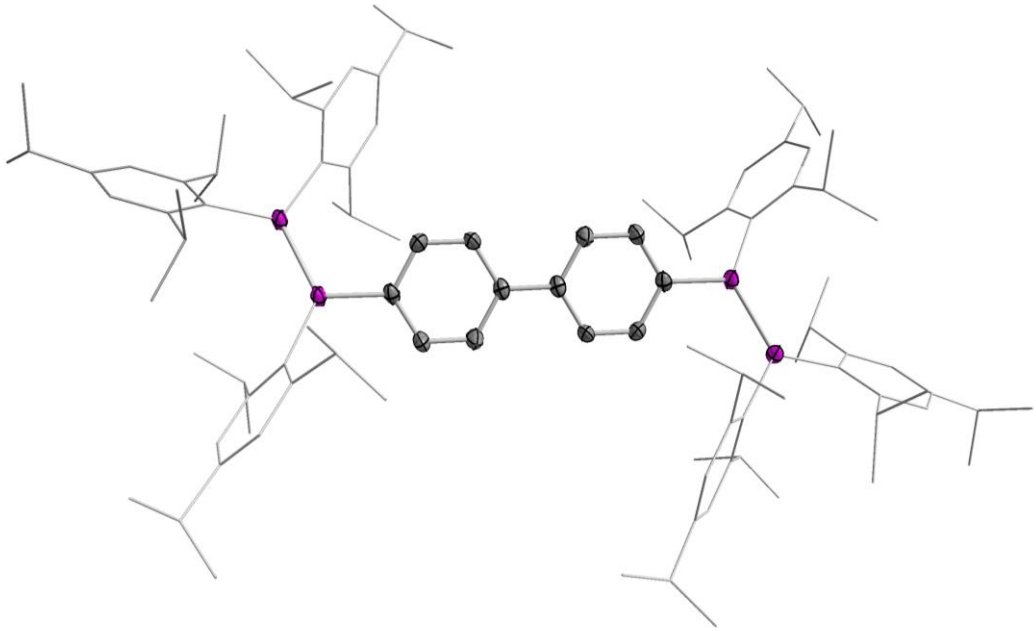


Figure S64: Solid state molecular structure of **3a** (50% probability ellipsoids), H atoms and disordered *i*Pr groups are omitted for clarity). Selected bond lengths [Å]: Si1-Si2 2.1460(8), Si1-C1 1.855(2).

Table S4: Crystal data and structure refinement for **3a.**

CCDC	1529970	
Empirical formula	C_{102} H_{146} Si_4	
Formula weight	1484.54	
Temperature	122(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 37.053(5) Å	α= 90°.
	b = 18.096(2) Å	β= 111.333(7)°.
	c = 15.4097(18) Å	γ = 90°.
Volume	9625(2) $Å^3$	
Z	4	
Density (calculated)	1.025 Mg/m^3	
Absorption coefficient	0.104 mm^{-1}	
F(000)	3256	
Crystal size	0.671 x 0.231 x 0.066 mm^3	
Theta range for data collection	1.180 to 27.150°.	
Index ranges	-46<=h<=47, -23<=k<=23, -19<=l<=14	
Reflections collected	73251	
Independent reflections	10663 [R(int) = 0.0848]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6793	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10663 / 0 / 770	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0521, wR2 = 0.1053	
R indices (all data)	R1 = 0.1098, wR2 = 0.1278	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.375 and -0.358 $e.Å^{-3}$	

The X-ray crystal structure of 3b

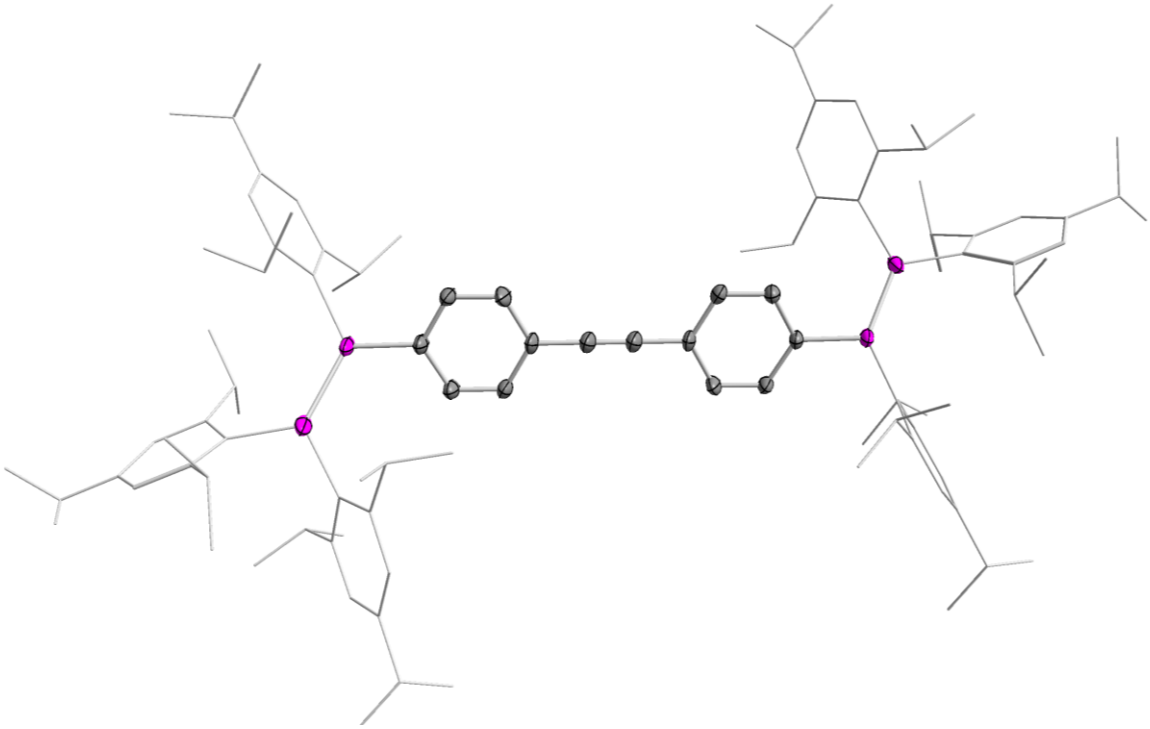


Figure S65: Solid state molecular structure of **3b** (50% probability ellipsoids), H atoms and disordered *i*Pr groups are omitted for clarity). Selected bond lengths [Å]: Si1-Si2 2.1530(8), Si1-C1 1.8587(18).

Table S5: Crystal data and structure refinement for **3b.**

CCDC	1529971	
Empirical formula	C_{104} H_{146} Si_4 x 4(C_6 H_6)	
Formula weight	1820.99	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.0556(12) Å	α= 76.026(4)°.
	b = 13.8116(15) Å	β= 80.911(4)°.
	c = 20.163(2) Å	γ = 72.584(3)°.
Volume	2838.5(5) $Å^3$	
Z	1	
Density (calculated)	1.065 Mg/m^3	
Absorption coefficient	0.099 mm^{-1}	
F(000)	994	
Crystal size	0.428 x 0.369 x 0.080 mm^3	
Theta range for data collection	1.045 to 26.462°.	
Index ranges	-13<=h<=13, -15<=k<=17, -25<=l<=24	
Reflections collected	39573	
Independent reflections	11469 [R(int) = 0.0344]	
Completeness to theta = 25.242°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6675	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11469 / 709 / 961	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0524, wR2 = 0.1197	
R indices (all data)	R1 = 0.0850, wR2 = 0.1391	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.382 and -0.357 e.$Å^{-3}$	

The X-ray crystal structure of 3c

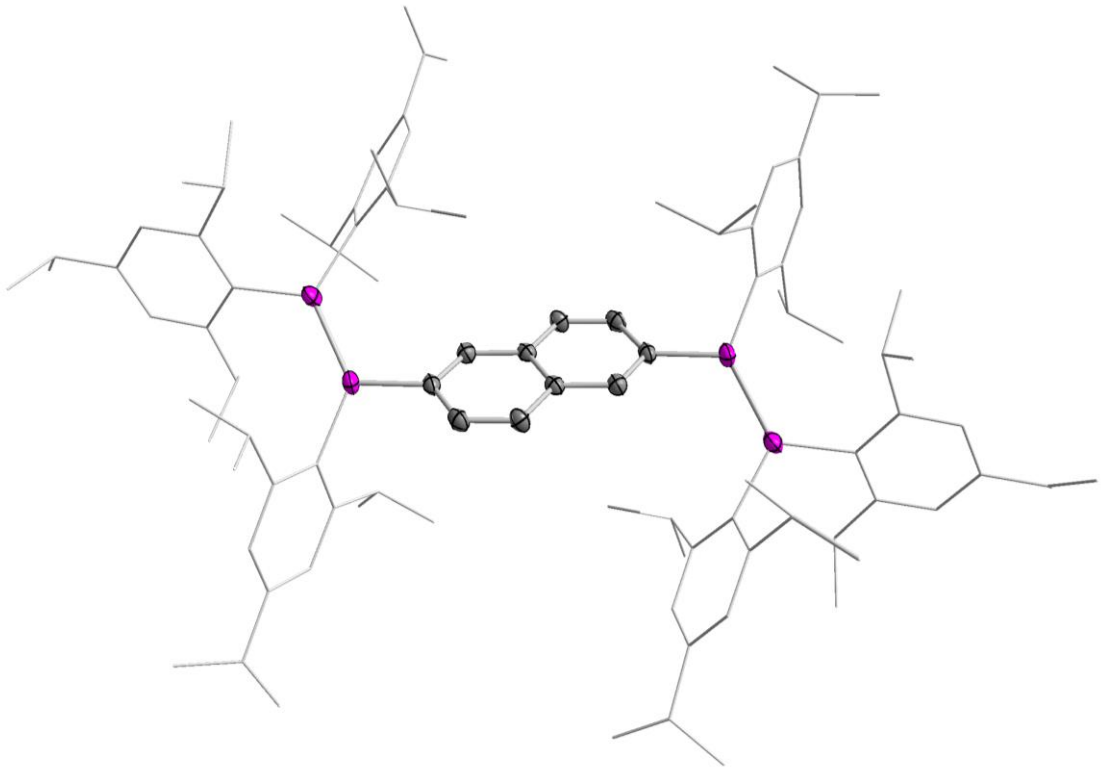


Figure S66: Solid state molecular structure of **3c** (50% probability ellipsoids), H atoms and disordered *i*Pr groups are omitted for clarity). Selected bond lengths [Å]: Si1-Si2 2.1622(6), Si1-C1 1.8547(19).

Table S6: Crystal data and structure refinement for **3c.**

CCDC	1529969	
Empirical formula	C_{100} H_{144} Si_4 x 0.5(C_{18} H_{18}) x 2(C_6 H_6)	
Formula weight	1692.83	
Temperature	122(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.4614(5) Å	α= 114.7130(10)°.
	b = 16.0181(7) Å	β= 98.7550(10)°.
	c = 18.0405(9) Å	γ = 93.023(2)°.
Volume	2691.3(2) $Å^3$	
Z	1	
Density (calculated)	1.044 Mg/m^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	926	
Crystal size	0.650 x 0.522 x 0.306 mm^3	
Theta range for data collection	1.266 to 29.661°.	
Index ranges	-14<=h<=14, -22<=k<=22, -25<=l<=25	
Reflections collected	56249	
Independent reflections	15141 [R(int) = 0.0288]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7459 and 0.7068	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15141 / 638 / 691	
Goodness-of-fit on F^2	1.254	
Final R indices [I>2sigma(I)]	R1 = 0.0623, wR2 = 0.1567	
R indices (all data)	R1 = 0.0844, wR2 = 0.1684	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.384 and -0.359 e.$Å^{-3}$	

The X-ray crystal structure of 3d

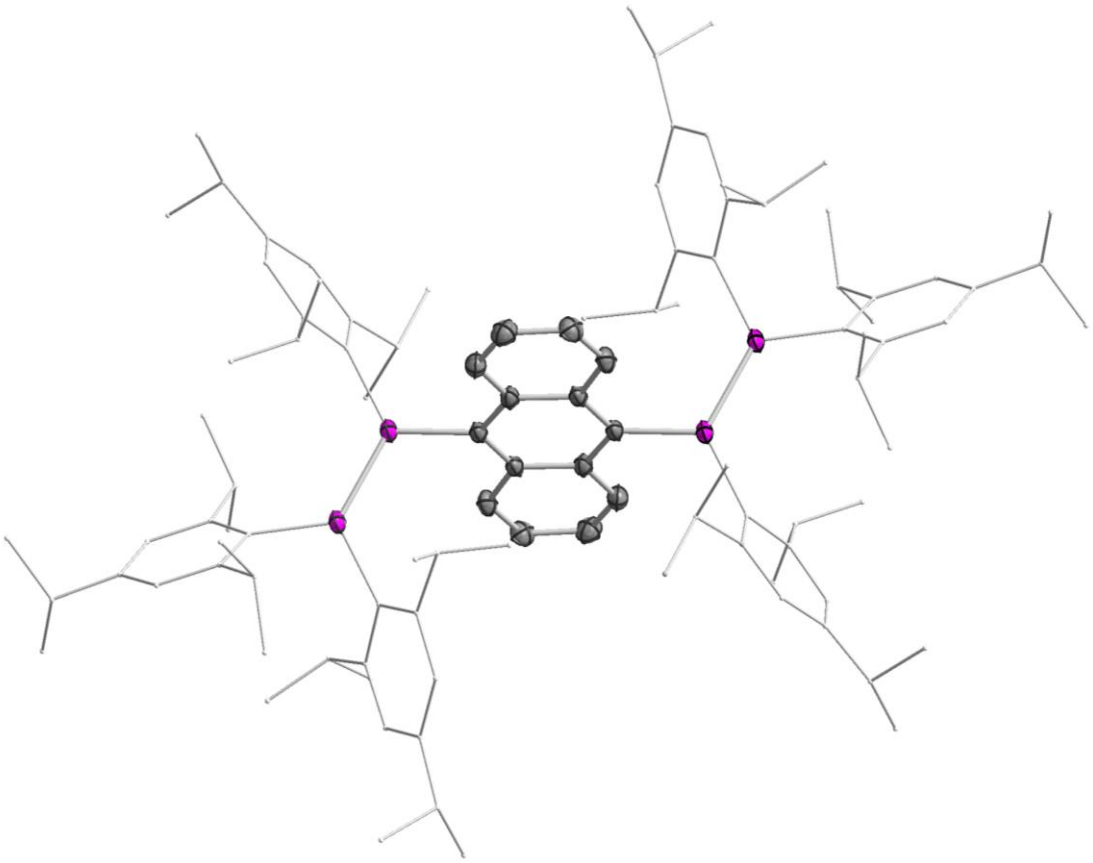
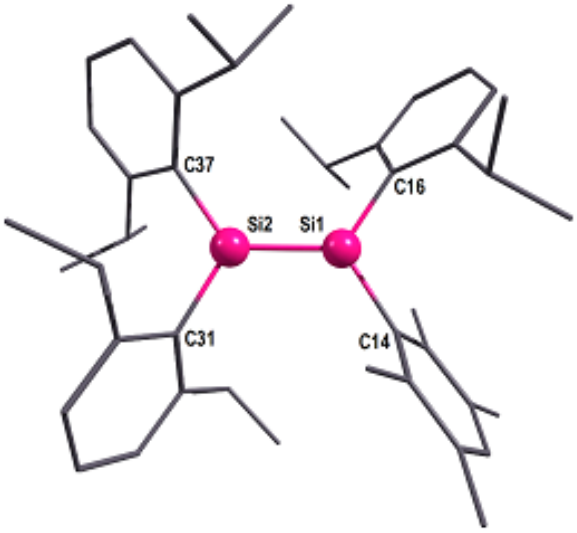


Figure S67: Solid state molecular structure of **3d** (50% probability ellipsoids), H atoms and disordered *i*Pr groups are omitted for clarity). Selected bond lengths [Å]: Si1-Si2 2.1483 (8), Si1-C1 1.899(2).

Table S7: Crystal data and structure refinement for **3d.**

CCDC	1529973	
Empirical formula	C_{104} H_{146} Si_4,C_{12} H_{12},3(C_1 H_4),2()n,2(H_1)	
Formula weight	1703.83	
Temperature	192(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.9487(6) Å	α= 83.163(3)°.
	b = 12.7883(8) Å	β= 77.072(3)°.
	c = 21.4719(14) Å	γ = 65.079(3)°.
Volume	2656.3(3) $Å^3$	
Z	1	
Density (calculated)	1.065 Mg/m^3	
Absorption coefficient	0.102 mm^{-1}	
F(000)	931	
Crystal size	0.525 x 0.115 x 0.102 mm^3	
Theta range for data collection	0.973 to 27.174°.	
Index ranges	-14<=h<=14, -16<=k<=16, -27<=l<=27	
Reflections collected	38197	
Independent reflections	11426 [R(int) = 0.0529]	
Completeness to theta = 25.242°	98.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6215	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11426 / 216 / 628	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0595, wR2 = 0.1467	
R indices (all data)	R1 = 0.1008, wR2 = 0.1665	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.614 and -0.510 $e.Å^{-3}$	

6. DFT calculations



Bond lengths (Pm):	
Si1-Si2	216.75(5)
Si1-C14	190.70(8)
Si1-C16	190.99(1)
Si2-C31	191.67(4)
Si2-C37	191.55(6)

Bond Angles (°):	
Si2-Si1-C14	121.46(4)
Si2-Si1-C16	124.67(5)
Si1-Si2-C31	120.89(3)
Si1-Si2-C37	123.77(0)
Σ°(Si1)	359.95(5)
Σ°(Si2)	360.0(0)
θ(Si1)	1.97(1)
θ(Si2)	0.25(9)
τ	2.37(8)

Deviation from planarity (°):	
(Si1-Si2)-Duryl	59.26(6)

Figure S68: Optimized structure of **2bDip** including selected bond distances and bond angles.

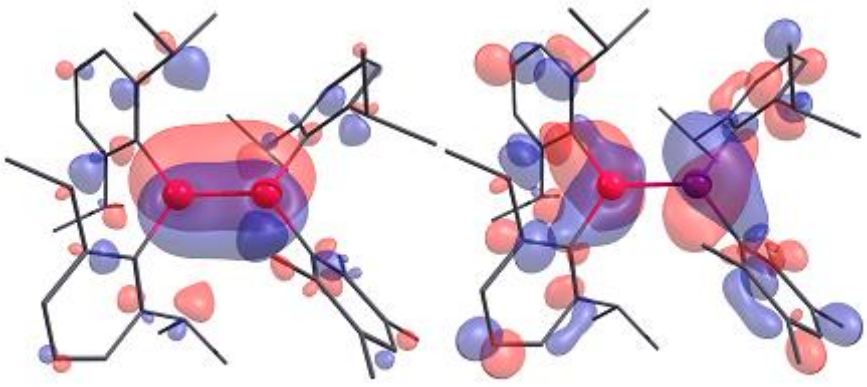


Figure S69: Selected Frontier orbitals of **2bDip**.

