Supplementary materials

Synthesis of fused chalcogenophenocarbazoles: towards dual emission resulting from hybridized local and charge-transfer states

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Instrumentation

Thermogravimetric analysis (TGA) was performed on a TA Instruments Q50 apparatus. The samples were heated at a rate of 20 °C/min.

Cyclic Voltammetry. CV measurements were carried out with a glassy carbon working electrode in a three−electrode cell using a μ-Autolab Type III (EcoChemie, Netherlands) potentiostat. A platinum wire as counter electrode, a glassy carbon working electrode, and a silver wire as reference electrode. Tetrabutylammonium hexafluorophosphate (n-Bu_4NPF_6) (0.1 M solution in dichloromethane) was used as supporting electrolyte at a scan rate of 100 mV/s. The reference electrode was calibrated versus ferrocene/ferrocenium redox couple as an internal standard.

The Edinburgh Instruments FLS980 and Avantes spectrometers were exploited for recording of emission and UV/Vis absorbance spectra of the compounds **7-11**, respectively. The PicoQuant LDH-D-C-375 laser (wavelength 374 nm) as the excitation source was used for taking of their photoluminescence decay curves. The integrated sphere (inner diameter of 120 mm) on Edinburgh Instruments FLS980 spectrometer was used for measuring of photoluminescence quantum yields (PLQYs).

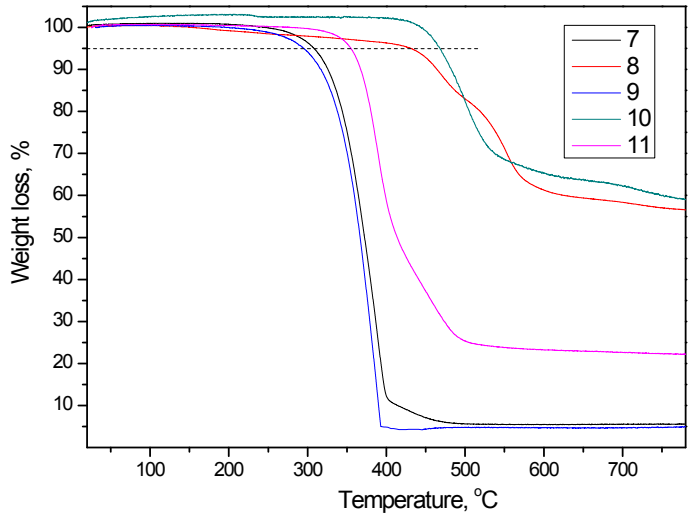


Figure S1. TGA curves of compounds **7-11** (scan rate of 20 ºC/min. N_2 atmosphere)

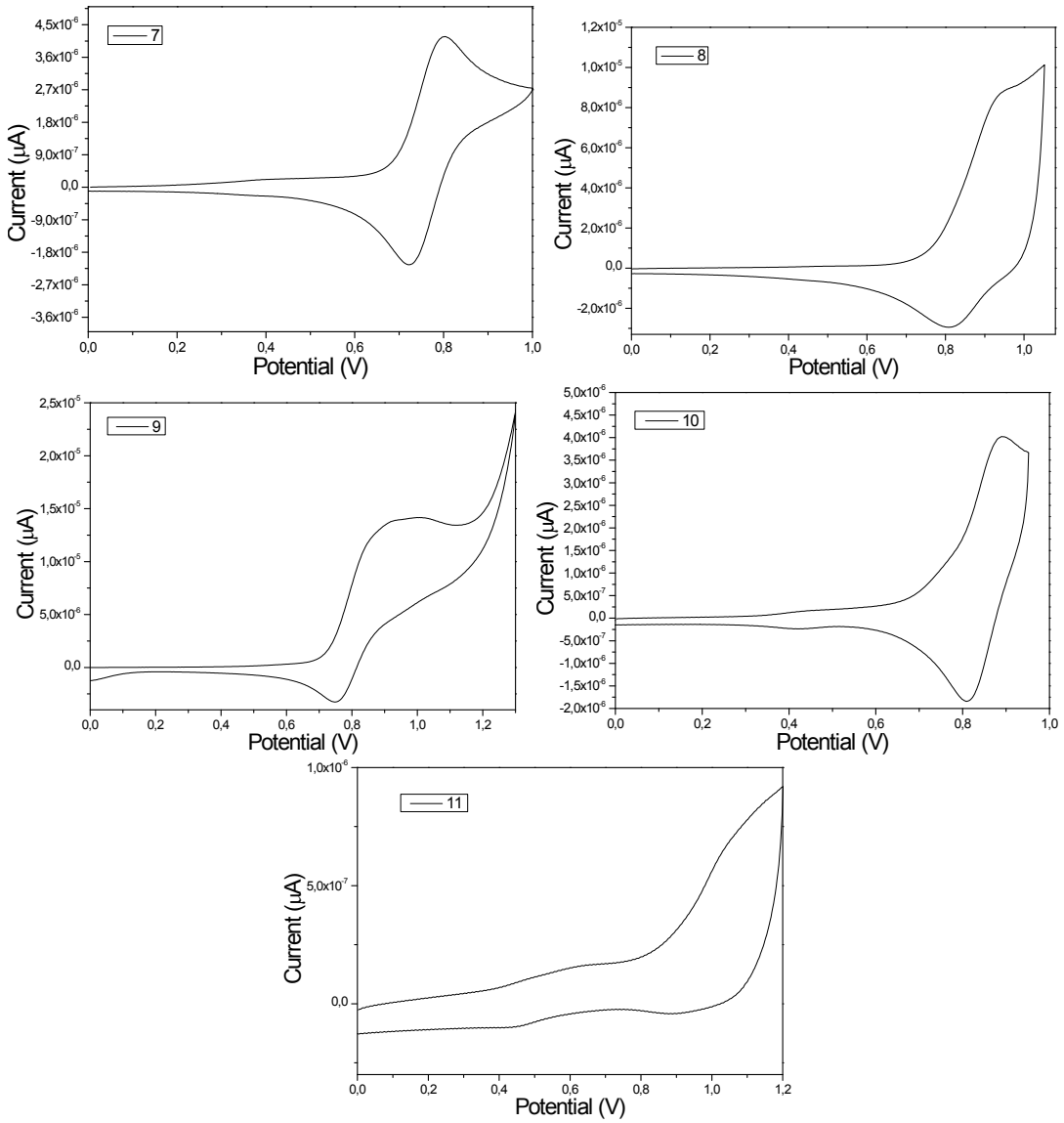
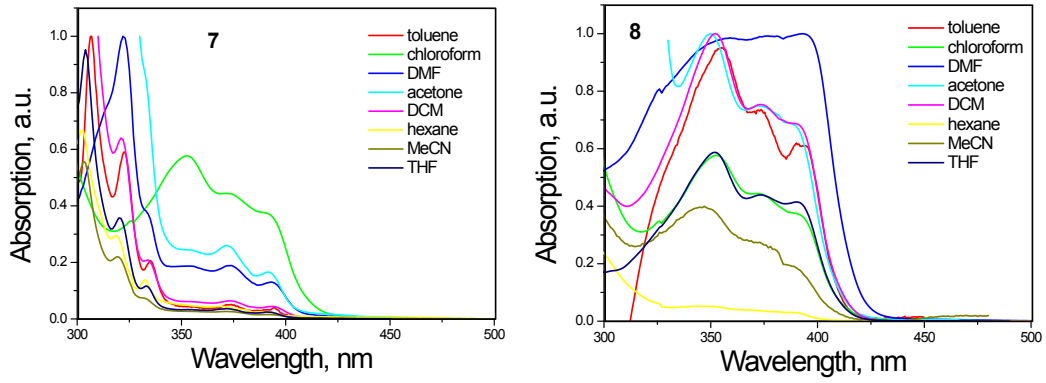


Figure S2. Cyclic voltammograms of dilute solutions of compounds **8**–**11** in dichloromethane (room temperature) recorded at sweep rate of 0.1 V/s



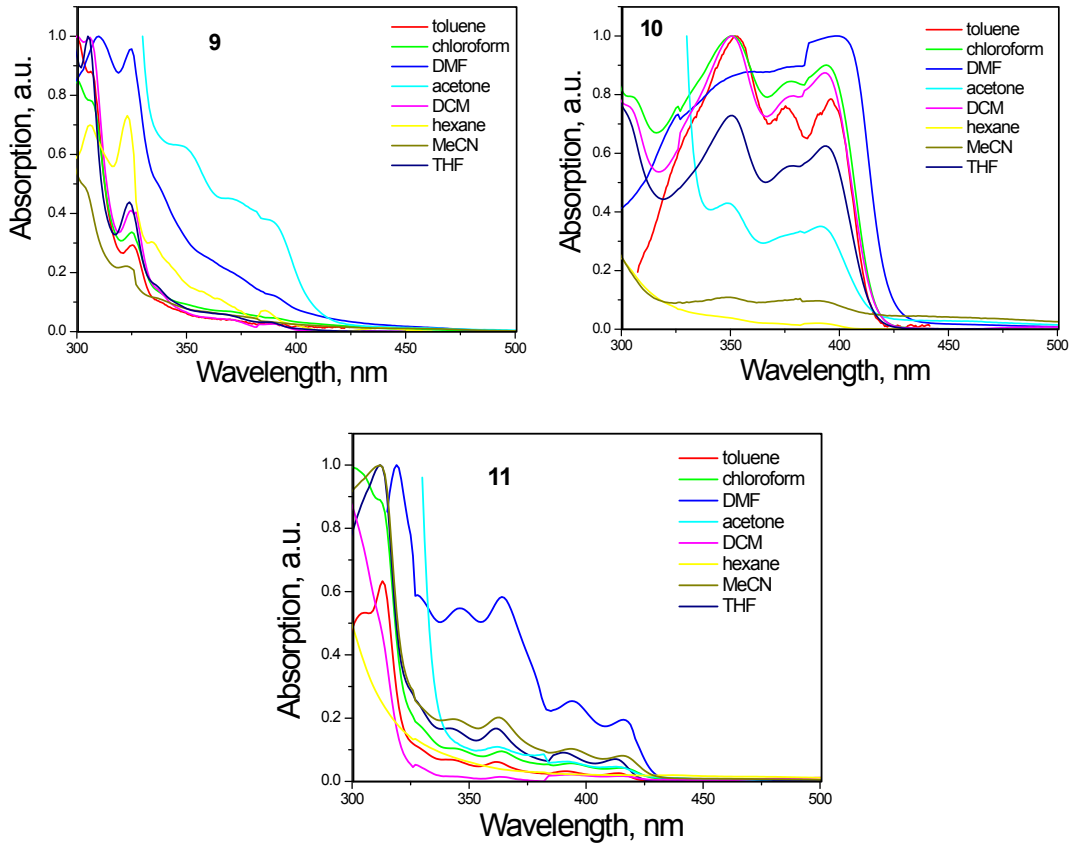


Figure S3. Absorption spectra of compounds **7-11** in different solutions.

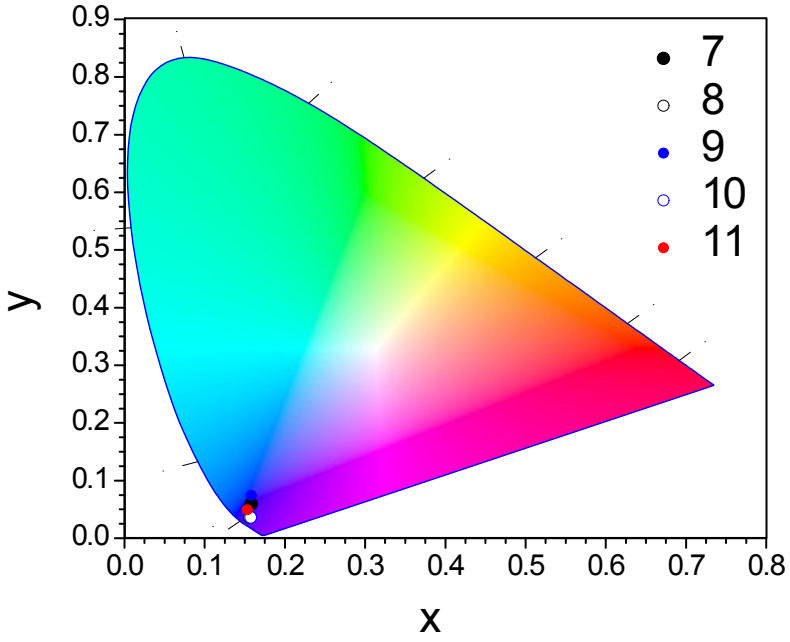


Figure S4. CIE coordinates of emission colors of compounds **7-11** in toluene.

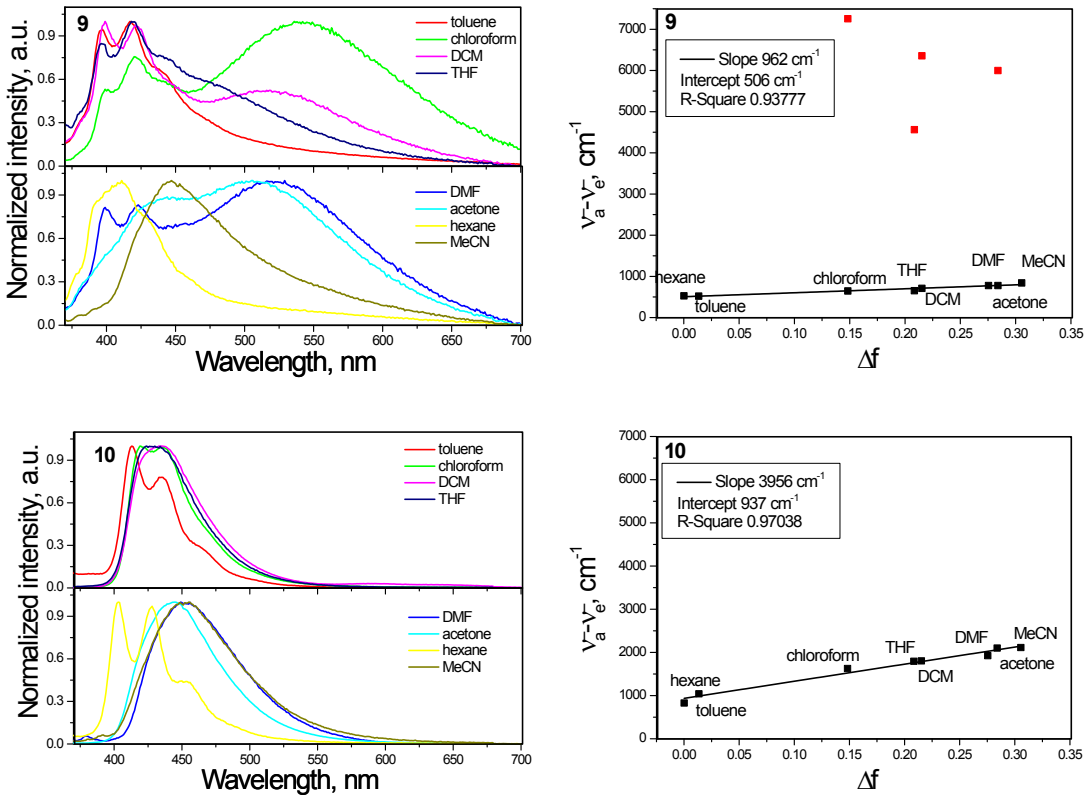


Figure S5. Solvatofluorochromism (left) and corresponding Lippert–Mataga plots (right) (Stokes shift (ν_{abs}-ν_{em}) versus orientation polarizability of solvent (Δf)) for compounds **9** and **10.**

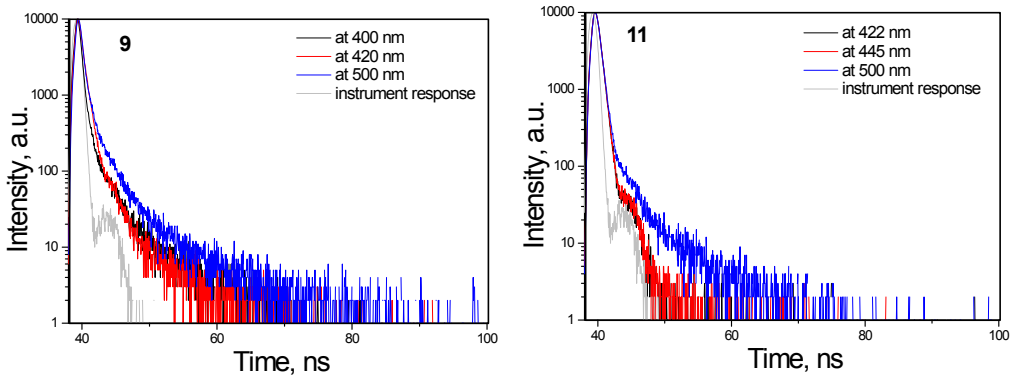


Figure S6. PL decays for compounds **9, 10** and **11** in THF at different emission wavelengths.