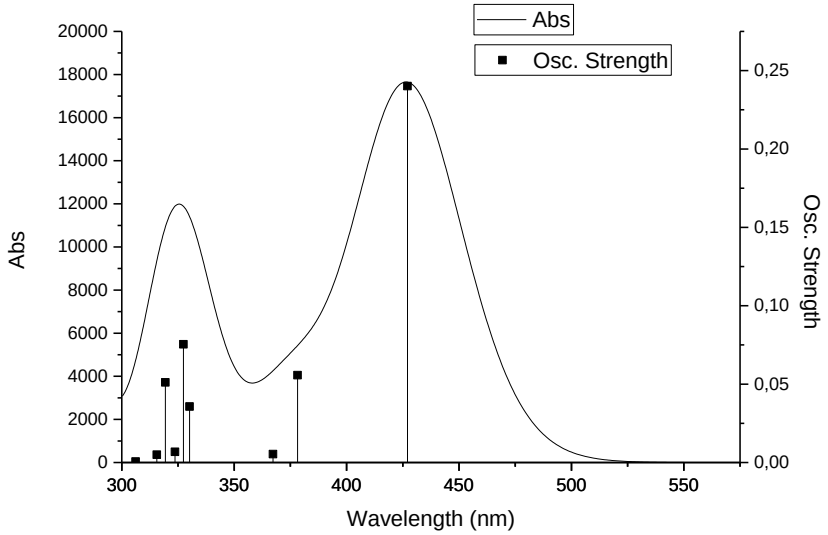
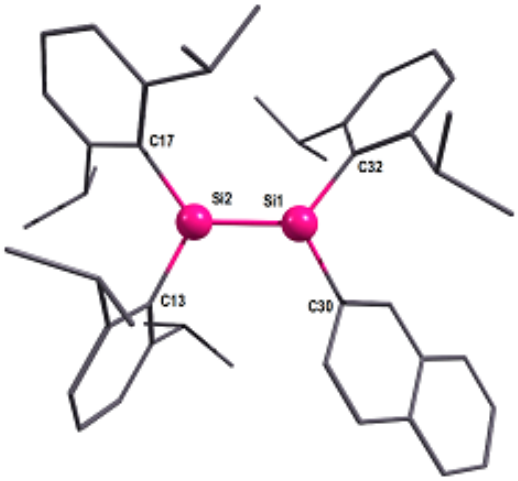


Figure S70: Calculated transitions (vertical bars) and simulated UV–vis absorption spectrum of **2bDip**.

Table S8: Selected electronic transitions and optical parameters of the theoretical calculations of **2bDip.**

Transition No.	$\lambda_{calc.\ max}$ (nm)	Transition energy (eV)	Transitions	*f c*	Contribution (%)
1	4 2 7.0 8	2.90	H→L	0.2401	90
2	378.02	3.27	H→L+1	0.0557	99
5	327.42	3.78	H→L+4	0.0754	91



Bond lengths (Pm):	
Si1-Si2	217.87(5)
Si1-C30	187.9(4)
Si1-C32	190.0(6)
Si2-C13	191.4(8)
Si2-C17	191.7(3)

Bond Angles (°):	
Si2-Si1-C30	119.61(3)
Si2-Si1-C32	126.73(9)
Si1-Si2-C13	116.79(4)
Si1-Si2-C17	125.56(6)
Σ°(Si1)	358.59(5)
Σ°(Si2)	357.91(9)
θ(Si1)	10,956
θ(Si2)	13,767
τ	3,013

Deviation from planarity (°):	
(Si1-Si2)-Naphthyl	42.46(0)

Figure S71: Optimized structure of **2cDip** including selected bond distances and bond angles.

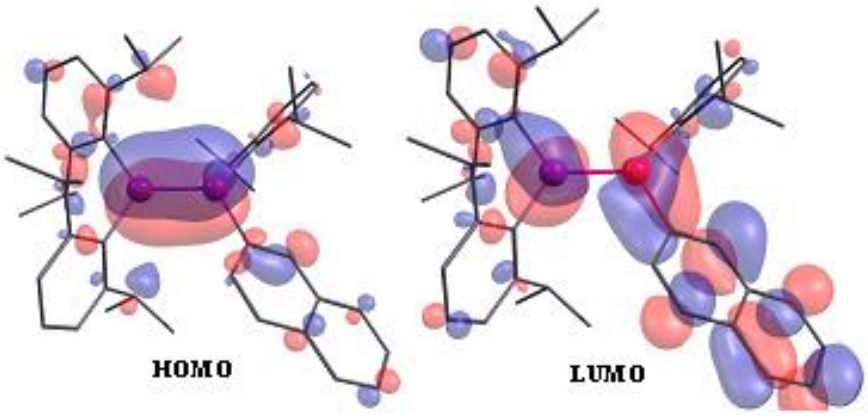


Figure S72: Selected Frontier orbitals of **2cDip.**

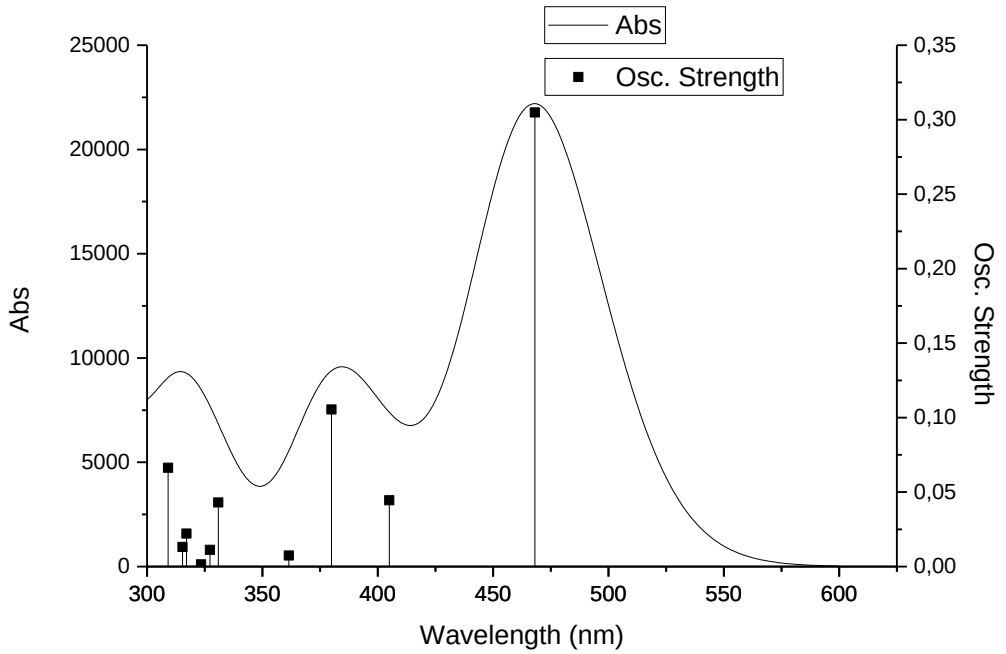
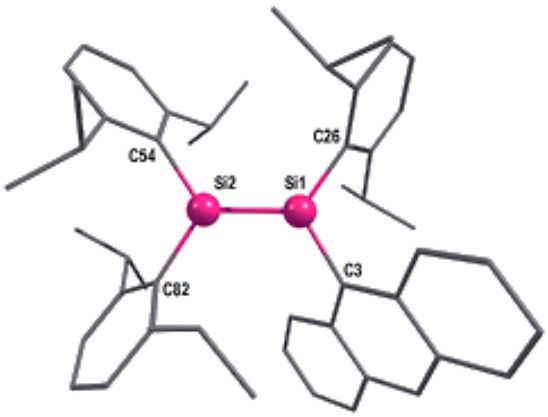


Figure S73: Calculated transitions (vertical bars) and simulated UV–vis absorption spectrum of **2cDip.**

Table S9: Selected electronic transitions and optical parameters of the theoretical calculations of **2cDip.**

Transition No.	$\lambda_{calc.\ max}$ (nm)	Transition energy (eV)	Transitions	f c	Contribution (%)
1	468.11	2.64	H→L	0.3048	93
2	404.97	3.06	H→L+1	0.0445	87
3	379.95	3.27	H→L+2	0.1054	87



Bond lengths (Pm):	Angles (°):		Deviation from planarity (°):	
216.88(8)	Si2-Si1-C3	120.42(2)	(Si1-Si2)-Anthracyl	63.70(6)
190.66(3)	Si2-Si1-C26	125.10(3)		
190.91(9)	Si1-Si2-C54	123.75(7)		
191.43(6)	Si1-Si2-C82	121.76(7)		
191.53(7)	Σ°(Si1)	359.99(6)		
	Σ°(Si2)	359.99(5)		
	θ(Si1)	1.49(9)		
	θ(Si2)	0.62(2)		
	τ	2.32(4)		

Figure S74: Optimized structure of **2dDip** including selected bond distances and bond angles.

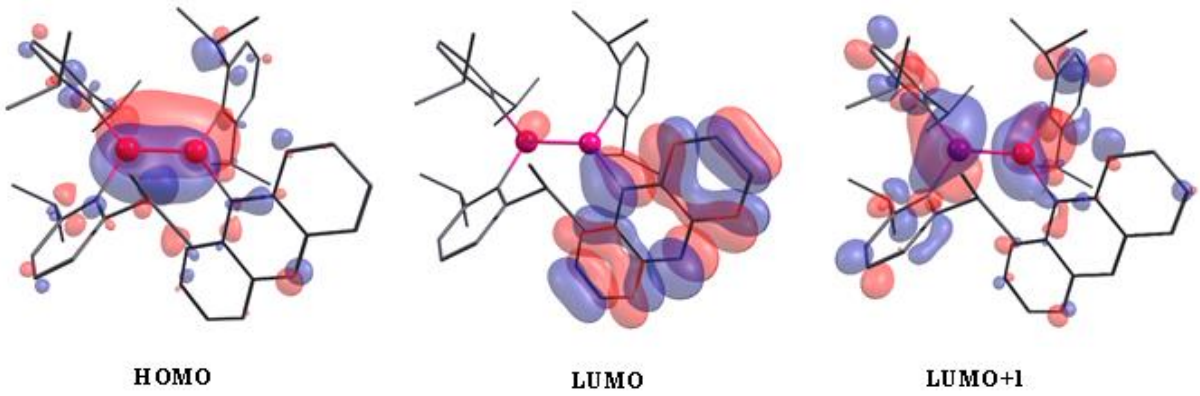


Figure S75: Selected Frontier orbitals of **2dDip.**

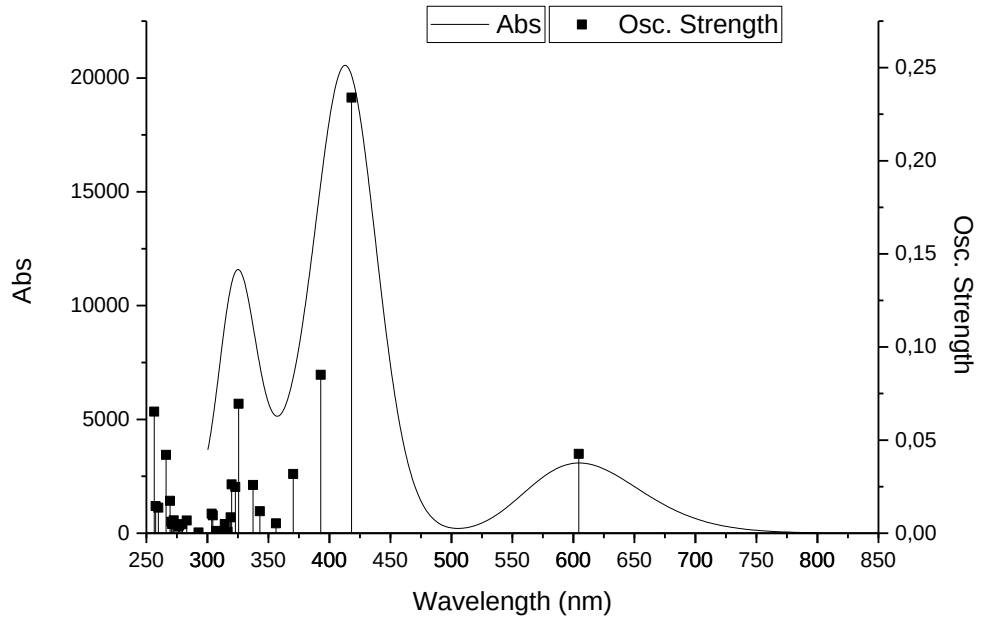
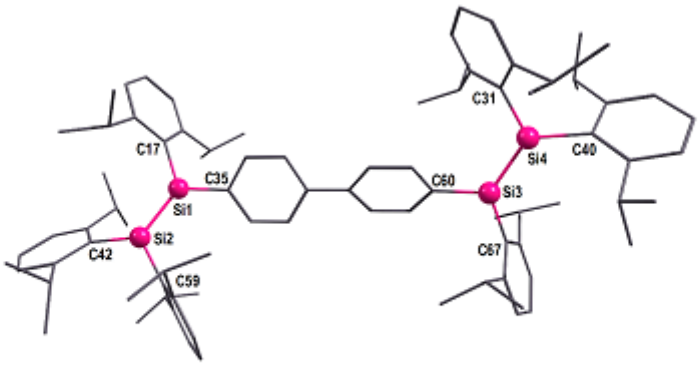


Figure S76: Calculated transitions (vertical bars) and simulated UV–vis absorption spectrum of **2dDip.**

Table S10: Selected electronic transitions and optical parameters of the theoretical calculations of **2dDip.**

Transition No.	$\lambda_{calc.\ max}$ (nm)	Transition energy (eV)	Transitions	*f c*	Contribution (%)
1	604.41	2.05	H→L	0.0426	98
2	418.10	2.96	H→L+1	0.2339	81
8	325.56	3.80	H→L+5	0.1054	70
			H→L+6		10



Bond lengths (pm):	
Si1-Si2	217.8(3)
Si1-C42	191.7(0)
Si1-C59	191.5(5)
Si2-C17	189.9(9)
Si2-C35	187.8(3)
Si3-Si4	217.3(2)
Si3-C60	187.8(4)
Si3-C67	189.9(1)
Si4-C31	191.4(4)
Si4-C40	191.6(4)

Bond angles (°):	
Si1-Si2-C17	126.86(9)
Si1-Si2-C35	119.60(0)
Si2-Si1-C42	125.83(0)
Si2-Si1-C59	116.16(5)
Si3-Si4-C31	117.24(8)
Si3-Si4-C40	125.55(3)
Si4-Si3-C60	119.54(4)
Si4-Si3-C67	127.28(2)
Σ°(Si1)	357,915
Σ°(Si2)	358,685
Σ°(Si3)	359,516
Σ°(Si4)	358,835
θ(Si1)	13,819
θ(Si2)	10,594
θ(Si3)	6,442
θ(Si4)	10,328
τ(Si1-Si2)	3,353
τ(Si3-Si4)	4,067

Deviation from planarity (°):	
(Si1-Si2)-Biphenyl	40.79(0)
Biphenyl-(Si3-Si4)	41.69(0)
(Si1-Si2)-(Si3-Si4)	34.10(2)

Figure S77: Optimized structure of **3aDip** including selected bond distances and bond angles.

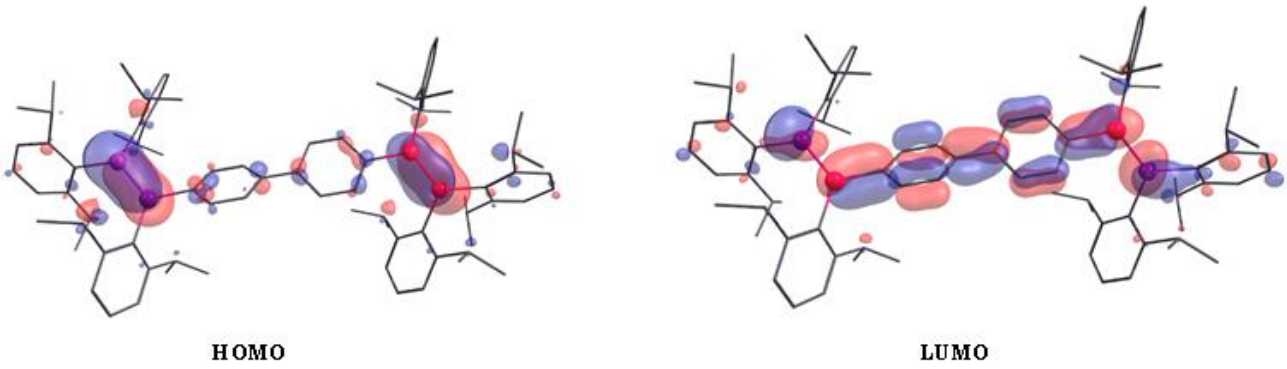


Figure S78: Selected Frontier orbitals of **3aDip**.