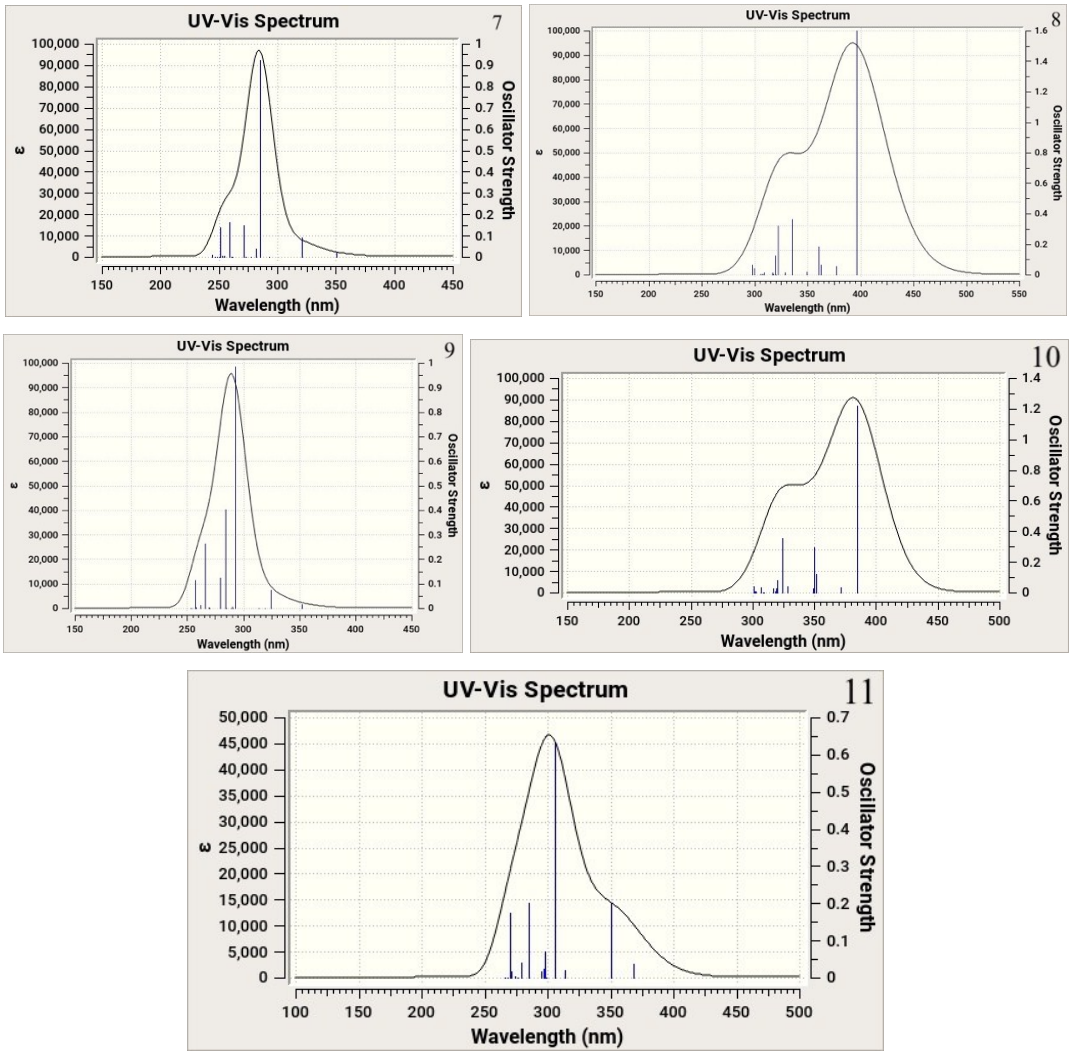


Figure S7. Theoretically calculated (B3LYP/6-31+G*) UV/Vis spectra of compounds **7-11.**

Table S1. Photophysical parameters of compounds **7-11**.

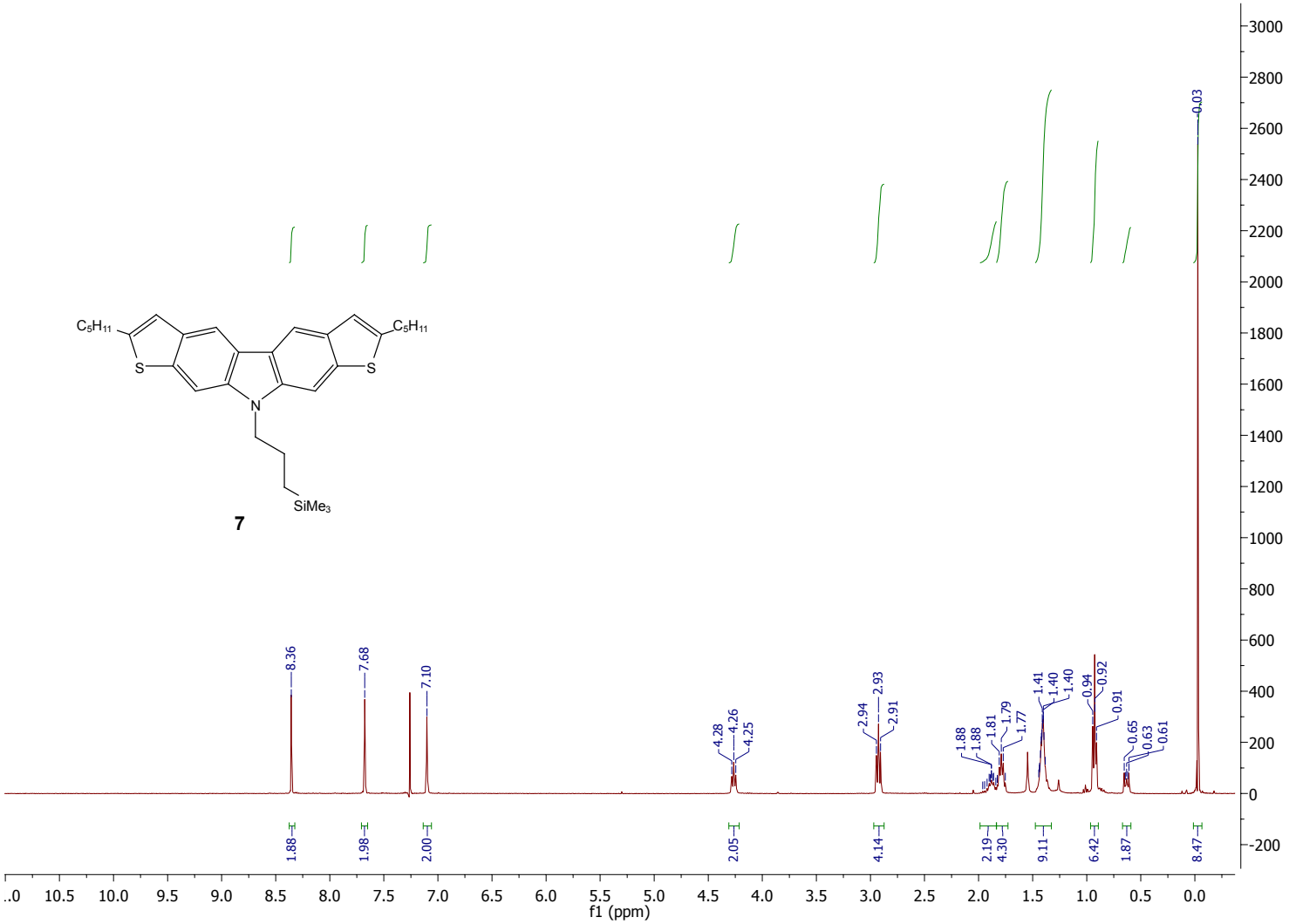
Compound	Φ_{tol}, %	$\Phi_{chloroform}$, %	τ, ns (χ^2)
7	2	2	0.78 (97 %), 3.23 (3%) at 400 nm (1.067); 0.83 (96%), 3.96 (4%) at 424 nm (1.008); 1.21 (41%), 3.06 (52%), 11.51 (7%) at 500 nm (1.129)
8	9	9	0.73 at 424 nm (1.003); 0.74 at 440 nm (1.008); 0.78 at 500 nm (1.170)
9	0.1	0.1	0.04 (81 %), 0.89 (17%), 5.49 (2%) at 400 nm (1.032); 0.08 (51 %), 0.73 (47%), 4.86 (2%) at 420 nm (1.006); 0.19 (70 %), 1.05 (26 %), 5.28 (4%) at 500 nm (1.061)
10	0.3	0.5	-[a]

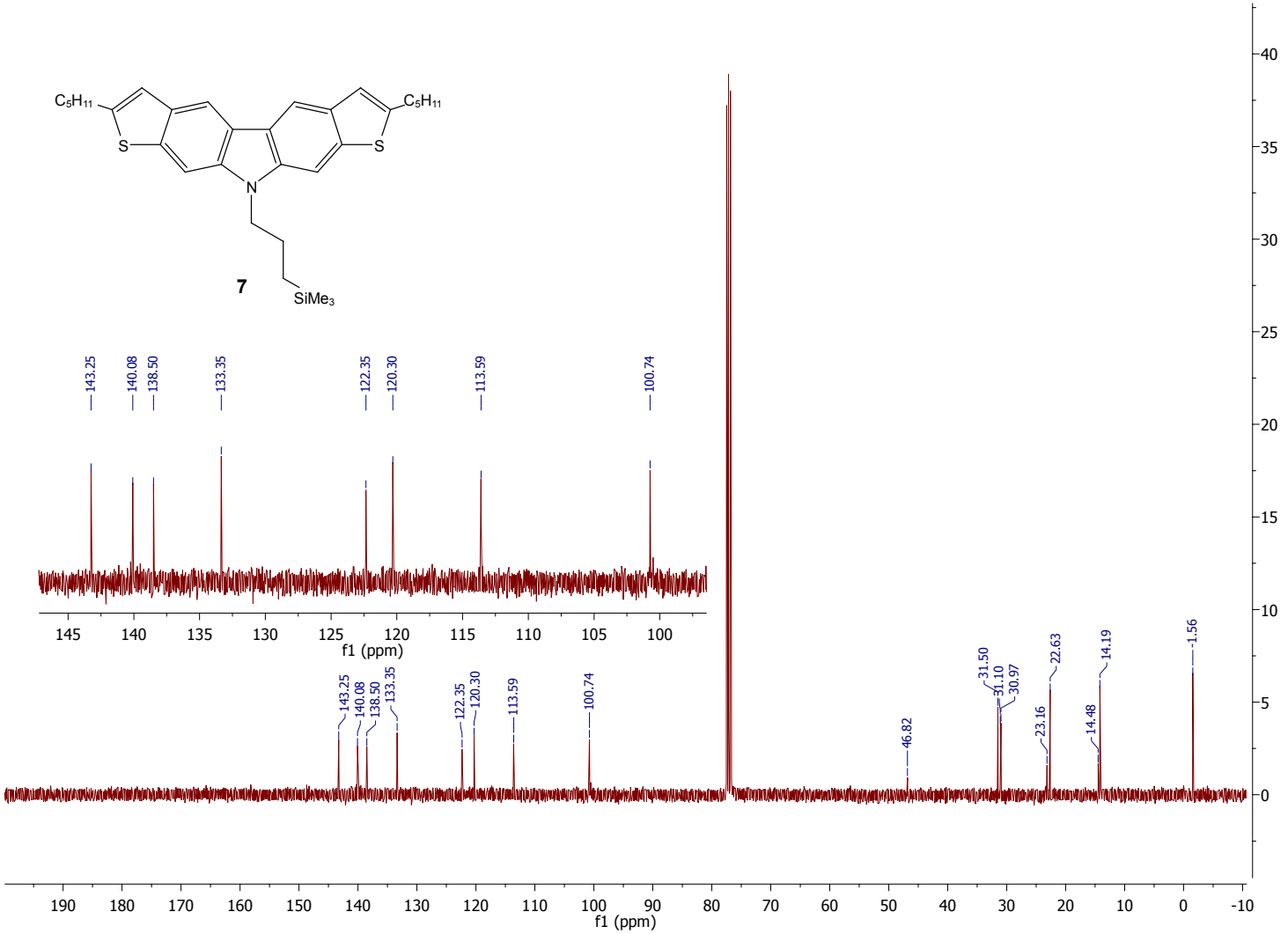
11	1	1	0.51 at 422 nm (1.042); 0.52 at 445 nm (1.028); 0.53 (97%), 4.71 (3%) at 500 nm (1.021)