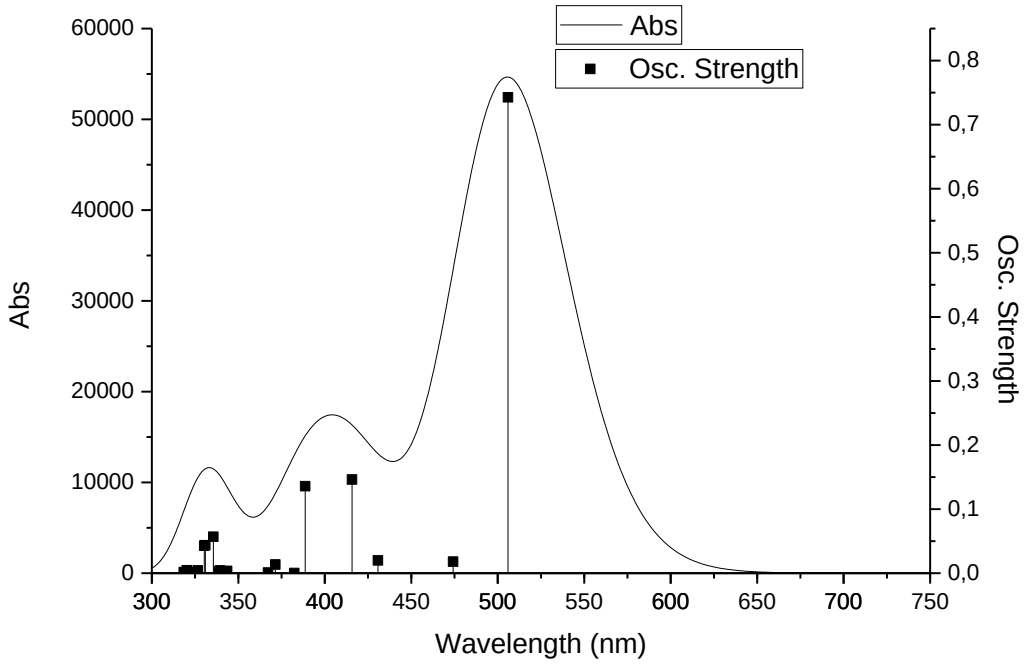
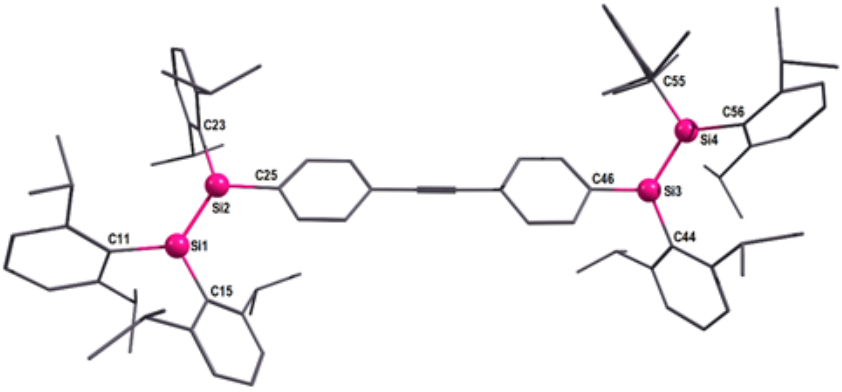


Figure S79: Calculated transitions (vertical bars) and simulated UV–vis absorption spectrum of **3aDip.**

Table S11: Selected electronic transitions and optical parameters of the theoretical calculations of **3aDip.**

Transition No.	$\lambda_{calc.\ max}$ (nm)	Transition energy (eV)	Transitions	*f c*	Contribution (%)
1	505.93	2.45	H→L	0.7427	97
4	415.77	2.98	H-1→L+1	0.1462	75
			H→L+2		14
5	388.71	3.18	H-1→L+1	0.1357	20
			H-1→L+3		13
			H→L+2		60



Bond lengths (Pm):	
Si1-Si2	217.7(3)
Si1-C11	191.6(5)
Si1-C15	191.4(1)
Si2-C23	189.9(8)
Si2-C25	187.8(2)
Si3-Si4	217.4(8)
Si3-C44	189.8(9)
Si3-C46	187.8(0)
Si4-C55	191.4(2)
Si4-C56	191.5(6)

Bond angles (°):	
Si1-Si2-C23	127.61(2)
Si1-Si2-C25	118.85(9)
Si2-Si1-C11	125.79(6)
Si2-Si1-C15	116.53(1)
Si3-Si4-C55	116.23(8)
Si3-Si4-C56	126.14(7)
Si4-Si3-C44	127.44(9)
Si4-Si3-C46	119.27(4)
Σ°(Si1)	358,209
Σ°(Si2)	359,252
Σ°(Si3)	359,410
Σ°(Si4)	358,704
θ(Si1)	12,801
θ(Si2)	9,463
θ(Si3)	7,112
θ(Si4)	10,910
τ(Si1-Si2)	3,551
τ(Si3-Si4)	4,291

Deviation from planarity (°):	
(Si1-Si2)-Diphenylacetylen	42.61(3)
Diphenylacetylen-(Si3-Si4)	38.43(8)
(Si1-Si2)-(Si3-Si4)	12.50(4)

Figure S80: Optimized structure of **3bDip** including selected bond distances and bond angles.

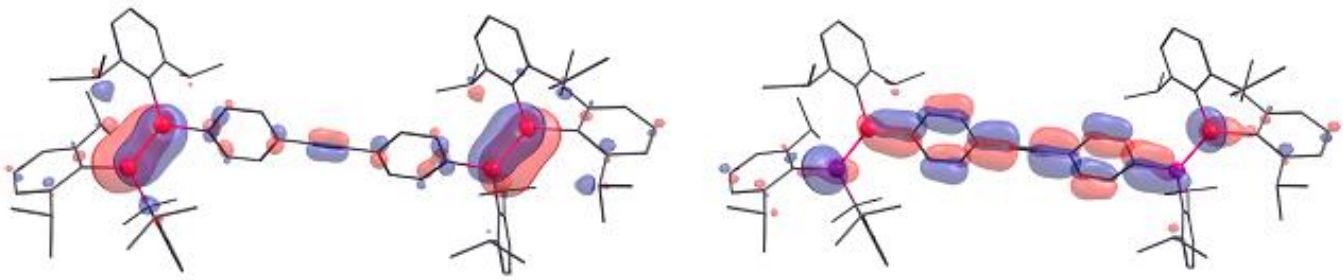


Figure S81: Selected Frontier orbitals of **3bDip.**

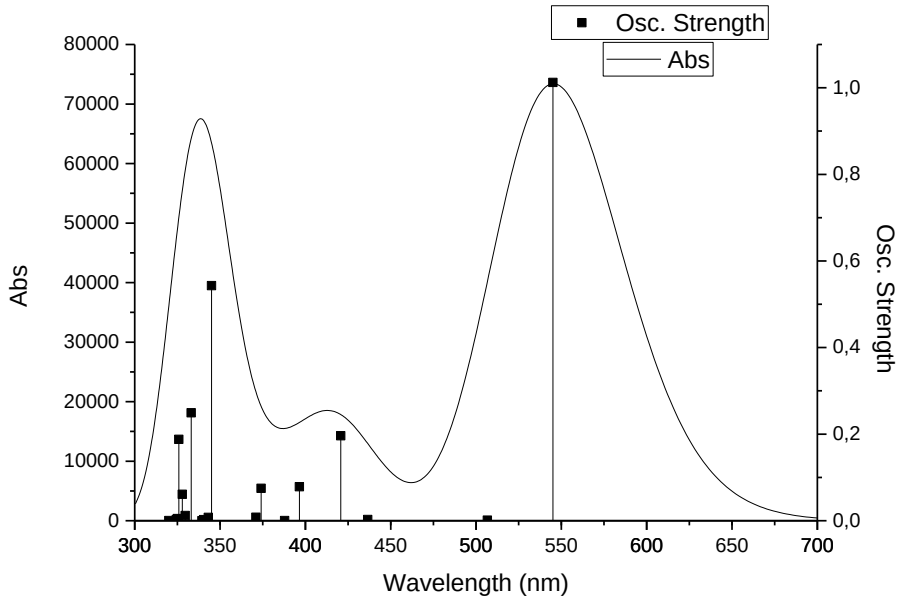
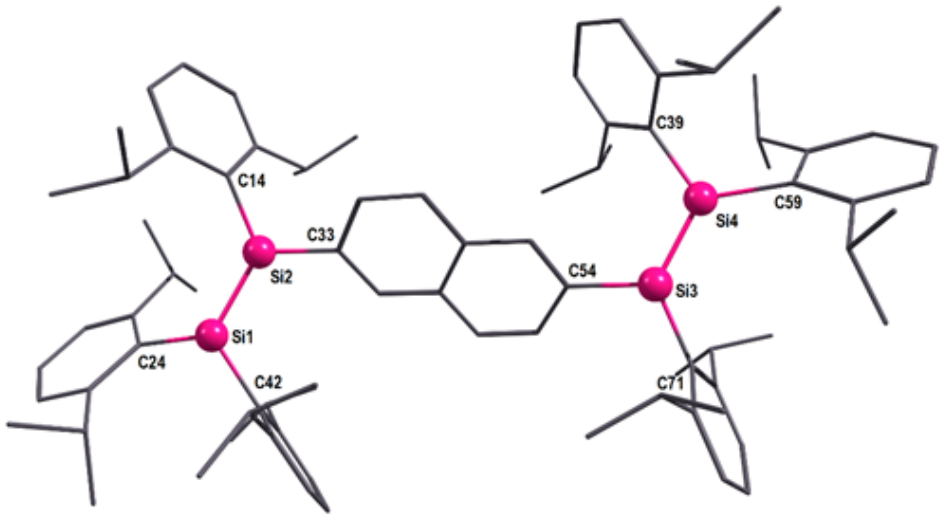


Figure S82: Calculated transitions (vertical bars) and simulated UV–vis absorption spectrum of **3bDip.**

Table S12: Selected electronic transitions and optical parameters of the theoretical calculations of **3bDip.**

Transition No.	$\lambda_{calc.\ max}$ (nm)	Transition energy (eV)	Transitions	*f c*	Contribution (%)
1	545.03	2.27	H→L	1.0124	98
4	420.77	2.94	H-1→L+1	0.1962	75
			H→L+2		13
9	345.00	3.59	H-2→L	0.5431	45
			H-1→L+5		18
			H→L+8		13



Bond lengths (Pm):	
Si1-Si2	217.9(4)
Si1-C24	191.7(1)
Si1-C42	191.5(7)
Si2-C14	190.0(7)
Si2-C33	187.9(8)
Si3-Si4	217.4(5)
Si3-C54	187.8(9)
Si3-C71	190.0(2)
Si4-C39	191.5(5)
Si4-C59	191.6(3)

Bond angles (°):	
Si1-Si2-C14	127.46(0)
Si1-Si2-C33	118.90(8)
Si2-Si1-C24	125.49(0)
Si2-Si1-C42	116.53(1)
Si3-Si4-C39	116.30(8)
Si3-Si4-C59	125.92(9)
Si4-Si3-C54	119.55(2)
Si4-Si3-C71	127.38(9)
Σ°(Si1)	357,566
Σ°(Si2)	358,413
Σ°(Si3)	359,294
Σ°(Si4)	358,485
θ(Si1)	14,899
θ(Si2)	11,615
θ(Si3)	7,756
θ(Si4)	11,804
τ(Si1-Si2)	3,295
τ(Si3-Si4)	4,249

Deviation from planarity (°):	
(Si1-Si2)-Naphthyl	46.82(4)
Naphthyl-(Si3-Si4)	39.81(1)
(Si1-Si2)-(Si3-Si4)	7.50(7)

Figure S83: Optimized structure of **3cDip** including selected bond distances and bond angles.

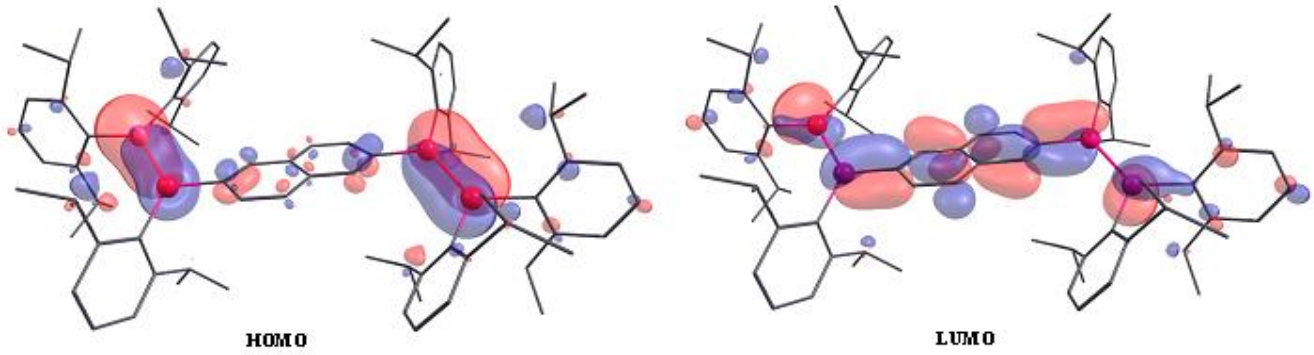


Figure S84: Selected Frontier orbitals of **3cDip**.

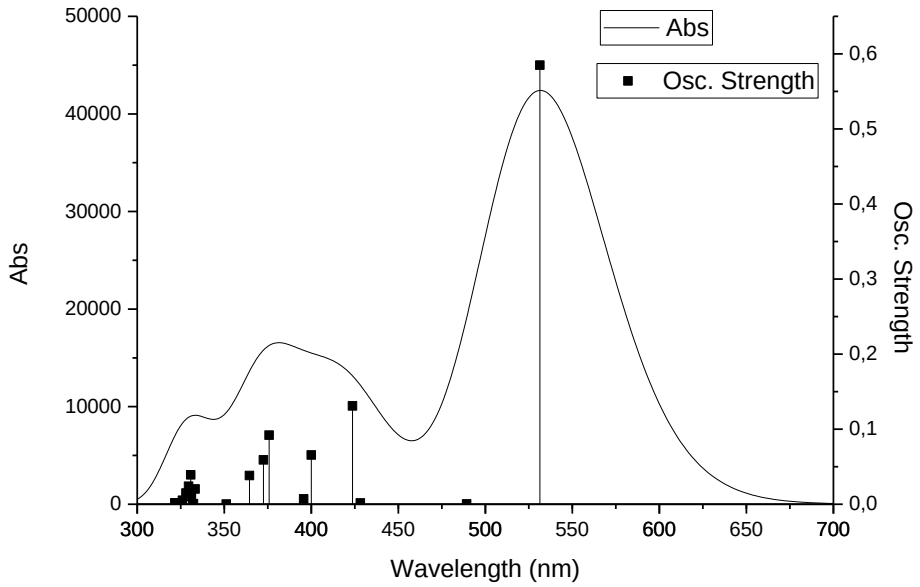
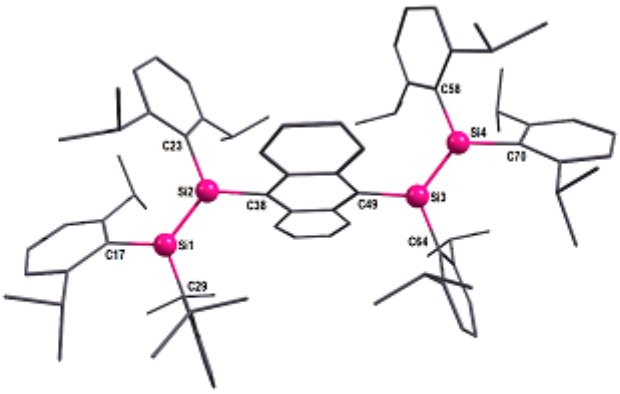


Figure S85: Calculated transitions (vertical bars) and simulated UV–vis absorption spectrum of **3cDip.**

Table S13: Selected electronic transitions and optical parameters of the theoretical calculations of **3cDip.**

Transition No.	$\lambda_{calc.\ max}$ (nm)	Transition energy (eV)	Transitions	*f c*	Contribution (%)
1	531.34	2.33	H→L	0.585	98
4	423.67	2.92	H→L+2	0.131	82



Bond lengths (Pm):	
Si1-Si2	218.2(6)
Si1-C17	192.6(4)
Si1-C29	191.2(6)
Si2-C23	191.5(2)
Si2-C38	193.2(0)
Si3-Si4	218.2(7)
Si3-C49	193.2(0)
Si3-C64	191.5(2)
Si4-C58	191.2(6)
Si4-C70	192.6(4)

Bond angles (°):	
Si1-Si2-C38	124.17(7)
Si1-Si2-C23	120.68(5)
Si2-Si1-C17	125.79(2)
Si2-Si1-C29	120.95(8)
Si3-Si4-C58	120.95(4)
Si3-Si4-C70	125.79(3)
Si4-Si3-C49	124.17(6)
Si4-Si3-C64	120.68(4)
Σ°(Si1)	359,909
Σ°(Si2)	359,993
Σ°(Si3)	359,993
Σ°(Si4)	359,908
θ(Si1)	2,819
θ(Si2)	0.800
θ(Si3)	0.788
θ(Si4)	2,830
τ(Si1-Si2)	4,970
τ(Si3-Si4)	4,971

Deviation from planarity (°):	
(Si1-Si2)-Anthracyl	65.23(6)
Anthracyl-(Si3-Si4)	65.24(1)
(Si1-Si2)-(Si3-Si4)	0.0(6)

Figure S86: Optimized structure of **3dDip** including selected bond distances and bond angles.

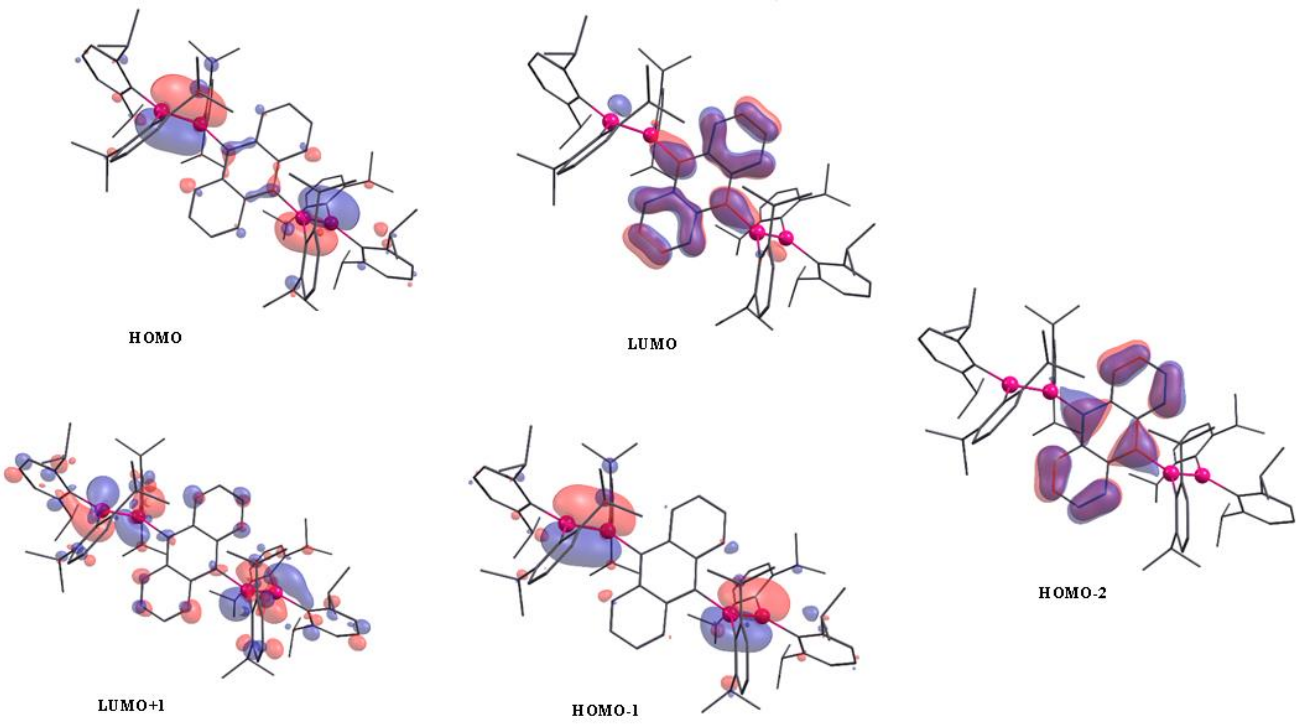


Figure S87: Selected Frontier orbitals of **3dDip.**

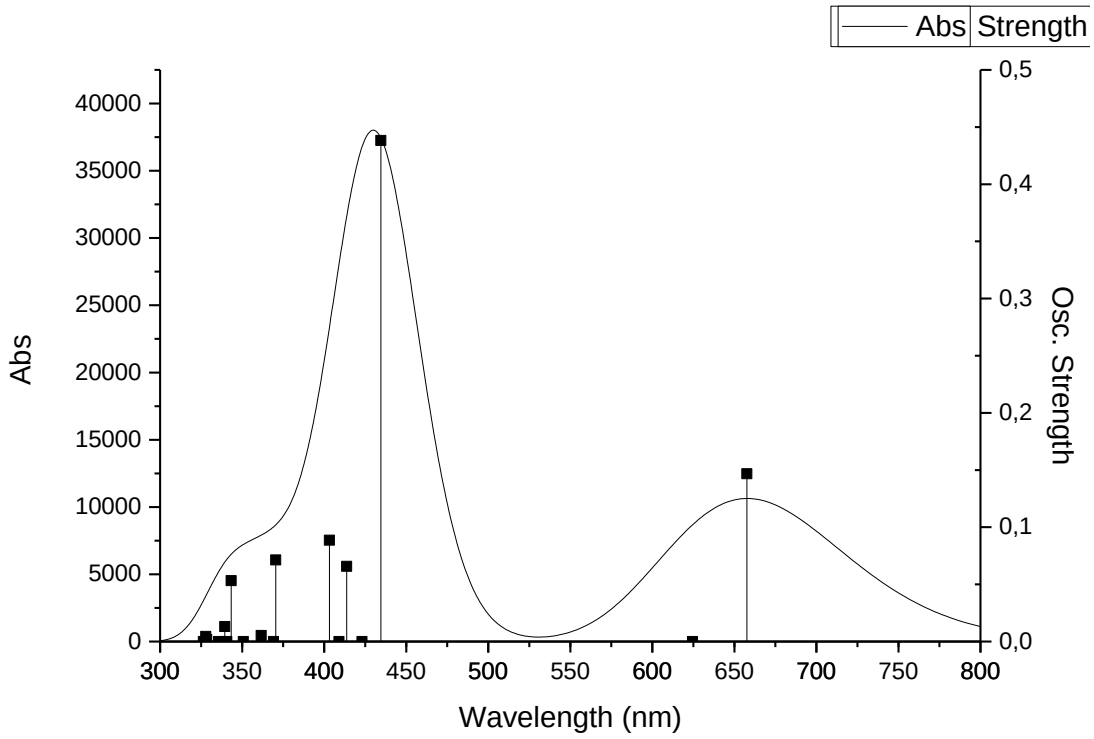


Figure S88: Calculated transitions (vertical bars) and simulated UV–vis absorption spectrum of **3dDip.**

Table S14: Selected electronic transitions and optical parameters of the theoretical calculations of **3dDip.**

Transition No.	$\lambda_{calc.\ max}$ (nm)	Transition energy (eV)	Transitions	*f c*	Contribution (%)
1	657.60	1.88	H→L	0.1468	99
2	624.57	1.98	H-1→L	0	99
3	423.67	2.85	H-2→L	0.4382	30
			H→L+1		60

Table S15: Atomic coordinates of **2bDip.**

C	3.859117000	-3.800943000	2.217357000
C	5.432105000	-2.058851000	-2.212460000
C	4.462378000	1.273080000	2.016134000
C	4.555246000	-2.840734000	0.006502000
C	3.658774000	-2.832861000	1.073674000
C	4.420461000	-1.989354000	-1.090256000
C	2.977066000	1.679681000	2.033755000
C	3.172166000	3.816624000	0.746593000
C	2.586421000	-1.915958000	1.066440000
C	3.334867000	-1.093894000	-1.123562000
C	2.610833000	2.536679000	0.822085000
C	2.880411000	4.668054000	-0.312168000
C	1.650804000	-1.932055000	2.254392000
C	2.421879000	-1.034317000	-0.035428000
C	3.166066000	-0.212146000	-2.340996000
C	1.736594000	2.084418000	-0.209006000
C	2.019447000	4.240383000	-1.315277000
C	1.440240000	2.963801000	-1.290401000
C	0.817836000	-3.689213000	-1.960603000
C	1.236118000	2.673750000	-3.814176000
C	-2.161011000	-1.860409000	3.857780000
C	-0.915303000	3.852902000	1.776962000
C	0.513989000	2.603410000	-2.453217000
C	-2.589925000	-4.669204000	0.576015000
C	-1.816563000	-4.349311000	-0.532315000
C	-2.858110000	-3.689562000	1.523716000
C	-1.310367000	-3.056977000	-0.730515000
C	-0.469790000	-2.842171000	-1.991209000
C	-1.561052000	2.469103000	1.988076000
C	-2.366262000	-2.386969000	1.376713000
C	-1.592368000	-2.041171000	0.230731000
C	-2.687849000	-1.390107000	2.488448000
C	-2.179425000	2.383947000	3.397955000
C	-0.744429000	3.492684000	-2.477168000
C	-1.259514000	-3.137733000	-3.282252000
C	-2.579233000	2.151039000	0.890832000
C	-2.458239000	1.068106000	-0.030786000
C	-4.192131000	-1.068355000	2.555713000
C	-3.691274000	3.001022000	0.809584000
C	-3.398617000	0.399287000	-3.514309000
C	-3.469776000	0.903771000	-1.021884000
C	-3.416380000	-0.186964000	-2.089807000
C	-4.682893000	2.817291000	-0.145288000
C	-4.566060000	1.773874000	-1.054663000
C	-4.556170000	-1.209210000	-1.925754000
H	4.713948000	-4.455133000	2.026713000
H	6.243603000	-2.746480000	-1.959491000
H	5.387369000	-3.541509000	0.027453000
H	5.114320000	2.151036000	2.086519000
H	4.043522000	-3.282646000	3.166451000
H	5.878280000	-1.080784000	-2.424305000
H	4.691553000	0.619591000	2.865020000
H	4.715274000	0.735571000	1.098274000
H	2.979738000	-4.436529000	2.373626000
H	4.983325000	-2.412053000	-3.149263000
H	3.842158000	4.153316000	1.532442000
H	2.205593000	-1.901492000	3.199044000
H	2.389023000	0.757857000	1.980840000
H	3.753947000	0.711100000	-2.264891000
H	3.482023000	-0.723981000	-3.254138000

H	1.047868000	-2.848322000	2.269209000
H	0.955839000	-1.091822000	2.238067000
H	2.121742000	0.079285000	-2.479754000
H	1.409252000	-3.490558000	-1.064810000
H	1.792342000	4.910679000	-2.139130000
H	2.140650000	2.059779000	-3.828355000
H	-1.088400000	-2.071796000	3.819827000
H	-0.159807000	4.043780000	2.546343000
H	0.587070000	-4.760149000	-1.986208000
H	1.440527000	-3.465300000	-2.833648000
H	1.528928000	3.699963000	-4.061541000
H	-2.669660000	-2.769371000	4.195711000
H	-0.424809000	3.924994000	0.803727000
H	-2.329210000	-1.088457000	4.616640000
H	-0.763079000	1.722326000	1.933445000
H	-1.409809000	2.547594000	4.160341000
H	-1.599947000	-5.120471000	-1.265710000
H	0.180139000	1.570221000	-2.306054000
H	0.573883000	2.321586000	-4.612747000
H	-3.453510000	-3.940678000	2.396810000
H	-1.659847000	4.654007000	1.842197000
H	-0.171326000	-1.789383000	-2.020538000
H	-0.482640000	4.546622000	-2.622545000
H	-2.163692000	-0.456062000	2.256601000
H	-1.315279000	3.409412000	-1.549584000
H	-2.636055000	1.408038000	3.583531000
H	-2.953660000	3.144723000	3.544971000
H	-1.540401000	-4.194324000	-3.349611000
H	-0.647252000	-2.905072000	-4.160499000
H	-1.401969000	3.200962000	-3.303372000
H	-4.779115000	-1.966194000	2.778582000
H	-4.396148000	-0.335595000	3.344092000
H	-2.564431000	1.094700000	-3.645941000
H	-2.177431000	-2.547598000	-3.344458000
H	-2.473105000	-0.728493000	-1.965175000
H	-3.781531000	3.824371000	1.512039000
H	-4.552273000	-0.654507000	1.609938000
H	-3.293881000	-0.401390000	-4.254571000
H	-4.323401000	0.939246000	-3.742729000
H	-4.483087000	-1.994379000	-2.685987000
H	-4.520845000	-1.687694000	-0.943314000
H	-5.335063000	1.637075000	-1.809468000
H	-5.536021000	-0.732021000	-2.036065000
Si	1.061899000	0.301290000	-0.095026000
Si	-1.038697000	-0.216176000	0.039056000
C	2.605737000	2.355528000	3.367017000
H	1.541440000	2.606009000	3.402726000
H	2.824514000	1.684983000	4.205202000
H	3.172167000	3.278740000	3.528672000
H	-2.975365000	-5.677113000	0.703440000
H	3.319604000	5.661053000	-0.354323000
H	-5.537332000	3.487353000	-0.184530000

Table S16: Atomic coordinates of **2cDip.**

C	-3.866405000	-1.641949000	2.929858000
C	-2.351813000	-1.530736000	2.675911000
C	-1.556481000	-1.603712000	3.992434000
C	-2.619421000	2.498908000	3.063528000
C	-1.970890000	-3.913605000	2.005363000
C	-1.864863000	-2.560958000	1.658675000
C	-1.529682000	-4.911025000	1.144007000
C	-4.449957000	2.293038000	0.643768000
C	-2.156238000	2.457796000	1.593929000
C	-5.442762000	1.762112000	-0.168679000
C	-3.159155000	1.747966000	0.685951000
C	-4.503718000	-2.284980000	-1.597033000
C	-1.307774000	-2.193549000	0.401050000
C	-0.980058000	-4.561688000	-0.083567000
C	-5.144667000	0.673964000	-0.978075000
C	-1.862769000	3.880183000	1.076128000
C	-2.852791000	0.609149000	-0.117160000
C	-3.869652000	0.096626000	-0.975752000
C	-0.862784000	-3.222771000	-0.480811000
C	1.608055000	3.425365000	3.148151000
C	-3.634700000	-1.061706000	-1.941693000
C	-1.069019000	-3.641181000	-2.990375000
C	-0.261814000	-2.962504000	-1.865479000
C	2.233713000	2.622042000	1.993723000
C	2.321004000	-1.636221000	1.137614000
C	3.453080000	-2.395179000	1.314152000
C	-3.835666000	-0.630080000	-3.407196000
C	1.859990000	3.168397000	0.614612000
C	3.762147000	2.528885000	2.163654000
C	2.305979000	-0.515046000	0.248677000
C	1.212363000	-3.403319000	-1.952774000
C	1.239131000	2.366999000	-0.387080000
C	2.179125000	4.501068000	0.331333000
C	4.656672000	-2.093284000	0.620076000
C	-0.972287000	2.658435000	-3.266657000
C	5.843907000	-2.854305000	0.779964000
C	0.988550000	2.931436000	-1.667777000
C	1.898563000	5.058099000	-0.911968000
C	1.315589000	4.274790000	-1.900812000
C	0.407620000	2.131777000	-2.832635000
C	3.478495000	-0.209519000	-0.430949000
C	4.665399000	-0.973153000	-0.272752000
C	6.988839000	-2.528074000	0.087155000
C	5.863475000	-0.662972000	-0.972545000
C	1.379940000	2.078025000	-4.026719000
C	6.998357000	-1.422076000	-0.797788000
H	-4.130540000	-2.612260000	3.364545000
H	-4.196825000	-0.865084000	3.628000000
H	-4.432057000	-1.522732000	2.001233000
H	-2.399389000	-4.187880000	2.965288000
H	-1.700180000	-2.563947000	4.499399000
H	-2.826229000	1.495992000	3.449033000
H	-1.880781000	-0.815116000	4.680317000
H	-3.528699000	3.096519000	3.187473000
H	-1.844810000	2.948932000	3.694018000
H	-2.171805000	-0.536258000	2.254359000
H	-4.299971000	-2.642815000	-0.584057000
H	-0.483934000	-1.476632000	3.815131000

H	-4.678780000	3.156907000	1.260542000
H	-2.765837000	4.500218000	1.087053000
H	-1.217737000	1.895946000	1.567199000
H	-5.911730000	0.269424000	-1.631983000
H	-4.309415000	-3.108967000	-2.291861000
H	-5.570171000	-2.044242000	-1.663631000
H	-1.113239000	4.374426000	1.701935000
H	0.518693000	3.463870000	3.065360000
H	1.858658000	2.963673000	4.109230000
H	-0.636777000	-5.345882000	-0.751984000
H	-2.586647000	-1.365496000	-1.850148000
H	-2.123007000	-3.354516000	-2.971099000
H	1.979046000	4.455556000	3.172709000
H	1.418240000	-1.892195000	1.683401000
H	-1.479841000	3.860501000	0.052413000
H	-1.022244000	-4.732968000	-2.914425000
H	3.441247000	-3.241240000	1.996937000
H	1.836534000	1.600740000	2.069902000
H	-0.289060000	-1.880816000	-2.040983000
H	4.013474000	2.083541000	3.132353000
H	-0.659077000	-3.363946000	-3.967709000
H	-4.875459000	-0.349982000	-3.606198000
H	-3.579109000	-1.450857000	-4.085714000
H	-1.688872000	2.626267000	-2.440613000
H	1.307858000	-4.487632000	-1.825238000
H	-3.205301000	0.228832000	-3.656153000
H	5.834027000	-3.702654000	1.459469000
H	2.653967000	5.112050000	1.093697000
H	4.224869000	3.521292000	2.122199000
H	1.826448000	-2.920532000	-1.191513000
H	4.212541000	1.913266000	1.381078000
H	-1.372809000	2.050235000	-4.085571000
H	0.265476000	1.102728000	-2.485468000
H	1.624253000	-3.150089000	-2.935930000
H	-0.914967000	3.693355000	-3.622033000
H	1.118980000	4.709883000	-2.876422000
H	7.890684000	-3.119190000	0.216848000
H	3.510203000	0.640747000	-1.108326000
H	0.978568000	1.431959000	-4.815100000
H	2.355135000	1.680290000	-3.728162000
H	1.544406000	3.068813000	-4.464111000
H	5.867784000	0.187073000	-1.650022000
H	7.907408000	-1.175136000	-1.338353000
Si	-1.186980000	-0.338287000	-0.057229000
Si	0.787287000	0.575773000	0.059820000
H	-1.613211000	-5.956539000	1.428087000
H	2.144284000	6.097382000	-1.112576000
H	-6.436323000	2.201567000	-0.180722000

Table S17: Atomic coordinates of **2dDip.**

Si	-0.819277000	0.556092000	-0.004971000
Si	1.184122000	-0.273403000	-0.053584000
C	-2.339950000	-0.593759000	0.020146000
C	-3.275360000	-0.518848000	-1.051375000
C	-3.060448000	0.292256000	-2.210872000
H	-2.137397000	0.855598000	-2.284053000
C	-3.970973000	0.358959000	-3.232950000
H	-3.764741000	0.980597000	-4.099327000
C	-5.181159000	-0.387238000	-3.175877000
H	-5.895697000	-0.320960000	-3.990829000
C	-5.428091000	-1.194852000	-2.099650000
H	-6.339742000	-1.784313000	-2.046079000
C	-4.494189000	-1.297287000	-1.021187000
C	-4.731480000	-2.152264000	0.056566000
H	-5.646169000	-2.740562000	0.075800000
C	-3.820189000	-2.277186000	1.107438000
C	-4.080664000	-3.169734000	2.194488000
H	-4.997337000	-3.753209000	2.168785000
C	-3.206400000	-3.287879000	3.239525000
H	-3.416005000	-3.967365000	4.060217000
C	-2.016792000	-2.508352000	3.250413000
H	-1.328650000	-2.595044000	4.086290000
C	-1.730036000	-1.648535000	2.221901000
H	-0.812634000	-1.070932000	2.245038000
C	-2.605582000	-1.487285000	1.098756000
C	-1.235163000	2.418105000	0.065530000
C	-1.935545000	2.910265000	1.205098000
C	-2.270130000	4.266921000	1.282611000
H	-2.810800000	4.634962000	2.149671000
C	-1.918654000	5.153103000	0.271530000
C	-1.234326000	4.682437000	-0.841980000
H	-0.965651000	5.378298000	-1.631396000
C	-0.890412000	3.329603000	-0.973144000
C	-2.367152000	2.011083000	2.362064000
H	-1.925157000	1.022541000	2.201429000
C	-1.847922000	2.500523000	3.726570000
H	-0.758827000	2.604248000	3.725277000
H	-2.119975000	1.785813000	4.510616000
H	-2.276414000	3.469611000	4.002933000
C	-3.896106000	1.826722000	2.391192000
H	-4.403610000	2.778794000	2.582607000
H	-4.183058000	1.127263000	3.183581000
H	-4.266987000	1.434213000	1.440550000
C	-0.168231000	2.922938000	-2.257730000
H	-0.033149000	1.835575000	-2.235164000
C	-0.994733000	3.265730000	-3.514182000
H	-1.075274000	4.348291000	-3.659889000
H	-2.011828000	2.867681000	-3.450716000
H	-0.518041000	2.849759000	-4.408502000
C	1.233899000	3.554283000	-2.351824000
H	1.733657000	3.240530000	-3.274947000
H	1.864900000	3.258873000	-1.509909000
H	1.175519000	4.648301000	-2.365632000
C	2.775574000	0.790296000	-0.078343000
C	3.089354000	1.751626000	0.928160000
C	4.329486000	2.404215000	0.892677000
H	4.565701000	3.133640000	1.661733000
C	5.263665000	2.142435000	-0.101106000

C	4.956189000	1.226048000	-1.098990000
H	5.678227000	1.033071000	-1.887041000
C	3.727564000	0.555086000	-1.113418000
C	2.144985000	2.145596000	2.065134000
H	1.232516000	1.549730000	1.965732000
C	2.741856000	1.846316000	3.454729000
H	3.637939000	2.446226000	3.647215000
H	3.019292000	0.793868000	3.559863000
H	2.014210000	2.083761000	4.238700000
C	1.742460000	3.630654000	1.969881000
H	1.019464000	3.882707000	2.752441000
H	1.283503000	3.862885000	1.006193000
H	2.610518000	4.286617000	2.099428000
C	3.468338000	-0.398366000	-2.277990000
H	2.444408000	-0.773447000	-2.177327000
C	4.410564000	-1.615780000	-2.250015000
H	5.456498000	-1.308235000	-2.358454000
H	4.179435000	-2.300570000	-3.072967000
H	4.314998000	-2.170686000	-1.313134000
C	3.537788000	0.320916000	-3.638635000
H	4.544144000	0.699383000	-3.846586000
H	2.848116000	1.168948000	-3.674855000
H	3.272688000	-0.368654000	-4.447538000
C	1.493174000	-2.163675000	-0.052510000
C	1.038771000	-3.035504000	-1.085250000
C	1.415782000	-4.385056000	-1.059246000
H	1.070286000	-5.046501000	-1.848145000
C	2.217671000	-4.899467000	-0.048509000
C	2.640900000	-4.062932000	0.976720000
H	3.250548000	-4.467914000	1.779341000
C	2.284308000	-2.709227000	0.999366000
C	0.129667000	-2.600540000	-2.235218000
H	-0.054375000	-1.526773000	-2.128704000
C	0.768408000	-2.827005000	-3.619624000
H	1.731221000	-2.318058000	-3.714975000
H	0.106506000	-2.447923000	-4.405883000
H	0.935101000	-3.891469000	-3.817193000
C	-1.235280000	-3.314196000	-2.166050000
H	-1.128612000	-4.390173000	-2.344234000
H	-1.912352000	-2.915652000	-2.928735000
H	-1.707681000	-3.181673000	-1.190517000
C	2.752315000	-1.884176000	2.196146000
H	2.334353000	-0.876627000	2.087751000
C	2.203155000	-2.446189000	3.521782000
H	1.115773000	-2.559023000	3.481390000
H	2.450695000	-1.777598000	4.353645000
H	2.630669000	-3.428189000	3.750104000
C	4.284439000	-1.744791000	2.246081000
H	4.766779000	-2.722221000	2.356585000
H	4.589134000	-1.127697000	3.098410000
H	4.670536000	-1.277884000	1.336055000
H	6.220534000	2.657168000	-0.103822000
H	-2.178736000	6.205193000	0.349662000
H	2.501146000	-5.948392000	-0.053706000