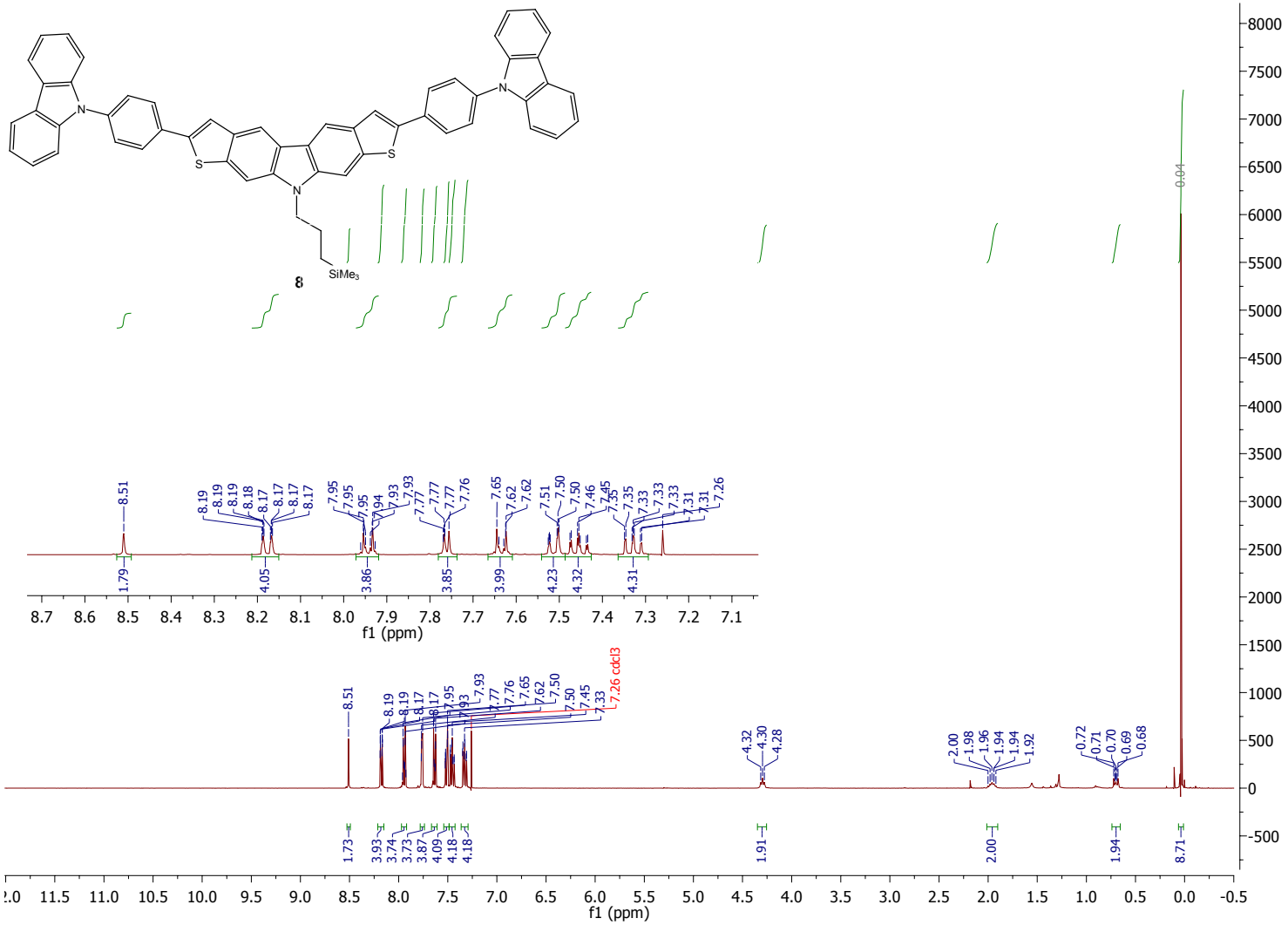
[a] PL decays were not recorded due to the very weak emission.

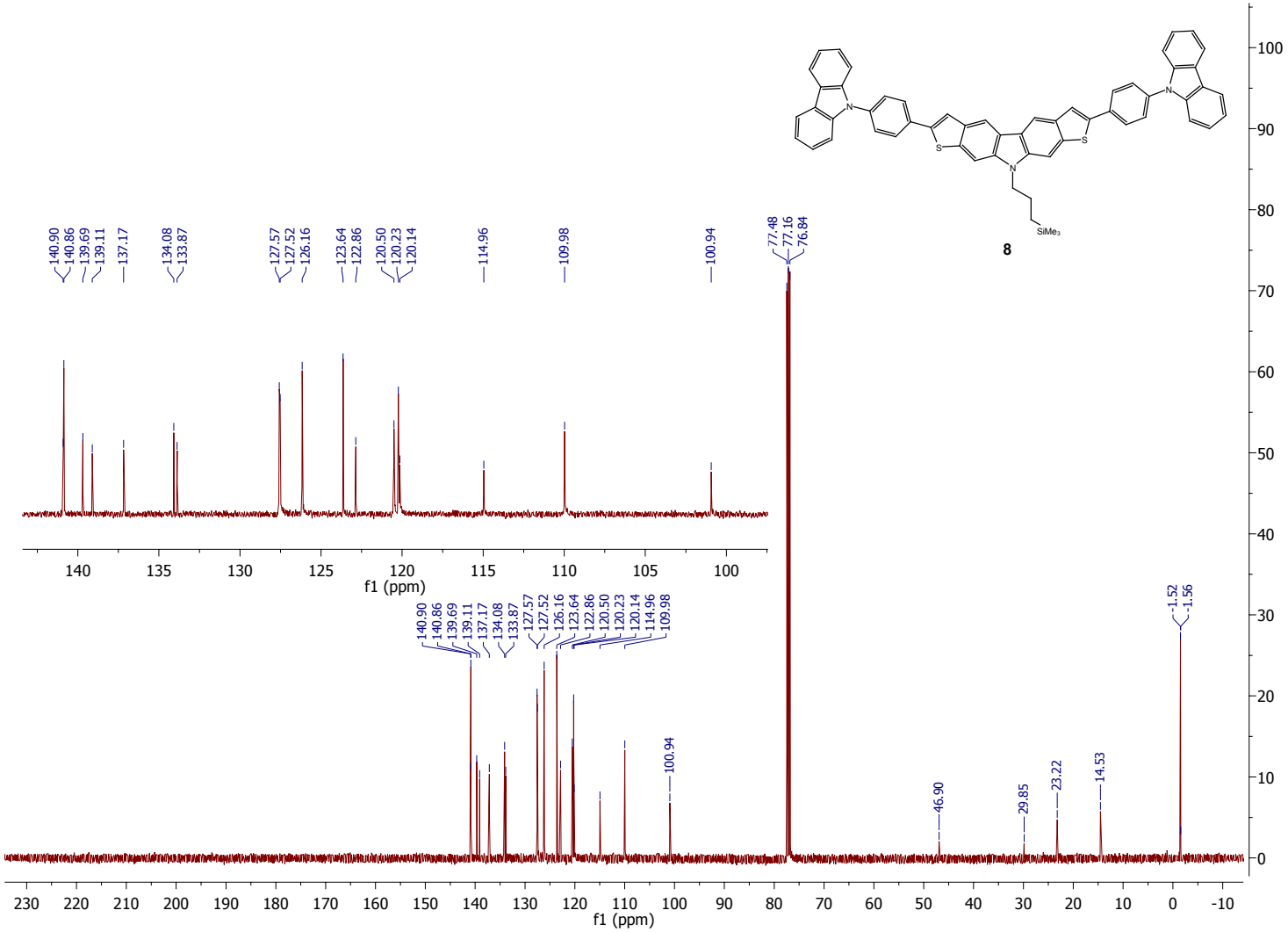
Table S2. Results of theoretical characterization of compounds **7-11.**