Table S18: Atomic coordinates of **3aDip.**

C	-5.660076000	3.610117000	3.316413000
C	5.914936000	0.874500000	4.362886000
C	-6.511871000	2.938569000	2.222124000
C	-7.999989000	2.914675000	2.615652000
C	8.190853000	1.904050000	3.891751000
C	-6.579026000	4.949206000	0.726145000
C	6.883775000	1.373529000	3.275075000
C	-6.287713000	3.584044000	0.855925000
C	-6.351810000	5.625752000	-0.466356000
C	5.743547000	3.578021000	2.935354000
C	8.738325000	-2.204527000	3.054067000
C	-9.179871000	-1.169143000	3.753344000
C	-5.421711000	-2.709980000	3.896730000
C	6.229922000	2.401007000	2.353160000
C	5.110745000	4.548529000	2.167876000
C	-3.426886000	-1.736676000	2.706110000
C	-5.770086000	2.874307000	-0.262351000
C	-5.810704000	4.944971000	-1.551961000
C	-4.935534000	-2.033088000	2.599574000
C	5.199475000	-4.537211000	1.883890000
C	-2.634760000	1.605251000	0.244422000
C	-8.772297000	-1.821576000	2.418241000
C	8.519184000	-1.986106000	1.543956000
C	10.685629000	-0.819610000	1.172852000
C	-5.514406000	3.579496000	-1.473872000
C	-1.261947000	1.378642000	0.205179000
C	11.504265000	0.202147000	0.711055000
C	9.293663000	-0.781226000	1.011689000
C	-10.838676000	-1.163240000	1.188710000
C	-9.439963000	-1.134434000	1.230148000
C	6.093058000	2.194658000	0.951039000
C	4.961004000	4.349707000	0.800854000
C	9.288202000	3.891557000	-0.158264000
C	8.878293000	-3.261307000	0.755056000
C	-3.553225000	0.655916000	-0.247671000
C	1.563072000	0.411247000	0.665048000
C	-11.541551000	-0.528567000	0.173299000
C	10.931968000	1.283591000	0.054609000
C	-9.040188000	-3.337866000	2.431562000
C	8.693723000	0.338233000	0.361038000
C	-9.171548000	2.521183000	-1.808737000
C	-8.706783000	-0.462920000	0.207435000
C	2.933202000	0.170864000	0.645393000
C	4.527185000	-3.754222000	0.741690000
C	-3.468024000	3.448166000	-2.966819000
C	9.547985000	1.365251000	-0.138169000
C	-5.278627000	-2.852253000	1.351697000
C	5.442792000	3.194967000	0.169336000
C	-10.839692000	0.157550000	-0.808447000
C	-0.735995000	0.190117000	-0.330604000
C	-9.438921000	0.212089000	-0.814497000
C	3.082792000	-4.244225000	0.522368000
C	-4.888648000	2.913215000	-2.700777000
C	0.724817000	-0.055322000	-0.363652000
C	9.030452000	2.574406000	-0.912817000
C	-3.019570000	-0.528471000	-0.794905000
C	-8.801766000	1.029890000	-1.936608000
C	-4.773993000	-4.158397000	1.292520000
C	-6.073169000	-2.364053000	0.272139000

C	3.539595000	-0.543836000	-0.407206000
C	-1.647550000	-0.757045000	-0.831306000
C	5.330863000	-3.790680000	-0.559526000
C	5.621164000	-5.042846000	-1.112781000
C	-5.761345000	3.041521000	-3.962287000
C	1.323502000	-0.770684000	-1.415606000
C	5.227823000	3.096183000	-1.343764000
C	5.761473000	-2.610178000	-1.232152000
C	2.694926000	-1.010025000	-1.434874000
C	9.606913000	2.625962000	-2.340875000
C	3.733142000	3.000040000	-1.707849000
C	-5.039278000	-4.992684000	0.213189000
C	-6.333582000	-3.223244000	-0.832383000
C	5.869657000	4.272259000	-2.106732000
C	-9.174815000	0.494569000	-3.333240000
C	6.326280000	-5.155016000	-2.306542000
C	-5.817310000	-4.525029000	-0.839182000
C	6.451933000	-2.730457000	-2.469369000
C	-7.153339000	-2.780831000	-2.042906000
C	6.730304000	-4.007061000	-2.977534000
C	8.416095000	-1.426754000	-3.424206000
C	-8.458008000	-3.586720000	-2.180950000
C	6.884594000	-1.526720000	-3.304378000
C	-6.327901000	-2.824207000	-3.342201000
C	6.218298000	-1.528475000	-4.693542000
H	-5.777907000	3.080258000	4.267954000
H	-5.953911000	4.652490000	3.481021000
H	-4.597227000	3.601425000	3.054351000
H	5.621126000	1.679852000	5.044325000
H	6.387056000	0.089556000	4.963656000
H	8.007900000	2.782225000	4.520738000
H	8.659748000	1.138562000	4.519756000
H	-8.130465000	2.424705000	3.587231000
H	-6.982577000	5.491687000	1.576365000
H	-8.411460000	3.926884000	2.698982000
H	5.854755000	3.732359000	4.004917000
H	-6.182301000	1.896658000	2.151080000
H	5.003001000	0.460201000	3.921858000
H	-5.244037000	-2.051585000	4.754074000
H	-8.965462000	-0.096170000	3.749487000
H	8.488782000	-1.309180000	3.631335000
H	8.906854000	2.188003000	3.115318000
H	-8.631606000	-1.624387000	4.585175000
H	9.777224000	-2.466751000	3.280908000
H	8.108358000	-3.025181000	3.414458000
H	-8.596874000	2.368246000	1.879491000
H	-3.226970000	-1.108751000	3.581560000
H	-10.249051000	-1.294780000	3.953656000
H	7.143591000	0.500447000	2.665708000
H	4.611612000	-4.443281000	2.803281000
H	-6.488505000	-2.943207000	3.863703000
H	-2.998847000	2.541869000	0.658012000
H	-4.885323000	-3.645820000	4.087922000
H	-5.449204000	-1.068373000	2.514442000
H	6.206191000	-4.162089000	2.086605000
H	11.136589000	-1.672813000	1.670460000
H	-0.585881000	2.144344000	0.573906000
H	-2.849968000	-2.660770000	2.825092000
H	5.279592000	-5.604850000	1.653272000

H	-7.691006000	-1.681230000	2.321842000
H	8.810490000	3.883826000	0.825382000
H	-3.051927000	-1.218117000	1.822732000
H	-8.861917000	2.927254000	-0.842128000
H	-5.616332000	5.484297000	-2.474578000
H	1.129807000	0.937810000	1.510182000
H	-11.384271000	-1.683128000	1.970726000
H	7.452438000	-1.792944000	1.397170000
H	3.540373000	0.537141000	1.467626000
H	10.360497000	4.061275000	-0.012963000
H	-2.820184000	3.309871000	-2.097383000
H	9.938506000	-3.511778000	0.870036000
H	8.295765000	-4.116230000	1.112399000
H	-8.537507000	-3.815085000	3.279585000
H	-3.487393000	4.516654000	-3.208644000
H	2.506898000	-4.163686000	1.450612000
H	4.467060000	-2.709066000	1.071315000
H	-10.251966000	2.672006000	-1.908165000
H	-10.110503000	-3.551628000	2.522491000
H	11.570426000	2.075959000	-0.324872000
H	4.460322000	5.109179000	0.207500000
H	8.893188000	4.745625000	-0.718665000
H	-8.681225000	3.110466000	-2.589842000
H	-4.163334000	-4.529407000	2.110394000
H	-11.391364000	0.668955000	-1.591492000
H	3.065566000	-5.293706000	0.208095000
H	-4.794885000	1.839259000	-2.491203000
H	8.673722000	-3.142600000	-0.312045000
H	-7.715136000	0.949191000	-1.839097000
H	-8.677866000	-3.811592000	1.514990000
H	-3.014208000	2.922802000	-3.814158000
H	5.292778000	-5.943571000	-0.602249000
H	7.946641000	2.463574000	-1.020063000
H	2.574630000	-3.652866000	-0.243604000
H	-5.886581000	4.086945000	-4.263551000
H	-3.688405000	-1.290567000	-1.183318000
H	10.690943000	2.780453000	-2.333337000
H	-6.756370000	2.617081000	-3.804728000
H	3.247281000	2.161431000	-1.207279000
H	3.200435000	3.915660000	-1.426727000
H	-1.276950000	-1.695865000	-1.231877000
H	6.931416000	4.382431000	-1.874228000
H	5.379138000	5.221996000	-1.867712000
H	5.708021000	2.173499000	-1.688774000
H	0.711546000	-1.119411000	-2.242307000
H	-10.246771000	0.594864000	-3.534045000
H	-5.295717000	2.511630000	-4.800190000
H	9.159353000	3.451552000	-2.904670000
H	-7.437761000	-1.734549000	-1.887662000
H	8.886873000	-1.347167000	-2.439989000
H	-8.643296000	1.053648000	-4.111017000
H	3.117391000	-1.564436000	-2.268803000
H	9.406725000	1.695910000	-2.881402000
H	-9.072169000	-3.499905000	-1.279982000
H	-8.914766000	-0.562685000	-3.441277000
H	3.614320000	2.868422000	-2.789070000
H	5.772507000	4.117814000	-3.186890000
H	6.543193000	-0.625494000	-2.783938000
H	-5.424581000	-2.211869000	-3.257491000

Table S19: Atomic coordinates of **3bDip.**

C	7.104158000	-1.620682000	-4.082304000
C	9.342393000	-2.662325000	-3.473951000
C	8.075458000	-1.969829000	-2.939597000
C	6.642040000	4.148622000	-2.676826000
C	11.978535000	0.476150000	-1.238452000
C	12.767325000	-0.483876000	-0.619452000
C	10.587141000	0.508543000	-1.072154000
C	6.854719000	-4.028529000	-2.197550000
C	7.397428000	-2.787586000	-1.842116000
C	5.907000000	3.603344000	-1.438926000
C	9.955513000	-0.472732000	-0.250755000
C	4.476388000	4.170790000	-1.363444000
C	6.197913000	-4.817358000	-1.260587000
C	12.164835000	-1.427065000	0.202412000
C	7.294028000	-2.327621000	-0.498864000
C	10.780243000	-1.432598000	0.407187000
C	6.674017000	3.847741000	-0.137760000
C	6.978955000	5.171379000	0.199325000
C	4.226369000	-0.293119000	-0.626297000
C	-6.660522000	3.289725000	-3.400257000
C	6.083594000	-4.371590000	0.050761000
C	2.855542000	-0.516089000	-0.638159000
C	7.057252000	2.794297000	0.742336000
C	6.623282000	-3.144244000	0.459139000
C	4.813081000	0.649620000	0.245043000
C	7.653136000	5.476489000	1.376932000
C	-4.674344000	2.080156000	-2.434501000
C	-6.170702000	2.396209000	-2.243078000
C	-8.009824000	-4.753573000	-1.559668000
C	7.718682000	3.115123000	1.960054000
C	2.001239000	0.207657000	0.220332000
C	8.012535000	4.455169000	2.248183000
C	-2.580639000	-1.413414000	-0.648559000
C	-7.699418000	-3.390340000	-1.457648000
C	0.595526000	-0.004075000	0.195891000
C	3.949258000	1.366830000	1.100097000
C	-3.957861000	-1.598449000	-0.683930000
C	6.448351000	-2.767489000	1.933411000
C	-0.608750000	-0.181828000	0.166101000
C	2.575491000	1.154838000	1.092779000
C	-7.749102000	-5.633159000	-0.515862000
C	-2.016172000	-0.379813000	0.127129000
C	4.969888000	-2.528968000	2.298297000
C	-7.123177000	-2.896270000	-0.255163000
C	-6.456768000	3.009438000	-0.869284000
C	-4.835066000	-0.765156000	0.042216000
C	-5.909304000	4.273738000	-0.612843000
C	7.050815000	-3.820870000	2.884764000
C	-10.674906000	1.451448000	-0.883957000
C	-7.160643000	-5.160404000	0.652447000
C	-2.883202000	0.453484000	0.864657000
C	-12.068196000	1.532661000	-0.778630000
C	-6.844511000	-3.805791000	0.805800000
C	-4.258073000	0.259644000	0.821989000
C	-7.236055000	2.371612000	0.140623000
C	-9.940900000	0.583694000	-0.022388000
C	-6.115962000	4.923824000	0.597946000
C	-4.743943000	-3.930773000	2.221408000

C	-12.766420000	0.760986000	0.140644000
C	-6.175521000	-3.371717000	2.111403000
C	-10.670053000	-0.227415000	0.897757000
C	-7.434854000	3.040598000	1.381381000
C	-6.876153000	4.308397000	1.585396000
C	-12.065950000	-0.115282000	0.958499000
C	-6.999344000	-3.741015000	3.358380000
C	-8.230808000	2.423524000	2.530248000
C	-9.495058000	3.237256000	2.860739000
C	-7.359407000	2.209605000	3.781876000
H	7.596240000	-0.976959000	-4.819505000
H	9.834507000	-2.037619000	-4.227485000
H	6.756422000	-2.517264000	-4.606340000
H	9.104510000	-3.623187000	-3.943640000
H	6.223667000	-1.090582000	-3.705722000
H	12.452576000	1.223667000	-1.867407000
H	6.082191000	3.905516000	-3.586275000
H	10.059850000	-2.848507000	-2.669616000
H	7.642351000	3.717743000	-2.769942000
H	6.941639000	-4.376743000	-3.222809000
H	6.748661000	5.237890000	-2.638309000
H	8.389758000	-1.018052000	-2.496514000
H	3.925000000	3.941993000	-2.281830000
H	5.817481000	2.518528000	-1.579844000
H	4.488901000	5.259871000	-1.244388000
H	4.854763000	-0.861259000	-1.305174000
H	6.685449000	5.975625000	-0.469147000
H	-6.518828000	2.776349000	-4.357555000
H	12.780070000	-2.168416000	0.703686000
H	2.426467000	-1.244656000	-1.318564000
H	3.923045000	3.745117000	-0.522562000
H	-6.098690000	4.228748000	-3.447721000
H	-7.718995000	3.543064000	-3.305139000
H	-4.511500000	1.591188000	-3.401390000
H	-8.455781000	-5.132049000	-2.475003000
H	-1.925764000	-2.062470000	-1.221278000
H	5.565637000	-4.991615000	0.776458000
H	-4.074423000	2.997060000	-2.423655000
H	-4.361703000	-2.405429000	-1.289436000
H	-6.714470000	1.446232000	-2.301424000
H	4.515773000	-1.761324000	1.670233000
H	-4.295213000	1.422014000	-1.651677000
H	6.979858000	-1.823527000	2.101238000
H	8.523039000	4.702212000	3.174514000
H	-5.310193000	4.758693000	-1.377935000
H	4.360554000	2.106222000	1.781814000
H	4.383048000	-3.447416000	2.185296000
H	8.101536000	-4.022432000	2.663256000
H	1.930958000	1.717098000	1.761048000
H	-12.613720000	2.203684000	-1.435611000
H	6.511805000	-4.772272000	2.823541000
H	4.885111000	-2.210187000	3.343152000
H	-4.130386000	-3.625459000	1.370030000
H	-6.944663000	-5.855828000	1.458409000
H	6.982626000	-3.473685000	3.921512000
H	-2.462109000	1.248864000	1.471229000
H	-4.897065000	0.918273000	1.402122000
H	-4.751217000	-5.025792000	2.258543000
H	-6.096854000	-2.276186000	2.100734000

H	-4.260617000	-3.568384000	3.135117000
H	-12.614899000	-0.732440000	1.663311000
H	-10.146780000	3.326568000	1.986823000
H	-7.102249000	-4.825607000	3.470178000
H	-8.563116000	1.430515000	2.208257000
H	-7.032423000	4.816812000	2.532691000
H	-8.004237000	-3.312208000	3.316135000
H	-6.507743000	-3.363704000	4.261436000
H	-9.243988000	4.248051000	3.200360000
H	-6.491457000	1.581492000	3.557601000
H	-10.066123000	2.751723000	3.659637000
H	-6.990403000	3.158463000	4.185337000
H	-7.937793000	1.716823000	4.571052000
Si	8.057284000	-0.631176000	-0.047443000
Si	6.656601000	1.007619000	0.239394000
Si	-6.688735000	-1.064794000	0.002324000
Si	-8.027793000	0.647931000	-0.116200000
H	13.843677000	-0.489600000	-0.767280000
H	5.775087000	-5.775235000	-1.551050000
H	7.889520000	6.509091000	1.618926000
H	-7.996293000	-6.686629000	-0.614866000
H	-13.848317000	0.831916000	0.210355000
H	-5.683947000	5.905559000	0.772038000
C	-10.014737000	2.302218000	-1.965552000
H	-8.940560000	2.092326000	-1.946493000
C	-10.195153000	3.808558000	-1.703917000
C	-10.508074000	1.914985000	-3.373151000
H	-10.358597000	0.847934000	-3.563920000
H	-11.574011000	2.130362000	-3.501151000
H	-9.962713000	2.478329000	-4.137978000
H	-11.254071000	4.088424000	-1.711140000
H	-9.693912000	4.400972000	-2.476749000
H	-9.775830000	4.094333000	-0.735335000
C	-10.035013000	-1.253207000	1.835231000
H	-8.949465000	-1.198209000	1.713113000
C	-10.473450000	-2.683913000	1.463712000
C	-10.340332000	-0.960113000	3.317479000
H	-10.025476000	0.048476000	3.601678000
H	-11.409525000	-1.048508000	3.537701000
H	-9.813780000	-1.671648000	3.962826000
H	-11.554393000	-2.812576000	1.586715000
H	-9.976958000	-3.419705000	2.104072000
H	-10.221664000	-2.922553000	0.427107000
C	-7.974978000	-2.507941000	-2.673466000
H	-7.631338000	-1.497489000	-2.428831000
C	-9.478959000	-2.407580000	-2.986607000
C	-7.180382000	-2.972835000	-3.908622000
H	-6.106800000	-3.014245000	-3.698586000
H	-7.492001000	-3.968156000	-4.243621000
H	-7.335034000	-2.280323000	-4.743165000
H	-9.906207000	-3.386077000	-3.232660000
H	-9.647190000	-1.748137000	-3.845563000
H	-10.034716000	-2.001855000	-2.136119000
C	8.104608000	2.065798000	3.001424000
H	7.746445000	1.096004000	2.639483000
C	7.419614000	2.327205000	4.356481000
C	9.630934000	1.948637000	3.165520000
H	10.112664000	1.683631000	2.219697000
H	10.071735000	2.888227000	3.516977000