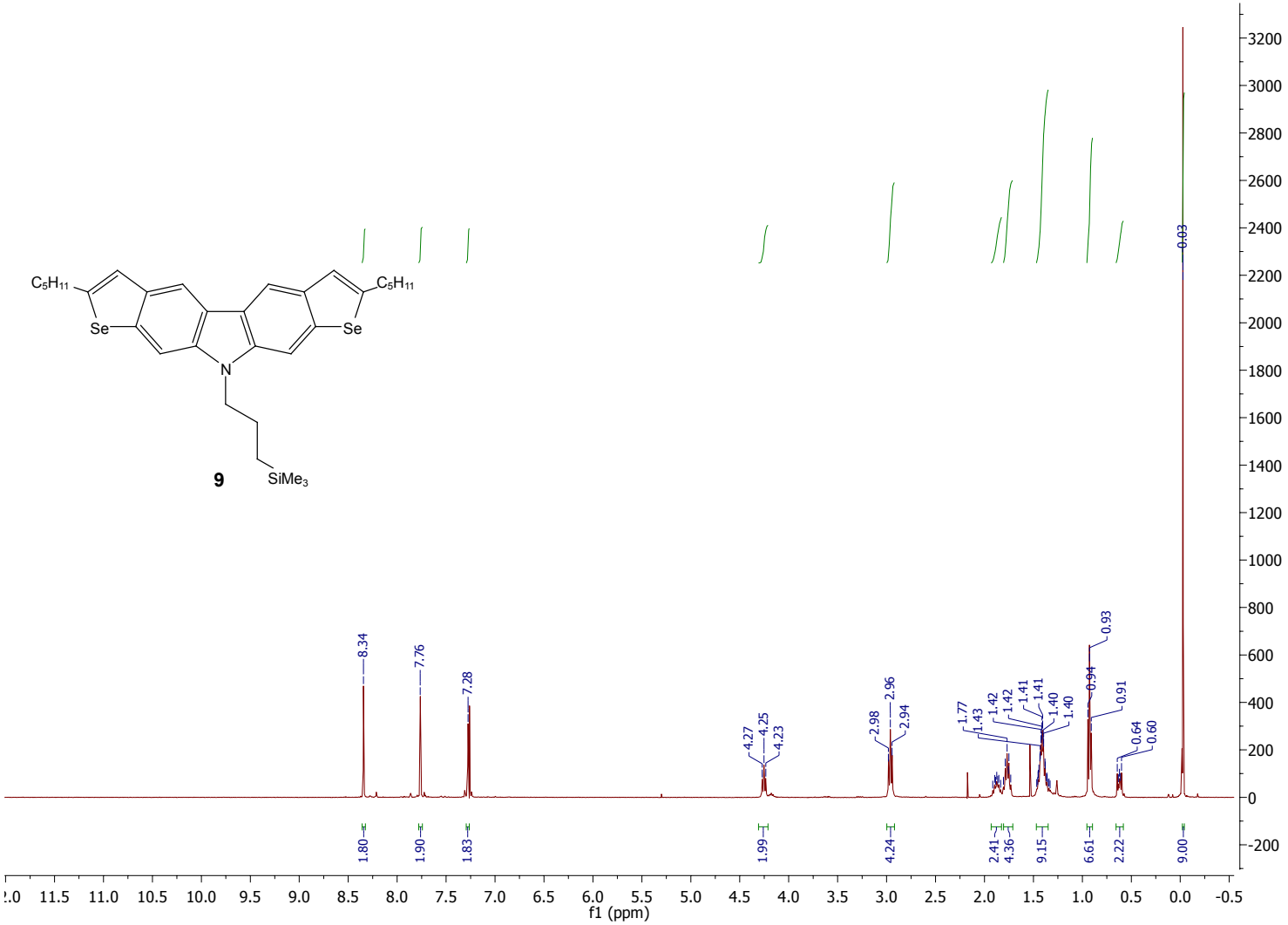
	7	**8**	**9**	**10**	**11**
HOMO	-5.1	-5.3	-5.1	-5.0	-6.2
LUMO	-1.1	-1.7	-1.1	-1.5	-2.3

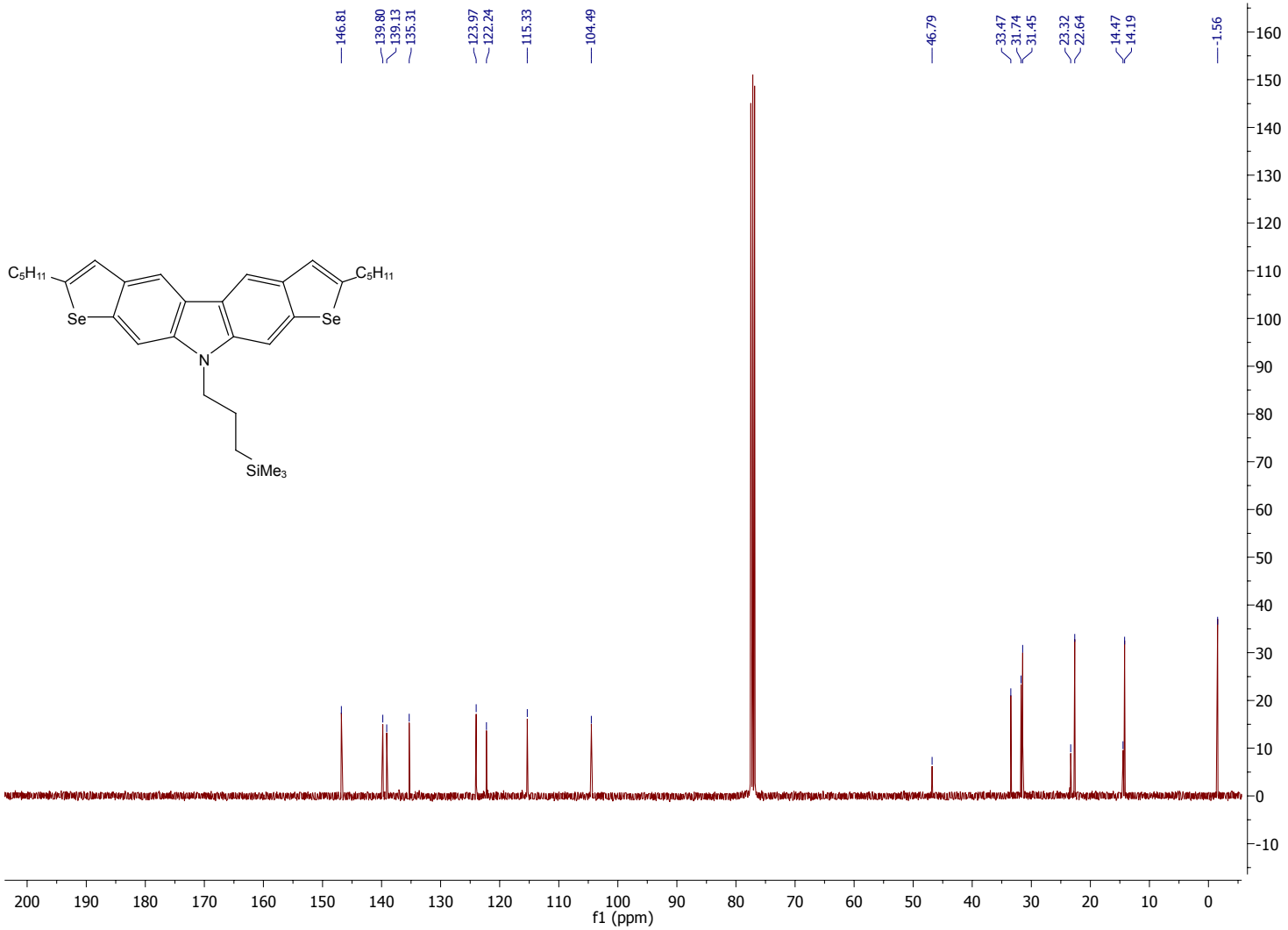

C5H11
C5H11
S
S
N
SiMe3
7
8.36
7.68
7.10
4.28
4.26
4.25
2.94
2.93
2.91
1.88
1.88
1.81
1.79
1.77
1.41
1.40
1.40
0.94
0.92
0.91
0.65
0.63
0.61
0.03
1.88
1.98
2.00
2.05
4.14
2.19
4.30
9.11
6.42
1.87
8.47
f1 (ppm)

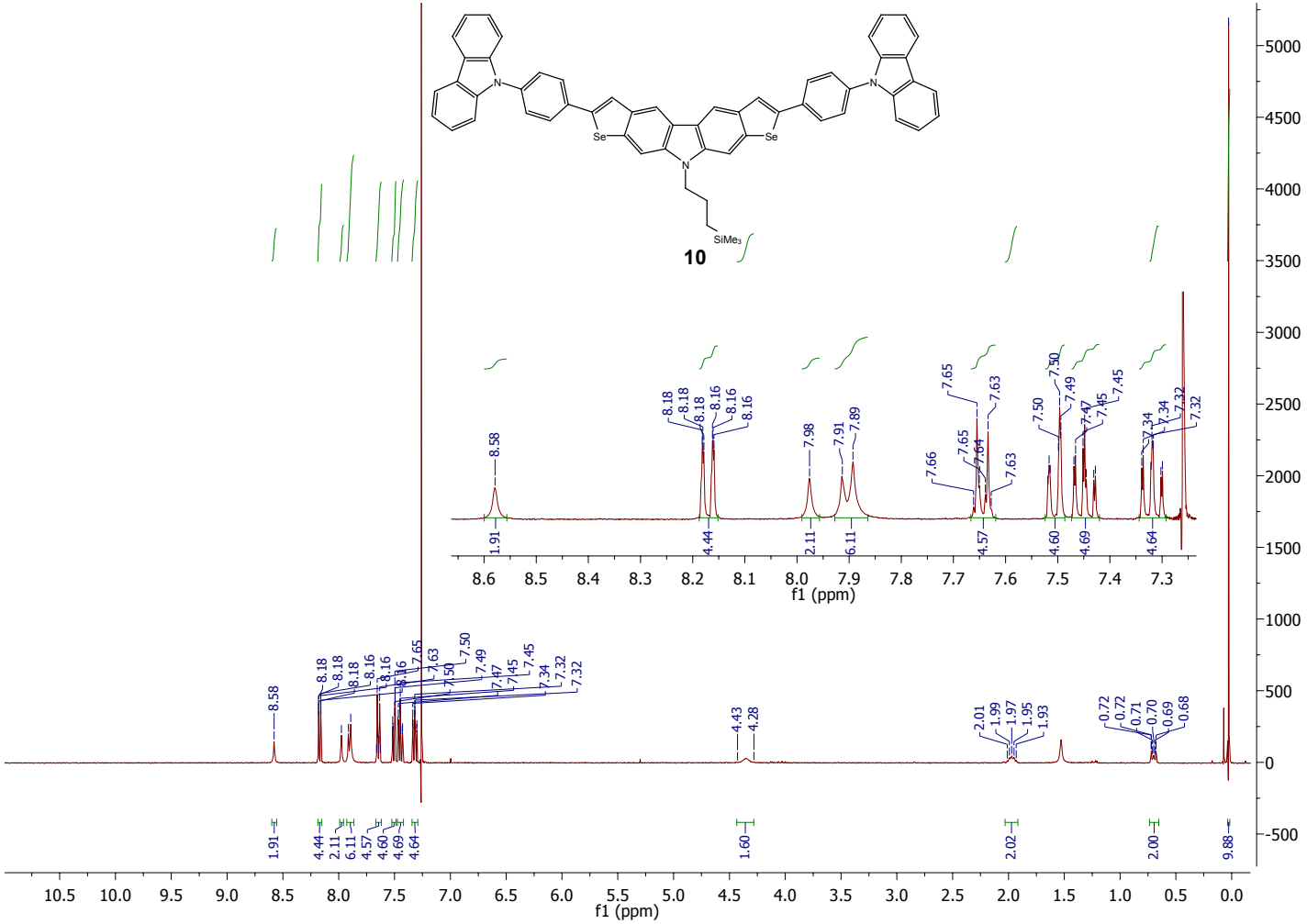

C5H11
S
S
C5H11
N
SiMe3
7
143.25
140.08
138.50
133.35
122.35
120.30
113.59
100.74
f1 (ppm)
46.82
31.50
31.10
30.97
23.16
22.63
14.48
14.19
-1.56
f1 (ppm)