H	9.877786000	1.172991000	3.899363000
H	7.756710000	3.265965000	4.808982000
H	7.649573000	1.520289000	5.060707000
H	6.331655000	2.381894000	4.248365000
C	9.849427000	1.636096000	-1.791764000
C	10.269461000	3.011441000	-1.236084000
C	10.047799000	1.581209000	-3.319345000
H	11.093806000	1.743354000	-3.600477000
H	9.741039000	0.614212000	-3.729221000
H	9.452741000	2.359275000	-3.809730000
H	9.700765000	3.813908000	-1.716090000
H	11.332581000	3.204949000	-1.416277000
H	10.092862000	3.077009000	-0.159256000
C	10.230949000	-2.484396000	1.366830000
C	10.439862000	-3.912529000	0.829946000
C	10.817951000	-2.327236000	2.782828000
H	11.895701000	-2.520277000	2.797214000
H	10.654729000	-1.315972000	3.167657000
H	10.346819000	-3.035378000	3.472941000
H	9.953990000	-4.044496000	-0.140851000
H	10.022783000	-4.653717000	1.519985000
H	11.504921000	-4.137807000	0.709121000
H	9.152701000	-2.323166000	1.458899000
H	8.779142000	1.515722000	-1.601766000
H	8.838577000	-2.302057000	-3.930155000
H	-6.021387000	-5.177294000	-1.683613000
H	7.264379000	-4.101757000	-3.918724000
H	-9.048694000	-3.221246000	-3.028208000
H	8.697349000	-0.541869000	-4.006271000
H	-8.256308000	-4.649867000	-2.352085000
H	-6.916945000	-2.442878000	-4.183463000
H	-6.018466000	-3.844900000	-3.591117000
H	5.127362000	-1.568552000	-4.611241000
H	6.537384000	-2.384337000	-5.298169000
H	6.482780000	-0.618819000	-5.243678000
Si	-5.397229000	1.011937000	-0.217616000
Si	-6.794641000	-0.589664000	0.259003000
Si	6.801660000	0.588477000	0.187579000
Si	5.377308000	-0.932126000	-0.430272000
H	-12.627477000	-0.557378000	0.153900000
H	-6.585493000	6.683874000	-0.546893000
H	-4.639882000	-6.003032000	0.192122000
H	6.551842000	-6.135421000	-2.717278000
H	12.580357000	0.150103000	0.851682000
H	4.732983000	5.454775000	2.633480000

Table S20: Atomic coordinates of **3cDip.**

C	4.182870000	-4.047229000	-2.824604000
C	5.361144000	-5.580717000	1.108587000
C	4.640774000	-5.218918000	-0.024816000
C	7.853597000	-2.943637000	-1.432961000
C	7.547786000	-1.412375000	-3.430821000
C	5.744413000	-4.604348000	2.020271000
C	7.400138000	-1.546970000	-1.902323000

C	3.492872000	-3.574987000	-1.531969000
C	4.311677000	-3.882179000	-0.276687000
C	2.069493000	-4.156949000	-1.431554000
C	9.533217000	-0.388066000	-1.360253000
C	8.148527000	-0.447650000	-1.150528000
C	5.429360000	-3.253732000	1.816534000
C	4.718906000	-2.873898000	0.644373000
C	10.330754000	0.550615000	-0.719921000
C	-4.447204000	-3.374878000	-3.340915000
C	7.374485000	-2.146097000	3.028243000
C	-3.555805000	-4.268079000	-0.558315000
C	-2.393390000	-2.168026000	-2.521690000
C	4.578869000	1.762532000	-3.944120000
C	5.844417000	-2.258939000	2.899123000
C	-3.707450000	-4.870078000	0.684932000
C	6.808043000	2.826437000	-3.339487000
C	7.533121000	0.483304000	-0.261178000
C	5.196180000	-2.590593000	4.256780000
C	-3.882755000	-2.450733000	-2.243513000
C	9.744786000	1.443934000	0.166988000
C	5.569399000	2.081436000	-2.809254000
C	-7.908721000	-3.805140000	-1.474517000
C	-4.107090000	-3.009919000	-0.835821000
C	8.367726000	1.420788000	0.416407000
C	-8.288827000	-1.942849000	-3.164162000
C	2.426205000	-0.747957000	0.361242000
C	-4.414776000	-4.210796000	1.683115000
C	1.619316000	-1.524612000	1.252437000
C	-7.726375000	-2.306618000	-1.776396000
C	1.791087000	0.203963000	-0.428343000
C	4.901295000	2.832717000	-1.659598000
C	-4.833373000	-2.327444000	0.184188000
C	0.259636000	-1.339396000	1.337405000
C	0.392777000	0.426099000	-0.358248000
C	4.842033000	2.310998000	-0.336315000
C	-4.975374000	-2.947323000	1.457808000
C	7.838208000	2.416027000	1.445206000
C	-0.397201000	-0.363787000	0.538226000
C	-0.262732000	1.407897000	-1.151612000
C	8.469369000	2.191424000	2.832738000
C	4.324228000	4.076436000	-1.944935000
C	-8.319783000	-1.423790000	-0.681722000
C	-1.797240000	-0.148074000	0.600458000
C	-1.622214000	1.593707000	-1.066080000
C	8.017503000	3.872551000	0.978395000
C	-9.704708000	-1.494621000	-0.492704000
C	-2.431381000	0.805512000	-0.187153000
C	4.185380000	3.072916000	0.674823000
C	-5.711757000	-2.283890000	2.620307000
C	-5.021767000	2.893420000	-4.034393000
C	-6.967127000	-3.073050000	3.034298000
C	-7.533507000	-0.534126000	0.108103000
C	4.065819000	2.631648000	2.136410000
C	3.677099000	4.809204000	-0.957104000
C	-5.732129000	2.468331000	-2.735215000
C	-7.253642000	2.361212000	-2.944389000
C	-4.783056000	-2.040250000	3.824500000
C	3.609622000	4.305008000	0.336154000
C	-10.344383000	-0.693279000	0.443604000

C	2.605228000	2.349434000	2.539482000
C	4.681846000	3.655887000	3.110623000
C	-8.203911000	0.308427000	1.044346000
C	-5.377084000	3.386636000	-1.567654000
C	-4.730619000	2.927201000	-0.387501000
C	-9.593938000	0.203615000	1.192271000
C	-7.509288000	1.360722000	1.906906000
C	-5.686357000	4.748195000	-1.694113000
C	-2.184623000	4.000272000	1.882215000
C	-4.381362000	3.868855000	0.623161000
C	-3.631626000	3.470273000	1.895412000
C	-7.724195000	1.121265000	3.414245000
C	-7.961597000	2.781398000	1.514411000
C	-5.357108000	5.659202000	-0.697711000
C	-4.699270000	5.220103000	0.446553000
C	-4.358646000	3.902672000	3.181380000
H	4.300264000	-5.135916000	-2.847335000
H	4.329343000	-5.987877000	-0.725843000
H	7.279324000	-3.727165000	-1.937035000
H	8.912754000	-3.113394000	-1.655129000
H	8.586213000	-1.547084000	-3.752000000
H	6.946471000	-2.173024000	-3.940548000
H	5.175279000	-3.601787000	-2.933340000
H	3.585873000	-3.762818000	-3.697751000
H	2.093104000	-5.251112000	-1.377900000
H	9.995075000	-1.096672000	-2.041160000
H	7.710587000	-3.067916000	-0.356409000
H	7.216994000	-0.430398000	-3.782352000
H	6.291486000	-4.895838000	2.912212000
H	1.480075000	-3.878551000	-2.312030000
H	6.335666000	-1.450471000	-1.670519000
H	-3.909496000	-4.328498000	-3.378266000
H	3.390710000	-2.484937000	-1.609938000
H	1.548826000	-3.785762000	-0.545138000
H	-4.340974000	-2.901577000	-4.323184000
H	-2.997434000	-4.786206000	-1.332371000
H	7.826176000	-3.100259000	3.322033000
H	5.066528000	1.163787000	-4.721122000
H	7.293741000	2.250030000	-4.134565000
H	-1.808360000	-3.094620000	-2.516300000
H	-5.505161000	-3.599319000	-3.185966000
H	5.542748000	-3.552193000	4.650822000
H	-2.273160000	-1.707443000	-3.508559000
H	7.831375000	-1.833403000	2.084609000
H	-7.456436000	-4.418301000	-2.261232000
H	5.916804000	1.119225000	-2.417563000
H	-7.792016000	-2.529504000	-3.944468000
H	3.719106000	1.196444000	-3.571938000
H	7.541454000	2.987644000	-2.544126000
H	4.105539000	-2.638532000	4.175426000
H	4.200041000	2.673855000	-4.418946000
H	7.639258000	-1.406587000	3.792507000
H	6.539601000	3.803980000	-3.755161000
H	-1.964890000	-1.495676000	-1.777522000
H	-8.969157000	-4.073342000	-1.418896000
H	5.475036000	-1.273201000	2.597588000
H	10.367623000	2.167496000	0.684672000
H	-7.440509000	-4.077085000	-0.524640000
H	5.446618000	-1.821714000	4.995794000

H	-9.362733000	-2.146939000	-3.230046000
H	-4.412648000	-1.493293000	-2.307254000
H	2.092178000	-2.279695000	1.874343000
H	2.368502000	0.808732000	-1.122598000
H	-6.649937000	-2.109813000	-1.817443000
H	-4.528711000	-4.681383000	2.655678000
H	-8.137288000	-0.882132000	-3.385795000
H	-0.334302000	-1.941608000	2.020424000
H	8.324740000	1.160421000	3.169872000
H	0.332821000	2.014519000	-1.829279000
H	4.377240000	4.472106000	-2.955315000
H	9.545781000	2.392151000	2.823866000
H	-10.290541000	-2.181201000	-1.096807000
H	6.764807000	2.238625000	1.560887000
H	7.500868000	4.050482000	0.031069000
H	-5.231203000	2.175069000	-4.834472000
H	9.076081000	4.116024000	0.837556000
H	-2.376999000	-0.760896000	1.285836000
H	-2.093944000	2.355527000	-1.680620000
H	-6.709685000	-4.075532000	3.393428000
H	4.619872000	1.692393000	2.245775000
H	-5.372199000	1.465369000	-2.484221000
H	-7.478772000	1.676813000	-3.770169000
H	-7.659854000	-3.182136000	2.194935000
H	-3.936508000	2.939529000	-3.897803000
H	8.014898000	2.859487000	3.572291000
H	-4.407894000	-2.979948000	4.243540000
H	2.147195000	1.596518000	1.896741000
H	7.615005000	4.571710000	1.719156000
H	-3.918749000	-1.431416000	3.540972000
H	-6.048771000	-1.298691000	2.281789000
H	-7.751473000	1.981873000	-2.047081000
H	-5.355265000	3.878032000	-4.379905000
H	-7.495948000	-2.557290000	3.843360000
H	5.718047000	3.892569000	2.857550000
H	-7.696309000	3.332859000	-3.190663000
H	2.560995000	1.989369000	3.573419000
H	-5.319967000	-1.513993000	4.621344000
H	1.997325000	3.259237000	2.480122000
H	3.100543000	4.881870000	1.102571000
H	4.663112000	3.261235000	4.132388000
H	-1.640417000	3.650971000	1.000974000
H	4.119477000	4.595813000	3.114109000
H	-6.433671000	1.293023000	1.719453000
H	-3.574240000	2.373347000	1.921581000
H	-6.186893000	5.100109000	-2.591716000
H	-10.098210000	0.843714000	1.910017000
H	-7.399740000	0.120337000	3.714057000
H	-1.643549000	3.660012000	2.771924000
H	-7.766860000	2.985547000	0.458358000
H	-2.167578000	5.095980000	1.878883000
H	-8.776907000	1.227783000	3.697394000
H	-9.033401000	2.920531000	1.693409000
H	-7.153217000	1.849813000	4.000167000
H	-7.426489000	3.533971000	2.102126000
H	-3.812970000	3.546994000	4.061859000
H	-5.372524000	3.495319000	3.223955000
H	-4.430136000	5.939050000	1.214940000
H	-4.432334000	4.992527000	3.259720000

Si	4.274477000	-1.068182000	0.253930000
Si	5.641171000	0.606561000	0.017571000
Si	-5.630346000	-0.610381000	-0.109704000
Si	-4.284724000	1.103861000	-0.088817000
H	11.401491000	0.577994000	-0.902182000
H	3.227016000	5.769519000	-1.193631000
H	5.615376000	-6.622385000	1.284740000
H	-11.420424000	-0.756965000	0.579626000
H	-5.605249000	6.710548000	-0.815330000
H	-3.273943000	-5.848078000	0.875618000

Table S21: Atomic coordinates of **3dDip**

C	-7.875986000	1.182472000	-3.194746000
C	-3.923536000	-2.901755000	-4.090008000
C	-6.148172000	-2.544875000	-2.935023000
C	-4.617370000	-2.487584000	-2.776515000
C	-7.392285000	1.610128000	-1.795188000
C	-4.499535000	3.387267000	-3.354176000
C	-7.898087000	3.023406000	-1.448406000
C	-9.149045000	0.347250000	-0.571755000
C	-7.779015000	0.593164000	-0.724144000
C	-9.619544000	-0.581860000	0.345721000
C	-4.318932000	-4.711576000	-1.688969000
C	-0.292819000	-1.189860000	-3.534114000
C	-4.137601000	-3.324549000	-1.590688000
C	1.096106000	-0.910726000	-3.460255000
C	-3.842470000	2.632036000	-2.182957000
C	-1.081655000	-1.000388000	-2.432442000
C	-6.830630000	-0.102352000	0.086794000
C	-3.896997000	-5.573293000	-0.684873000
C	-8.706790000	-1.291371000	1.112337000
C	-2.315027000	2.659991000	-2.337933000
C	-7.325073000	-1.081267000	1.000908000
C	-4.257996000	3.158486000	-0.808719000
C	-3.519360000	-2.780546000	-0.427547000
C	4.830359000	-2.325955000	-3.940866000
C	-4.136632000	4.536485000	-0.586124000
C	1.639307000	-0.444028000	-2.293313000
C	-6.636613000	-3.451145000	1.547016000
C	3.064907000	3.666237000	-3.160278000
C	-4.741326000	2.322257000	0.238609000
C	-0.566201000	-0.522638000	-1.185617000
C	0.906248000	3.614902000	-1.852687000
C	-3.280644000	-5.052205000	0.445795000
C	-4.499984000	5.110160000	0.626279000
C	-6.448059000	-1.960173000	1.891017000
C	-3.090857000	-3.673667000	0.596326000
C	0.854948000	-0.215469000	-1.116046000
C	2.384757000	3.197948000	-1.861592000
C	-1.426581000	-0.323649000	-0.070332000
C	-5.107169000	2.918153000	1.478189000
C	6.713916000	1.710226000	-3.389211000
C	-4.988153000	4.303089000	1.646717000
C	5.645744000	-2.105449000	-2.653300000
C	-7.142061000	2.377982000	2.896506000

C	7.141676000	-2.378238000	-2.896582000
C	-5.646091000	2.105484000	2.653143000
C	4.987201000	-4.302985000	-1.647125000
C	-6.713656000	-1.710168000	3.389303000
C	5.106604000	-2.918102000	-1.478435000
C	1.426633000	0.323949000	0.070138000
C	-2.384658000	-3.197281000	1.861983000
C	-0.854910000	0.215846000	1.115814000
C	3.091127000	3.673985000	-0.595897000
C	6.448247000	1.960077000	-1.890913000
C	4.498857000	-5.110043000	-0.626760000
C	3.281107000	5.052475000	-0.445155000
C	-0.906022000	-3.613769000	1.853103000
C	6.636840000	3.450999000	-1.546720000
C	4.740974000	-2.322246000	-0.238773000
C	0.566243000	0.522972000	1.185404000
C	-3.064625000	-3.665638000	3.160741000
C	-1.639299000	0.444528000	2.293040000
C	-4.830643000	2.326262000	3.940621000
C	4.135751000	-4.536417000	0.585740000
C	3.519660000	2.780633000	0.427762000
C	7.325190000	1.081032000	-1.000861000
C	4.257515000	-3.158479000	0.808500000
C	2.314890000	-2.659808000	2.338150000
C	8.706920000	1.291061000	-1.112258000
C	3.897670000	5.573299000	0.685517000
C	6.830667000	0.102092000	-0.086823000
C	1.081695000	1.000723000	2.432232000
C	3.842307000	-2.632134000	2.182878000
C	-1.096105000	0.911250000	3.459976000
C	4.138052000	3.324378000	1.590948000
C	9.619623000	0.581411000	-0.345712000
C	4.319592000	4.711360000	1.689431000
C	7.779006000	-0.593579000	0.724042000
C	0.292839000	1.190283000	3.533875000
C	9.149054000	-0.347757000	0.571669000
C	7.897955000	-3.023897000	1.448062000
C	4.499426000	-3.387674000	3.353866000
C	7.392225000	-1.610625000	1.794986000
C	4.617684000	2.487173000	2.776663000
C	6.148498000	2.544159000	2.935168000
C	3.923943000	2.901319000	4.090213000
C	7.875957000	-1.183134000	3.194584000
H	-8.968922000	1.171522000	-3.260017000
H	-7.508944000	1.881491000	-3.953962000
H	-7.516784000	0.181810000	-3.450241000
H	-4.186085000	-2.206069000	-4.894646000
H	-6.466046000	-1.933167000	-3.786786000
H	-4.230219000	-3.903070000	-4.410965000
H	-6.491700000	-3.568614000	-3.119734000
H	-9.857430000	0.890110000	-1.190257000
H	-2.834755000	-2.911299000	-3.984855000
H	-4.245819000	2.898549000	-4.301130000
H	-5.588324000	3.415560000	-3.269053000
H	-6.656557000	-2.174560000	-2.040942000
H	-7.597972000	3.743676000	-2.216797000
H	-8.991495000	3.045540000	-1.386938000
H	-0.729670000	-1.540198000	-4.464467000
H	-4.795416000	-5.123147000	-2.573832000