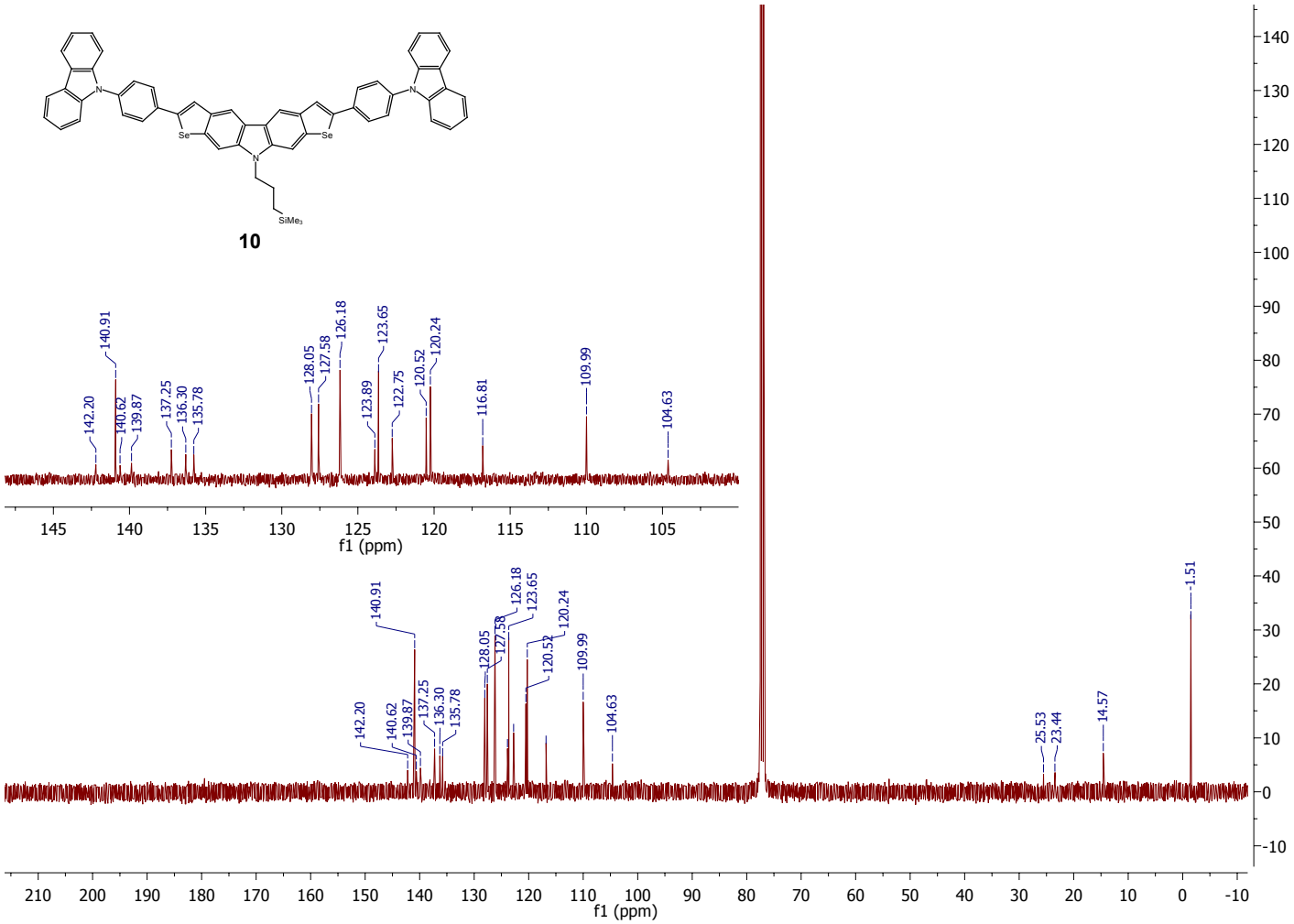

SiMe3
8
f1 (ppm)
cdcl3

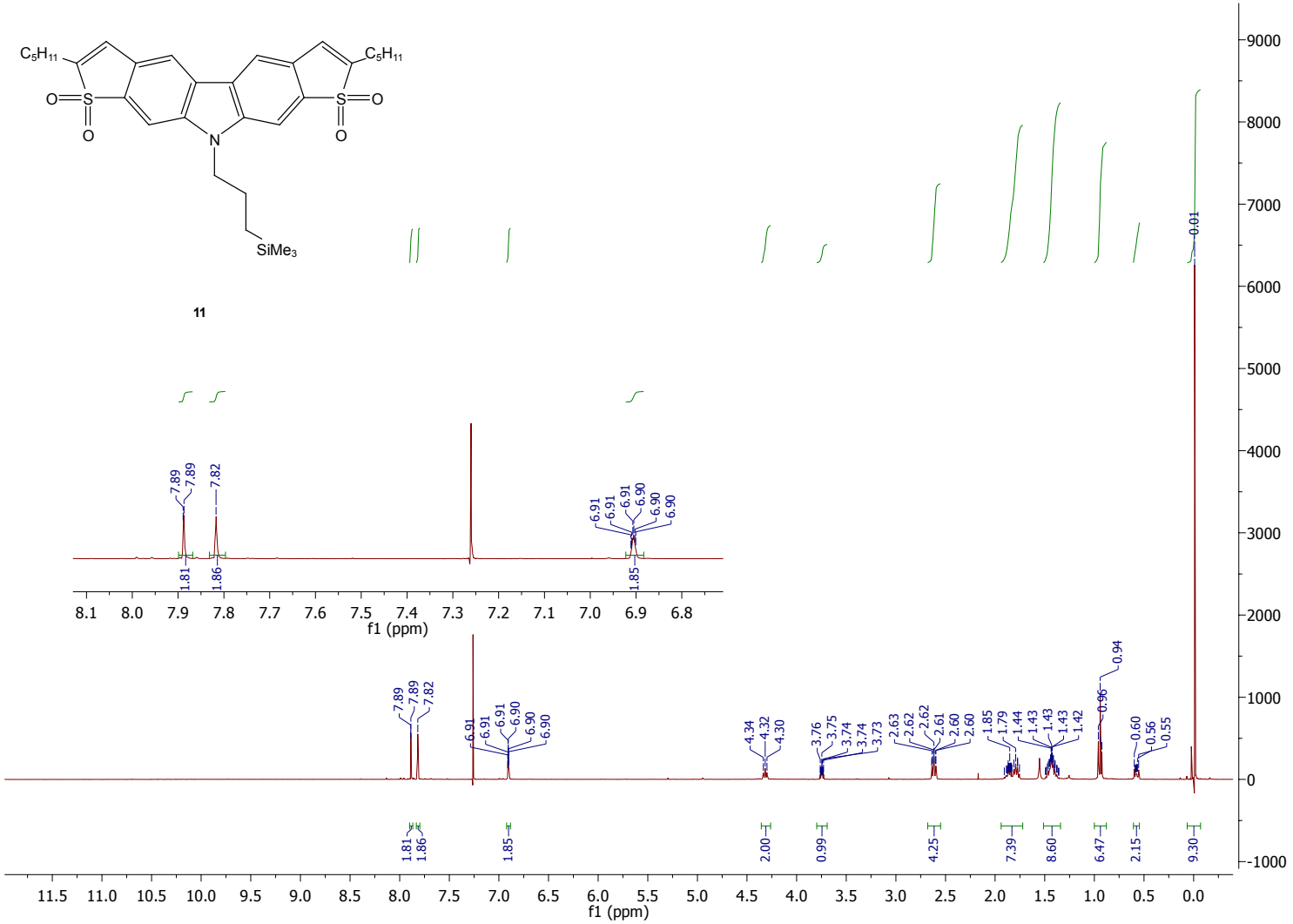

8
SiMe3
140.90
140.86
139.69
139.11
137.17
134.08
133.87
127.57
127.52
126.16
123.64
122.86
120.50
120.23
120.14
114.96
109.98
100.94
77.48
77.16
76.84
46.90
29.85
23.22
14.53
-1.52
-1.56
f1 (ppm)

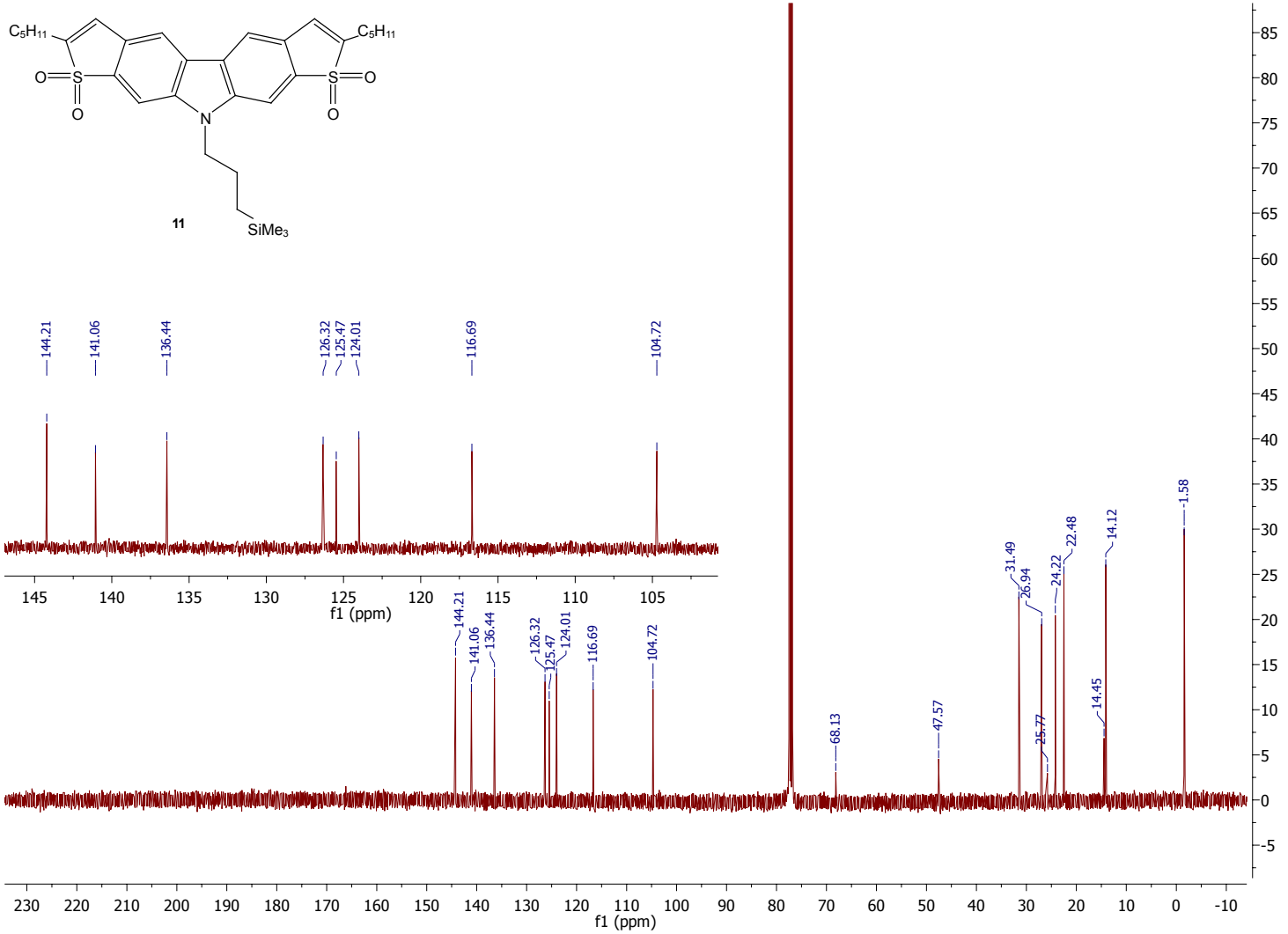

C5H11
Se
Se
C5H11
N
SiMe3
9
8.34
7.76
7.28
4.27
4.25
4.23
2.98
2.96
2.94
1.77
1.43
1.42
1.42
1.41
1.41
1.40
1.40
0.93
0.94
0.91
0.64
0.60
0.03
1.80
1.90
1.83
1.99
4.24
2.41
4.36
9.15
6.61
2.22
9.00
f1 (ppm)


146.81
139.80
139.13
135.31
123.97
122.24
115.33
104.49
46.79
33.47
31.74
31.45
23.32
22.64
14.47
14.19
-1.56
C5H11
C5H11
Se
Se
N
SiMe3
f1 (ppm)

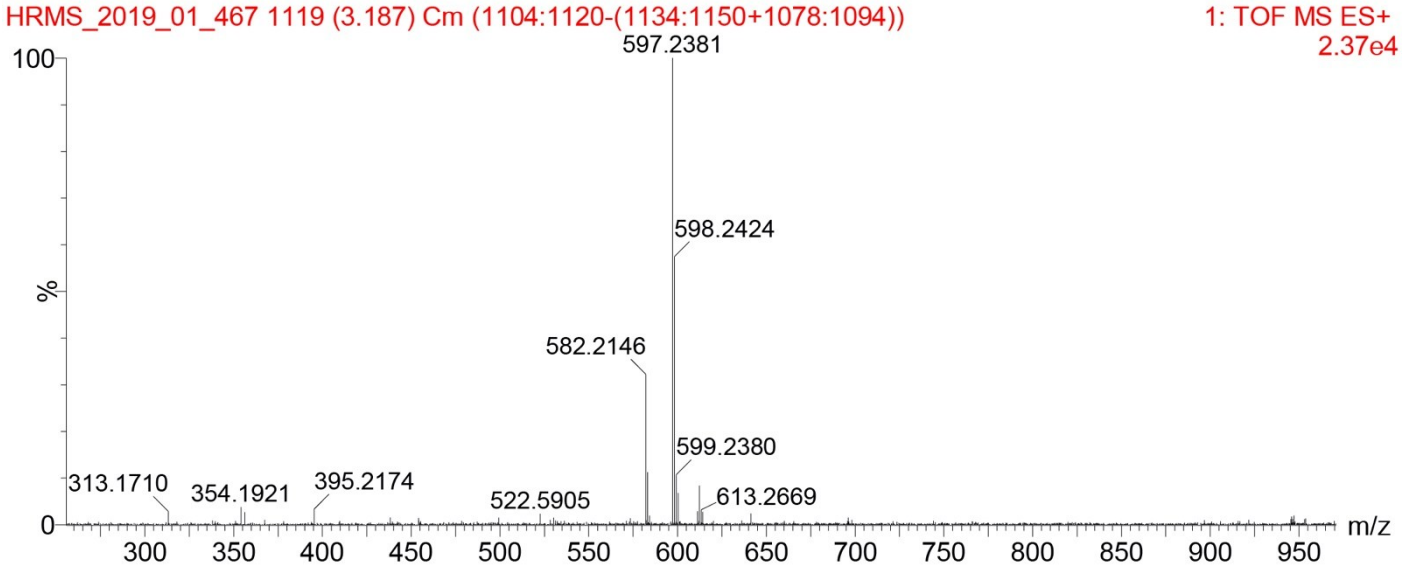

Se
Se
N
N
N
SiMe3
10
f1 (ppm)
f1 (ppm)


Se
Se
N
N
N
SiMe3
10
142.20
140.91
140.62
139.87
137.25
136.30
135.78
128.05
127.58
126.18
123.89
123.65
122.75
120.52
120.24
116.81
109.99
104.63
f1 (ppm)
-1.51
25.53
23.44
14.57
f1 (ppm)