H	-4.145114000	4.421370000	-3.420280000
H	-4.356089000	-1.442980000	-2.575417000
H	-6.301822000	1.649051000	-1.841637000
H	1.725321000	-1.054205000	-4.333449000
H	-7.497524000	3.366064000	-0.490907000
H	-2.145764000	-1.194369000	-2.499355000
H	-4.153153000	1.582849000	-2.245680000
H	-2.012767000	2.214615000	-3.292304000
H	2.533734000	3.259462000	-4.027447000
H	5.154446000	-1.628994000	-4.721643000
H	0.393673000	3.212210000	-2.730540000
H	-6.414513000	-3.647114000	0.495037000
H	-9.072819000	-2.031527000	1.817099000
H	-3.756274000	5.172662000	-1.379575000
H	4.962286000	-3.339599000	-4.334107000
H	-1.944328000	3.689552000	-2.313107000
H	3.762078000	-2.175643000	-3.763567000
H	-7.663128000	-3.778979000	1.743217000
H	0.804741000	4.705994000	-1.873897000
H	3.057293000	4.757414000	-3.253932000
H	2.700881000	-0.228313000	-2.240765000
H	-1.824132000	2.106254000	-1.535886000
H	-7.737660000	2.149571000	2.008744000
H	6.040540000	2.315589000	-4.005545000
H	4.103568000	3.332712000	-3.214251000
H	0.393571000	3.249295000	-0.959720000
H	-5.971423000	-4.075285000	2.150538000
H	6.561151000	0.660388000	-3.655993000
H	2.413719000	2.102796000	-1.871155000
H	-5.402700000	-1.705260000	1.696892000
H	-2.943563000	-5.726617000	1.227548000
H	7.517247000	-1.764800000	-3.723018000
H	5.275331000	-4.754098000	-2.592283000
H	7.739202000	1.976203000	-3.667615000
H	7.310136000	-3.428824000	-3.158334000
H	-5.543554000	1.044525000	2.391370000
H	5.543408000	-1.044494000	-2.391444000
H	-7.310736000	3.428565000	3.158138000
H	-7.738921000	-1.976135000	3.667790000
H	-5.276456000	4.754232000	2.591810000
H	-7.517435000	1.764573000	3.723054000
H	2.944009000	5.727064000	-1.226748000
H	5.402865000	1.705178000	-1.696866000
H	-6.560897000	-0.660299000	3.655969000
H	5.971719000	4.075243000	-2.150209000
H	-2.413991000	-2.102132000	1.871422000
H	-0.393462000	-3.248056000	0.960118000
H	-6.040229000	-2.315455000	4.005659000
H	-4.103448000	-3.332588000	3.214634000
H	7.737251000	-2.150071000	-2.008745000
H	1.823938000	-2.106033000	1.536168000
H	-2.700889000	0.228900000	2.240465000
H	-3.056497000	-4.756790000	3.254638000
H	-0.804209000	-4.704831000	1.874362000
H	7.663383000	3.778811000	-1.742814000
H	-3.762360000	2.176049000	3.763268000
H	9.073005000	2.031248000	-1.816958000
H	-4.962657000	3.339945000	4.333729000
H	1.943987000	-3.689305000	2.313474000

H	6.414684000	3.646844000	-0.494729000
H	3.755272000	-5.172586000	1.379138000
H	-5.154595000	1.629369000	4.721517000
H	-0.393566000	-3.210872000	2.730929000
H	-2.533655000	-3.258440000	4.027836000
H	2.012902000	-2.214314000	3.292552000
H	4.153205000	-1.583017000	2.245698000
H	7.497313000	-3.366467000	0.490563000
H	2.145814000	1.194655000	2.499155000
H	-1.725344000	1.054831000	4.333136000
H	6.301762000	-1.649489000	1.841433000
H	4.356200000	1.442645000	2.575439000
H	4.144831000	-4.421724000	3.419849000
H	4.796203000	5.122721000	2.574323000
H	8.991357000	-3.046058000	1.386515000
H	0.729682000	1.540621000	4.464230000
H	7.597871000	-3.744216000	2.216420000
H	6.656810000	2.173868000	2.041038000
H	9.857401000	-0.890738000	1.190109000
H	5.588196000	-3.416144000	3.268572000
H	4.245941000	-2.899065000	4.300939000
H	2.835167000	2.911107000	3.985069000
H	6.492225000	3.567806000	3.120019000
H	4.230842000	3.902530000	4.411295000
H	6.466260000	1.932277000	3.786847000
H	7.516739000	-0.182513000	3.450214000
H	4.186349000	2.205473000	4.894760000
H	8.968894000	-1.172163000	3.259824000
H	7.508960000	-1.882260000	3.953721000
Si	-4.982823000	0.437910000	0.017625000
Si	-3.268124000	-0.899283000	-0.171225000
Si	3.268214000	0.899444000	0.171089000
Si	4.982786000	-0.437947000	-0.017600000
H	-4.045008000	-6.645086000	-0.784799000
H	-10.685907000	-0.760002000	0.453240000
H	-4.404163000	6.182305000	0.774527000
H	4.045832000	6.645055000	0.785604000
H	10.685998000	0.759503000	-0.453200000
H	4.402722000	-6.182142000	-0.775138000

Table S22: Transition energy, wavelengths, and oscillator strength of the electronic transition of **2bDip.**

No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	23414,27507	427,08988	0,2401	Singlet-A	HOMO->LUMO (90%)	HOMO->L+4 (4%), HOMO->L+6 (4%)
2	26440,46729	378,20814	0,0557	Singlet-A	HOMO->L+1 (99%)	–
3	27226,85786	367,28439	0,0054	Singlet-A	HOMO->L+2 (99%)	–
4	30290,15158	330,14031	0,0357	Singlet-A	HOMO->L+3 (96%)	HOMO->LUMO (2%)
5	30541,79656	327,42016	0,0754	Singlet-A	HOMO->L+4 (91%)	HOMO->LUMO (4%)
6	30893,45429	323,69317	0,0068	Singlet-A	HOMO->L+5 (98%)	–
7	31310,44293	319,38226	0,0511	Singlet-A	HOMO->L+6 (90%)	HOMO->LUMO (3%), HOMO->L+4 (2%)
8	31684,68419	315,6099	0,005	Singlet-A	HOMO->L+7 (97%)	–
9	32663,84127	306,14893	6E-4	Singlet-A	HOMO->L+8 (96%)	–
10	34334,21549	291,25465	0,0061	Singlet-A	H-1->LUMO (96%)	–
11	35868,28201	278,79785	0,0703	Singlet-A	H-5->LUMO (80%)	H-6->LUMO (4%), H-3->LUMO (7%), H-2->LUMO (4%)
12	36415,93247	274,60508	0,0072	Singlet-A	H-2->LUMO (92%)	H-5->LUMO (3%)
13	36579,66302	273,37595	0,0056	Singlet-A	H-4->LUMO (34%), H-3->LUMO (58%)	H-5->LUMO (3%)
14	36600,63343	273,21932	0,0145	Singlet-A	H-4->LUMO (61%), H-3->LUMO (29%)	H-5->LUMO (6%)
15	38115,34265	262,36154	0,0045	Singlet-A	H-6->LUMO (87%)	H-5->LUMO (4%), HOMO->L+9 (3%)
16	38391,18427	260,47647	0,004	Singlet-A	HOMO->L+9 (95%)	H-6->LUMO (3%)
17	38853,33995	257,37813	0,0017	Singlet-A	H-7->LUMO (94%)	–
18	39759,10058	251,51474	0,0046	Singlet-A	H-8->LUMO (75%)	H-1->L+1 (8%), H-1->L+2 (7%)
19	39983,32271	250,10428	0,0097	Singlet-A	H-8->LUMO (19%), H-1->L+1 (35%), H-1->L+2 (28%)	H-6->L+7 (3%), H-5->L+7 (6%)
20	41125,40378	243,15871	0,013	Singlet-A	H-2->L+1 (49%), H-2->L+2 (12%)	H-7->L+4 (7%), H-5->L+4 (3%), H-3->L+1 (2%), H-1->L+1 (4%), H-1->L+2 (4%)
21	41391,56674	241,59511	0,0039	Singlet-A	H-4->L+1 (10%), H-1->L+1 (39%), H-1->L+2 (33%)	H-2->L+1 (5%)
22	41434,31413	241,34586	0,0203	Singlet-A	H-3->L+1 (30%), H-3->L+2 (16%)	H-8->L+3 (5%), H-6->L+5 (6%), H-5->L+1 (4%), H-4->L+1 (4%), H-4->L+2 (8%), H-1->L+1 (3%), H-1->L+2 (2%)
23	41441,57312	241,30358	0,0021	Singlet-A	H-4->L+1 (42%), H-3->L+2 (13%)	H-8->L+5 (3%), H-7->L+3 (2%), H-6->L+3 (4%), H-5->L+3 (3%), H-4->L+2 (3%), H-1->L+1 (6%), H-1->L+2 (6%)
24	42151,34101	237,24038	0,031	Singlet-A	HOMO->L+10 (59%), HOMO->L+11 (30%)	–
25	42756,25684	233,8839	0,0762	Singlet-A	H-5->L+1 (57%), H-3->L+1 (11%), HOMO->L+10 (14%)	HOMO->L+11 (9%)
26	43001,44938	232,5503	0,0279	Singlet-A	H-5->L+1 (16%), HOMO->L+10 (21%), HOMO->L+11 (52%)	H-3->L+1 (3%)
27	43547,48673	229,63438	0,0054	Singlet-A	H-1->L+3 (20%), H-1->L+4 (35%), H-1->L+6 (14%), H-1->L+8 (10%)	H-5->L+7 (3%), H-1->L+2 (5%), H-1->L+7 (3%)
28	43813,64969	228,23937	0,0046	Singlet-A	H-3->L+1 (31%), H-3->L+2 (22%), H-2->L+2 (25%)	H-5->L+1 (2%), H-5->L+2 (7%), H-4->L+1 (3%)
29	43899,14446	227,79487	0,0019	Singlet-A	H-3->L+2 (22%), H-2->L+1 (23%), H-2->L+2 (34%)	H-5->L+1 (3%), H-5->L+2 (3%), H-4->L+1 (2%), H-3->L+1 (6%)
30	43997,5441	227,28541	0,0012	Singlet-A	H-5->L+2 (41%), H-4->L+1 (12%), H-4->L+2 (25%)	H-2->L+2 (7%)

Table S23: Transition energy, wavelengths, and oscillator strength of the electronic transition of **2cDip.**

No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	21362,40061	468,11218	0,3048	Singlet-A	HOMO->LUMO (93%)	HOMO->L+1 (2%)
2	24692,66384	404,97858	0,0445	Singlet-A	HOMO->L+1 (87%)	HOMO->L+2 (7%)
3	26318,67757	379,9583	0,1054	Singlet-A	HOMO->L+2 (87%)	HOMO->LUMO (2%), HOMO->L+1 (6%), HOMO->L+3 (3%)
4	27668,04313	361,4278	0,0074	Singlet-A	HOMO->L+3 (95%)	HOMO->L+2 (3%)
5	30219,17479	330,91572	0,043	Singlet-A	HOMO->L+4 (87%)	HOMO->L+5 (5%)
6	30553,89488	327,29052	0,0112	Singlet-A	HOMO->L+5 (90%)	HOMO->L+4 (5%)
7	30917,65093	323,43984	0,0015	Singlet-A	HOMO->L+6 (95%)	–
8	31539,50439	317,06269	0,0221	Singlet-A	H-1->LUMO (79%)	HOMO->L+7 (4%), HOMO->L+8 (9%)
9	31704,84805	315,40918	0,0132	Singlet-A	H-1->LUMO (12%), HOMO->L+7 (49%), HOMO->L+8 (34%)	–
10	32350,89815	309,11043	0,0663	Singlet-A	HOMO->L+7 (43%), HOMO->L+8 (43%)	H-7->LUMO (3%)
11	34211,61921	292,29835	9E-4	Singlet-A	H-3->LUMO (55%), H-2->LUMO (42%)	–
12	34410,0316	290,61293	0,0085	Singlet-A	H-3->LUMO (42%), H-2->LUMO (51%)	–
13	34603,60467	288,98723	0,0091	Singlet-A	H-4->LUMO (87%)	H-5->LUMO (9%)
14	34781,8532	287,50624	0,0567	Singlet-A	H-5->LUMO (83%)	H-4->LUMO (9%)
15	35875,541	278,74144	0,0125	Singlet-A	H-7->LUMO (40%), H-1->L+1 (31%)	H-6->LUMO (3%), H-5->LUMO (3%), H-1->LUMO (3%), H-1->L+2 (8%), H-1->L+3 (4%)
16	36681,28888	272,61856	0,0055	Singlet-A	H-6->LUMO (84%)	H-8->LUMO (7%), H-7->LUMO (2%)
17	37338,63074	267,81914	0,0395	Singlet-A	H-1->L+1 (48%), H-1->L+2 (19%)	H-7->LUMO (6%), H-7->L+1 (3%), H-1->L+3 (5%), HOMO->L+9 (2%), HOMO->L+10 (8%)
18	37545,10867	266,34628	4E-4	Singlet-A	H-8->LUMO (81%)	H-6->LUMO (4%), H-1->L+1 (2%), HOMO->L+10 (6%)
19	38139,53928	262,19509	0,0031	Singlet-A	HOMO->L+9 (90%)	HOMO->L+11 (3%)
20	38352,46965	260,7394	0,0131	Singlet-A	HOMO->L+10 (76%)	H-8->LUMO (6%), H-6->LUMO (3%), H-1->L+2 (5%)
21	39751,84159	251,56067	0,0925	Singlet-A	H-7->LUMO (14%), H-4->L+1 (20%), H-3->L+1 (19%), H-2->L+1 (11%), H-1->L+2 (13%)	H-7->L+1 (4%), H-5->L+1 (3%), H-1->L+1 (3%)
22	39851,85434	250,92935	0,0227	Singlet-A	H-4->L+1 (57%), H-3->L+1 (10%)	H-8->L+4 (2%), H-7->LUMO (5%), H-4->L+2 (4%), H-1->L+2 (5%)
23	39902,66727	250,60981	0,0861	Singlet-A	H-3->L+1 (43%), H-2->L+1 (12%), H-1->L+2 (19%)	H-7->LUMO (8%), H-7->L+1 (4%), H-5->L+1 (3%), H-1->L+1 (2%)
24	40461,60949	247,14786	0,0062	Singlet-A	H-3->L+1 (18%), H-2->L+1 (63%)	H-4->L+1 (2%), H-2->LUMO (2%), H-2->L+3 (4%)
25	40585,01231	246,39638	0,0312	Singlet-A	H-7->L+1 (11%), H-5->L+1 (17%), H-1->L+2 (15%), H-1->L+3 (37%)	H-7->LUMO (5%), H-1->L+4 (4%), H-1->L+8 (3%), HOMO->L+11 (3%)
26	40749,54942	245,40149	0,0057	Singlet-A	H-3->L+2 (15%), HOMO->L+11 (44%)	H-5->L+1 (4%), H-5->L+5 (3%), H-3->L+3 (5%), H-2->L+2 (5%), H-1->L+3 (5%), HOMO->L+9 (2%)
27	40864,8867	244,70886	0,0223	Singlet-A	H-3->L+2 (21%), HOMO->L+11 (34%)	H-6->L+5 (3%), H-5->L+5 (4%), H-5->L+7 (2%), H-3->L+3 (6%), H-2->L+2 (7%), H-2->L+3 (2%), H-1->L+3 (4%)
28	41122,98412	243,17301	0,0146	Singlet-A	H-7->L+1 (13%), H-5->L+1 (62%)	H-7->LUMO (3%), H-1->L+3 (3%), HOMO->L+11 (2%)
29	41594,81846	240,41456	0,0143	Singlet-A	H-3->L+2 (11%), H-2->L+2 (32%), H-2->L+3 (19%)	H-8->L+6 (2%), H-6->L+6 (5%), H-3->L+3 (6%), H-2->L+1 (5%)
30	41619,01509	240,27479	0,0054	Singlet-A	H-4->L+1 (13%), H-4->L+2 (45%)	H-8->L+4 (4%), H-5->L+4 (4%), H-4->L+3 (6%), H-1->L+3 (4%), H-1->L+4 (5%)

Table S24: Transition energy, wavelengths, and oscillator strength of the electronic transition of **2dDip.**

No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	16544,851	604,41765	0,0426	Singlet-A	HOMO->LUMO (98%)	–
2	23917,56504	418,10276	0,2339	Singlet-A	HOMO->L+1 (81%)	H-1->LUMO (9%), HOMO->L+4 (3%)
3	25453,24467	392,87722	0,0851	Singlet-A	H-1->LUMO (87%)	HOMO->L+1 (6%)
4	27000,21607	370,36741	0,0318	Singlet-A	HOMO->L+2 (83%), HOMO->L+3 (14%)	–
5	28072,93346	356,215	0,0053	Singlet-A	HOMO->L+2 (13%), HOMO->L+3 (82%)	H-6->LUMO (3%)
6	29157,74916	342,962	0,0118	Singlet-A	H-1->L+1 (47%), HOMO->L+4 (47%)	HOMO->L+1 (2%)
7	29634,42283	337,44541	0,0259	Singlet-A	H-1->L+1 (44%), HOMO->L+4 (44%)	HOMO->L+5 (2%), HOMO->L+6 (2%), HOMO->L+7 (4%), HOMO->L+8 (2%)
8	30716,01232	325,56309	0,0695	Singlet-A	HOMO->L+5 (70%), HOMO->L+6 (10%)	H-1->L+1 (4%), HOMO->L+1 (3%), HOMO->L+7 (3%), HOMO->L+8 (2%)
9	30967,6573	322,91755	0,0248	Singlet-A	HOMO->L+5 (21%), HOMO->L+6 (64%)	HOMO->L+7 (7%)
10	31261,24311	319,88491	0,0262	Singlet-A	HOMO->L+6 (19%), HOMO->L+7 (64%)	HOMO->L+8 (6%)
11	31345,12477	319,02888	0,0085	Singlet-A	H-6->LUMO (47%), H-1->L+2 (16%), H-1->L+3 (24%)	HOMO->L+3 (2%), HOMO->L+7 (2%)
12	31579,83211	316,65779	7E-4	Singlet-A	H-2->LUMO (91%)	HOMO->L+8 (4%)
13	31814,53945	314,3217	0,0049	Singlet-A	HOMO->L+7 (13%), HOMO->L+8 (68%)	H-2->LUMO (6%), HOMO->L+9 (8%)
14	31902,45388	313,45551	1E-3	Singlet-A	H-4->LUMO (47%), H-3->LUMO (51%)	–
15	32553,34331	307,18811	0,0012	Singlet-A	HOMO->L+8 (10%), HOMO->L+9 (86%)	–
16	32842,08979	304,48732	0,0096	Singlet-A	H-5->LUMO (46%), H-4->LUMO (22%), H-3->LUMO (25%)	–
17	32942,9091	303,55546	0,0105	Singlet-A	H-5->LUMO (45%), H-4->LUMO (29%), H-3->LUMO (20%)	–
18	34158,38662	292,75387	4E-4	Singlet-A	H-8->LUMO (15%), H-7->LUMO (73%)	H-6->LUMO (6%)
19	35320,63155	283,12065	0,0068	Singlet-A	H-8->LUMO (74%), H-7->LUMO (19%)	H-9->LUMO (3%)
20	35781,98069	279,47028	0,0048	Singlet-A	H-9->LUMO (19%), H-1->L+2 (45%), H-1->L+3 (20%)	H-8->LUMO (3%), H-1->L+4 (5%), HOMO->L+10 (4%)
21	36094,92381	277,04727	0,0043	Singlet-A	H-9->LUMO (16%), HOMO->L+10 (75%)	–
22	36196,54966	276,26943	0,0035	Singlet-A	H-9->LUMO (49%), H-1->L+2 (19%), H-1->L+3 (10%), HOMO->L+10 (15%)	H-1->L+9 (3%)
23	36699,83963	272,48075	0,0069	Singlet-A	H-2->L+1 (95%)	–
24	36887,76681	271,09258	0,0049	Singlet-A	H-1->L+4 (73%)	H-4->L+1 (4%), H-3->L+1 (9%), H-1->L+3 (7%)
25	36981,32712	270,40674	0,0061	Singlet-A	H-4->L+1 (27%), H-3->L+1 (53%), H-1->L+4 (13%)	–
26	37124,08726	269,36689	0,0174	Singlet-A	H-4->L+1 (60%), H-3->L+1 (33%)	–
27	37570,91841	266,16331	0,0421	Singlet-A	H-5->L+1 (89%)	H-4->L+1 (3%)
28	38496,8429	259,76156	0,0137	Singlet-A	HOMO->L+11 (89%)	H-1->L+6 (2%)
29	38822,69089	257,58132	0,0146	Singlet-A	H-1->L+5 (36%), H-1->L+6 (34%), H-1->L+7 (13%)	H-6->L+1 (3%), H-1->L+8 (3%), H-1->L+9 (2%), HOMO->L+11 (3%)
30	38990,45421	256,47303	0,0653	Singlet-A	H-6->L+1 (79%)	H-6->LUMO (6%), H-1->L+3 (4%)

Table S25: Transition energy, wavelengths, and oscillator strength of the electronic transition of **3aDip.**

No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	19765,42284	505,93403	0,7427	Singlet-A	HOMO->LUMO (97%)	–
2	21088,1721	474,19947	0,0181	Singlet-A	H-1->LUMO (97%)	–
3	23216,66924	430,72501	0,0199	Singlet-A	HOMO->L+1 (86%)	H-1->L+2 (6%), HOMO->L+3 (3%)
4	24051,45307	415,7753	0,1462	Singlet-A	H-1->L+1 (75%), HOMO->L+2 (14%)	H-1->L+3 (4%)
5	25725,86007	388,71392	0,1357	Singlet-A	H-1->L+1 (20%), H-1->L+3 (13%), HOMO->L+2 (60%)	HOMO->L+4 (4%)
6	26152,52736	382,37222	2E-4	Singlet-A	H-1->L+2 (35%), H-1->L+4 (12%), HOMO->L+3 (43%)	HOMO->L+1 (9%)
7	26926,01306	371,38807	0,0136	Singlet-A	H-1->L+3 (19%), H-1->L+5 (11%), HOMO->L+2 (11%), HOMO->L+4 (53%)	–
8	27229,27752	367,25176	1E-3	Singlet-A	H-1->L+2 (32%), H-1->L+4 (24%), HOMO->L+3 (12%), HOMO->L+5 (23%)	HOMO->L+4 (2%)
9	29109,3559	343,53216	0,0036	Singlet-A	HOMO->L+6 (69%)	H-1->L+4 (2%), H-1->L+7 (9%), H-1->L+8 (3%), H-1->L+9 (2%), HOMO->L+3 (5%), HOMO->L+5 (2%)
10	29461,82018	339,42234	0,0043	Singlet-A	H-1->L+6 (42%), HOMO->L+7 (37%)	H-1->L+3 (2%), H-1->L+7 (4%), HOMO->L+8 (5%), HOMO->L+9 (3%)
11	29523,92487	338,70835	0,0028	Singlet-A	H-1->L+2 (19%), HOMO->L+3 (19%), HOMO->L+5 (33%)	H-1->L+4 (4%), H-1->L+6 (4%), H-1->L+7 (7%), H-1->L+10 (3%), HOMO->L+6 (5%), HOMO->L+13 (2%)
12	29802,18615	335,54585	0,0568	Singlet-A	H-1->L+3 (37%), H-1->L+5 (21%), HOMO->L+2 (11%), HOMO->L+7 (10%)	H-1->L+13 (2%), HOMO->L+4 (7%), HOMO->L+10 (5%)
13	30213,52891	330,97756	0,0435	Singlet-A	H-1->L+8 (26%), HOMO->L+8 (42%)	H-1->L+9 (4%), H-1->L+10 (5%), HOMO->L+9 (6%), HOMO->L+10 (7%)
14	30269,98772	330,36023	0,0428	Singlet-A	H-1->L+9 (20%), HOMO->L+9 (41%), HOMO->L+10 (16%)	H-1->L+7 (4%), H-1->L+10 (8%), HOMO->L+7 (3%)
15	30624,06511	326,54058	0,0043	Singlet-A	H-1->L+3 (19%), H-1->L+5 (11%), HOMO->L+4 (21%), HOMO->L+10 (16%)	H-1->L+4 (2%), H-1->L+12 (3%), H-1->L+13 (4%), HOMO->L+9 (2%), HOMO->L+12 (7%)
16	30699,88123	325,73416	4E-4	Singlet-A	##	H-1->L+10 (3%), H-1->L+11 (4%), HOMO->L+3 (7%), HOMO->L+5 (4%), HOMO->L+13 (4%)
17	30753,11382	325,17032	9E-4	Singlet-A	H-1->L+11 (31%), HOMO->L+11 (40%), HOMO->L+12 (12%)	HOMO->L+10 (2%)
18	30778,92357	324,89765	4E-4	Singlet-A	H-1->L+4 (26%), H-1->L+12 (13%), HOMO->L+12 (22%)	##
19	31224,94816	320,25674	0,0044	Singlet-A	H-1->L+14 (13%), HOMO->L+13 (43%)	H-1->L+4 (4%), H-1->L+5 (4%), H-1->L+7 (6%), H-1->L+10 (3%), HOMO->L+5 (9%), HOMO->L+15 (5%)
20	31395,9377	318,51254	0,0016	Singlet-A	H-1->L+13 (20%), H-1->L+15 (10%), HOMO->L+14 (41%)	H-1->L+5 (9%), H-1->L+6 (2%), H-1->L+14 (4%), HOMO->L+7 (3%), HOMO->L+13 (4%)

Table S26: Transition energy, wavelengths, and oscillator strength of the electronic transition of **3bDip.**

No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	18347,50015	545,03338	1,0124	Singlet-A	HOMO->LUMO (98%)	–
2	19737,99999	506,63694	0,0011	Singlet-A	H-1->LUMO (98%)	–
3	22908,56545	436,51795	0,0028	Singlet-A	HOMO->L+1 (88%)	H-1->L+2 (5%), HOMO->L+3 (2%)
4	23765,9328	420,77036	0,1962	Singlet-A	H-1->L+1 (75%), HOMO->L+2 (13%)	H-1->L+3 (4%)
5	25219,34389	396,52102	0,0784	Singlet-A	H-1->L+1 (20%), HOMO->L+2 (64%)	H-1->L+3 (9%), HOMO->L+4 (3%)
6	25782,31888	387,86271	2E-4	Singlet-A	H-1->L+2 (47%), HOMO->L+3 (32%)	H-1->L+4 (9%), HOMO->L+1 (9%)
7	26730,82689	374,09991	0,0748	Singlet-A	H-1->L+3 (21%), H-1->L+5 (11%), HOMO->L+4 (50%)	H-1->L+2 (2%), HOMO->L+2 (8%), HOMO->L+3 (3%)
8	26948,59658	371,07684	0,008	Singlet-A	H-1->L+2 (22%), H-1->L+4 (27%), HOMO->L+3 (18%), HOMO->L+5 (23%)	HOMO->L+4 (5%)
9	28985,14652	345,00429	0,5431	Singlet-A	H-2->LUMO (45%), H-1->L+5 (18%), HOMO->L+8 (13%)	H-1->L+3 (7%), HOMO->L+2 (4%), HOMO->L+6 (7%)
10	29139,19841	343,18034	0,0077	Singlet-A	H-1->L+2 (20%), HOMO->L+3 (22%), HOMO->L+5 (41%)	H-1->L+4 (2%), H-1->L+6 (2%), H-1->L+8 (5%)
11	29376,32541	340,41017	0,0024	Singlet-A	H-1->L+6 (25%), HOMO->L+6 (46%), HOMO->L+7 (10%)	H-1->L+7 (4%), H-1->L+8 (3%), HOMO->L+8 (8%)
12	29461,01363	339,43163	1E-4	Singlet-A	H-1->L+7 (31%), HOMO->L+7 (50%)	H-1->L+6 (4%), HOMO->L+6 (6%), HOMO->L+8 (5%)
13	30017,53618	333,1386	0,2492	Singlet-A	H-2->LUMO (21%), H-1->L+3 (25%), HOMO->L+10 (13%)	H-1->L+5 (7%), H-1->L+9 (9%), HOMO->L+2 (4%), HOMO->L+4 (3%), HOMO->L+9 (8%), HOMO->L+16 (2%)
14	30337,73829	329,62246	0,012	Singlet-A	H-1->L+9 (13%), H-1->L+10 (15%), HOMO->L+9 (51%)	H-1->L+3 (4%), H-1->L+8 (3%), HOMO->L+10 (4%)
15	30495,01641	327,92243	0,0609	Singlet-A	##	H-2->LUMO (5%), H-1->L+9 (7%)
16	30688,58947	325,85401	0,1879	Singlet-A	H-2->LUMO (12%), HOMO->L+4 (11%), HOMO->L+8 (19%)	##
17	30713,59266	325,58874	0,0034	Singlet-A	H-1->L+4 (36%), HOMO->L+3 (14%), HOMO->L+11 (12%)	H-1->L+8 (5%), H-1->L+11 (8%), HOMO->L+5 (6%), HOMO->L+12 (3%), HOMO->L+13 (7%)
18	30765,21214	325,04245	0,0048	Singlet-A	H-1->L+4 (11%), H-1->L+11 (26%), HOMO->L+11 (47%)	HOMO->L+3 (4%), HOMO->L+4 (2%), HOMO->L+5 (2%)
19	30827,31683	324,38762	0,0026	Singlet-A	H-1->L+12 (35%), HOMO->L+12 (52%)	H-1->L+4 (4%)
20	31248,33824	320,01702	2E-4	Singlet-A	H-1->L+14 (22%), HOMO->L+13 (45%)	H-1->L+4 (5%), H-1->L+8 (3%), HOMO->L+5 (7%), HOMO->L+14 (5%), HOMO->L+15 (4%)

Table S27: Transition energy, wavelengths, and oscillator strength of the electronic transition of **3cDip.**

No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs	
1	18820,14105	531,34565	0,585	Singlet-A	HOMO->LUMO (98%)		--
2	20436,47612	489,32115	3E-4	Singlet-A	H-1->LUMO (95%)		--
3	23352,97694	428,21093	0,0016	Singlet-A	HOMO->L+1 (80%)	H-1->L+2 (8%), HOMO->L+3 (3%), HOMO->L+6 (2%)	
4	23603,00881	423,6748	0,131	Singlet-A	HOMO->L+2 (82%)	H-1->L+1 (7%)	
5	24999,96108	400,00062	0,0656	Singlet-A	H-1->L+1 (70%)	H-1->L+2 (8%), HOMO->L+2 (9%), HOMO->L+4 (6%)	
6	25274,18959	395,66056	0,0071	Singlet-A	H-1->L+2 (73%)	H-1->L+1 (7%), HOMO->L+1 (9%), HOMO->L+3 (6%)	
7	26608,23061	375,82356	0,0921	Singlet-A	H-1->L+3 (21%), HOMO->L+3 (46%), HOMO->L+4 (10%)	H-1->L+1 (3%), H-1->L+2 (3%), H-1->L+5 (3%), HOMO->L+5 (9%)	
8	26842,1314	372,54866	0,0591	Singlet-A	H-1->L+4 (16%), H-1->L+5 (10%), HOMO->L+3 (15%), HOMO->L+4 (40%)	H-1->L+1 (2%), H-1->L+2 (4%), H-1->L+3 (3%), HOMO->L+5 (7%), HOMO->L+6 (2%)	
9	27434,14235	364,5093	0,0383	Singlet-A	HOMO->L+4 (21%), HOMO->L+5 (59%)	H-1->L+1 (5%), H-1->L+6 (9%), HOMO->L+3 (2%)	
10	28474,59756	351,19021	2E-4	Singlet-A	H-1->L+4 (28%), H-1->L+5 (29%), HOMO->L+6 (33%)	H-1->L+3 (3%), HOMO->L+1 (3%)	
11	30008,66409	333,23709	0,0203	Singlet-A	H-2->LUMO (23%), H-1->L+4 (15%), HOMO->L+7 (20%)	H-1->L+3 (2%), H-1->L+6 (9%), HOMO->L+3 (7%), HOMO->L+6 (8%), HOMO->L+8 (2%), HOMO->L+9 (3%)	
12	30094,15885	332,2904	7E-4	Singlet-A	##	H-1->L+7 (2%), H-1->L+8 (2%), HOMO->L+7 (7%)	
13	30195,78471	331,17205	0,0101	Singlet-A	H-1->L+7 (17%), HOMO->L+8 (51%)	H-2->LUMO (4%), H-1->L+3 (4%), H-1->L+4 (4%), H-1->L+6 (3%), HOMO->L+4 (5%)	
14	30231,27311	330,78329	0,0391	Singlet-A	H-1->L+3 (28%), H-1->L+4 (10%), HOMO->L+7 (13%)	H-2->LUMO (7%), H-1->L+6 (3%), H-1->L+7 (5%), HOMO->L+4 (8%), HOMO->L+5 (6%), HOMO->L+8 (6%)	
15	30345,80384	329,53485	0,0239	Singlet-A	H-2->LUMO (17%), H-1->L+3 (15%), HOMO->L+7 (26%)	H-1->L+4 (3%), H-1->L+8 (8%), H-1->L+9 (5%), HOMO->L+4 (6%), HOMO->L+5 (3%), HOMO->L+8 (2%), HOMO->L+9 (8%)	
16	30483,72464	328,0439	0,0148	Singlet-A	H-2->LUMO (15%), H-1->L+9 (13%), HOMO->L+9 (53%)	H-1->L+5 (5%), H-1->L+8 (3%)	
17	30672,45838	326,02538	0,0053	Singlet-A	H-1->L+10 (15%), HOMO->L+10 (40%), HOMO->L+12 (12%)	H-2->LUMO (3%), H-1->L+5 (4%), H-1->L+11 (6%), H-1->L+12 (4%), HOMO->L+11 (9%)	
18	30749,08105	325,21297	0,0019	Singlet-A	H-1->L+11 (14%), HOMO->L+11 (52%)	H-1->L+5 (8%), H-1->L+10 (6%), HOMO->L+6 (2%), HOMO->L+10 (8%)	
19	30882,96909	323,80306	0,0019	Singlet-A	H-1->L+5 (10%), H-1->L+12 (15%), HOMO->L+10 (20%), HOMO->L+12 (33%)	H-1->L+6 (2%), H-1->L+10 (6%), HOMO->L+6 (4%)	
20	31089,44702	321,65255	0,0018	Singlet-A	H-1->L+5 (27%), HOMO->L+6 (21%), HOMO->L+12 (18%)	##	

Table S28: Transition energy, wavelengths, and oscillator strength of the electronic transition of **3dDip.**

No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs	
1	15206,7772	657,60153	0,1468	Singlet-A	HOMO->LUMO (99%)		--
2	16010,91197	624,57404	0	Singlet-A	H-1->LUMO (99%)		--
3	23010,99786	434,57481	0,4382	Singlet-A	H-2->LUMO (30%), HOMO->L+1 (60%)	H-1->L+2 (5%)	
4	23635,27099	423,09648	0	Singlet-A	HOMO->L+2 (82%)	H-1->L+1 (7%), HOMO->L+7 (2%)	
5	24167,59691	413,77718	0,0658	Singlet-A	H-2->LUMO (53%), HOMO->L+1 (34%)	H-1->L+2 (9%)	
6	24448,27785	409,02677	0	Singlet-A	H-1->L+1 (85%), HOMO->L+2 (11%)		--
7	24801,54869	403,20063	0,0886	Singlet-A	H-2->LUMO (12%), H-1->L+2 (77%)		--
8	26988,9243	370,52236	0,0713	Singlet-A	H-1->L+4 (25%), HOMO->L+3 (65%)	HOMO->L+5 (5%)	
9	27092,96982	369,09944	0	Singlet-A	H-1->L+3 (24%), H-1->L+5 (12%), HOMO->L+4 (60%)		--
10	27649,49238	361,67029	0,0053	Singlet-A	H-1->L+4 (12%), HOMO->L+3 (17%), HOMO->L+5 (64%)	H-11->LUMO (4%)	
11	28509,2794	350,76299	0	Singlet-A	H-1->L+3 (56%), H-1->L+5 (38%)	HOMO->L+4 (4%)	
12	29129,51976	343,29437	0,0533	Singlet-A	H-1->L+7 (13%), HOMO->L+6 (73%)	H-2->L+1 (5%), H-1->L+2 (2%)	
13	29348,09601	340,73761	0	Singlet-A	H-2->L+2 (61%), H-1->L+6 (18%), HOMO->L+7 (18%)		--
14	29458,59396	339,45951	0,0131	Singlet-A	H-2->L+1 (87%)	HOMO->L+6 (5%)	
15	29795,73372	335,61852	0	Singlet-A	H-2->L+2 (33%), H-1->L+6 (33%), HOMO->L+7 (20%)	HOMO->L+10 (3%)	
16	30443,39692	328,47846	0,0018	Singlet-A	H-7->LUMO (19%), H-3->LUMO (62%)	H-9->LUMO (2%), H-6->LUMO (8%), H-1->L+4 (3%)	
17	30500,66229	327,86173	0,0045	Singlet-A	H-1->L+4 (50%), HOMO->L+3 (12%), HOMO->L+5 (19%)	H-5->LUMO (4%), H-4->LUMO (3%), H-3->LUMO (5%)	
18	30500,66229	327,86173	4E-4	Singlet-A	H-8->LUMO (15%), H-5->LUMO (44%), H-4->LUMO (32%)	H-1->L+4 (4%)	
19	30553,08832	327,29916	0	Singlet-A	H-1->L+3 (16%), H-1->L+5 (42%), HOMO->L+4 (30%)	H-1->L+6 (4%)	
20	30642,61587	326,3429	0	Singlet-A	H-8->LUMO (48%), H-4->LUMO (48%)	H-5->LUMO (3%)	

References

[X1] (a) SHELXTL, Bruker AXS, Madison, WI; (b) SHELX-97, G.M. Sheldrick, *Acta Cryst*., 2008, **A64**, 112-122; (c) SHELX-2013, G.M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3-8.