C5H11
C5H11
O
S
O
O
S
O
N
SiMe3
11
7.89
7.89
7.82
6.91
6.91
6.90
6.90
6.90
1.81
1.86
1.85
f1 (ppm)
4.34
4.32
4.30
3.76
3.75
3.74
3.74
3.73
2.63
2.62
2.62
2.61
2.60
2.60
1.85
1.79
1.44
1.43
1.43
1.43
1.42
0.94
0.96
0.60
0.56
0.55
0.01
2.00
0.99
4.25
7.39
8.60
6.47
2.15
9.30
f1 (ppm)


C5H11
C5H11
O
S
O
O
S
O
N
SiMe3
11
144.21
141.06
136.44
126.32
125.47
124.01
116.69
104.72
f1 (ppm)
68.13
47.57
31.49
26.94
25.77
24.22
22.48
14.45
14.12
-1.58
f1 (ppm)

Compound **11**:


HRMS_2019_01_467 1119 (3.187) Cm (1104:1120-(1134:1150+1078:1094))
1: TOF MS ES+
2.37e4
100
%
0
597.2381
598.2424
582.2146
599.2380
313.1710
354.1921
395.2174
522.5905
613.2669
m/z
300
350
400
450
500
550
600
650
700
750
800
850
900
950

2,7-dipentyl-10-(3-(trimethylsilyl)propyl)-10H-diselenopheno[2,3-b:3',2'-h]carbazole (9)

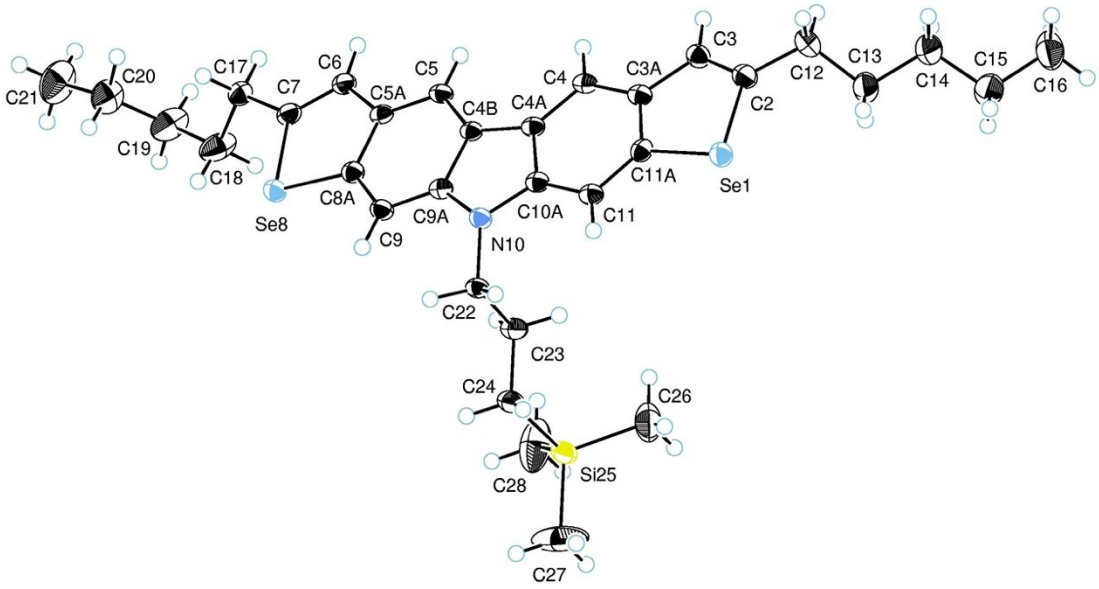


Table 1 Crystal data and structure refinement for **9**

Identification code	A184
Empirical formula	$C_{32}H_{43}NSe_2Si$
Formula weight	627.68
Temperature/K	140.0(1)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	19.8872(10)
b/Å	5.8066(2)
c/Å	26.9647(16)
α/°	90
β/°	103.393(5)
γ/°	90
Volume/Å^3	3029.1(3)
Z	4
ρ_{calc}g/cm^3	1.376
μ/mm^{-1}	2.502
F(000)	1296.0
Crystal size/mm^3	0.03 × 0.04 × 0.17
Radiation	MoKα (λ = 0.71073)
2Θ max. for data collection/°	67.0
Index ranges	-29 ≤ h ≤ 28, -8 ≤ k ≤ 7, -33 ≤ l ≤ 41
Reflections collected	47064
Independent reflections	10395 [R_{int} = 0.0469, R_{sigma} = 0.0514]
Data/restraints/parameters	10395/0/333

Goodness-of-fit on F^2	1.011
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0461$, $wR_2 = 0.0844$
Final R indexes [all data]	$R_1 = 0.0767$, $wR_2 = 0.0911$
Largest diff. peak/hole / e Å^{-3}	0.64/-0.43

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters (Å$^2 \times 10^3$) for A184. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	***U*(eq)**
Se1	9561.5(2)	4778.8(4)	5863.7(2)	23.39(6)
C2	9849.7(12)	7683(4)	6170.0(8)	24.6(4)
C3	9398.4(11)	8510(3)	6425.6(8)	22.1(4)
C3A	8801.8(11)	7089(3)	6432.0(8)	19.1(4)
C4	8272.2(10)	7562(3)	6675.7(7)	18.5(4)
C4A	7734.9(11)	5979(3)	6638.9(7)	17.7(4)
C4B	7105.9(10)	5954(3)	6821.0(7)	17.0(4)
C5	6807.5(11)	7494(3)	7101.6(7)	18.8(4)
C5A	6156.6(11)	6993(3)	7186.7(7)	17.9(4)
C6	5748.6(11)	8412(3)	7448.0(8)	20.5(4)
C7	5121.5(12)	7605(3)	7467.8(8)	22.1(4)
Se8	4942.4(2)	4687.3(4)	7141.7(2)	22.43(6)
C8A	5819.6(11)	4910(3)	6994.5(8)	19.2(4)
C9	6115.0(11)	3322(3)	6720.2(8)	20.3(4)
C9A	6752.8(11)	3880(3)	6634.9(8)	18.2(4)
N10	7148.5(9)	2628(3)	6363.0(6)	18.7(3)
C10A	7735.8(11)	3915(3)	6350.7(8)	18.5(4)
C11	8258.2(11)	3395(3)	6106.4(8)	19.6(4)
C11B	8787.7(11)	4995(3)	6153.8(8)	19.1(4)
C12	10521.5(12)	8733(4)	6127.9(9)	28.9(5)
C13	10693.8(13)	8562(5)	5611.2(10)	35.7(6)
C14	11281.0(14)	10184(5)	5569.7(10)	36.4(6)
C15	11487.4(15)	10091(5)	5067.1(11)	42.4(6)
C16	12017.5(15)	11923(5)	5030.0(12)	47.7(7)
C17	4598.9(11)	8654(4)	7719.1(8)	24.0(4)
C18	3863.5(14)	8662(5)	7400.3(10)	42.5(7)
C19	3343.8(15)	9800(5)	7658.2(11)	44.1(7)
C20	3280.3(14)	8692(5)	8152.2(11)	40.2(6)
C21	2701.6(17)	9692(6)	8365.2(13)	58.0(9)
C22	6845.1(11)	959(3)	5967.3(8)	19.0(4)
C23	6525.3(12)	2128(3)	5461.8(8)	23.9(4)
C24	6191.6(12)	442(4)	5043.3(8)	26.5(5)
Si25	5892.3(4)	1781.3(11)	4395.1(2)	28.13(15)
C26	6605.5(15)	3390(6)	4222.2(12)	53.2(8)
C27	5557(3)	-449(6)	3916.2(12)	89.1(17)

C28	5180.8(18)	3875(7)	4406.8(14)	65.6(10)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for A184. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Se1	23.07(11)	23.31(11)	25.07(12)	-2.06(8)	8.17(9)	-1.75(8)
C2	24.1(11)	23.6(10)	24.8(11)	0.7(8)	3.0(9)	-2.8(8)
C3	22.4(11)	19.9(10)	22.7(11)	1.5(8)	3.0(9)	-1.5(8)
C3A	20.6(10)	16.5(9)	17.2(10)	2.4(7)	-1.5(8)	0.5(7)
C4	20.2(10)	15.9(9)	17.2(10)	-0.7(7)	-0.2(8)	0.4(7)
C4A	19.9(10)	15.8(8)	15.5(9)	0.4(7)	0.3(8)	1.0(7)
C4B	19.0(10)	16.0(8)	14.1(9)	1.5(7)	-0.1(8)	-0.3(7)
C5	23.0(10)	14.8(9)	16.6(10)	-1.0(7)	0.4(8)	-2.2(7)
C5A	21.1(10)	17.3(9)	13.5(9)	0.0(7)	0.1(8)	0.5(7)
C6	24.7(11)	18.8(9)	17.4(10)	-1.7(7)	3.5(8)	-0.8(8)
C7	27.7(12)	20.7(10)	18.1(10)	-3.2(7)	5.5(9)	-0.6(8)
Se8	23.29(11)	21.33(10)	24.14(11)	-5.14(8)	8.48(9)	-4.75(8)
C8A	20.8(10)	18.4(9)	17.4(9)	1.0(7)	2.4(8)	-0.5(7)
C9	23.1(11)	17.3(9)	19.4(10)	-1.2(7)	2.4(8)	-3.7(8)
C9A	22.2(10)	14.0(8)	16.8(10)	0.9(7)	1.2(8)	1.2(7)
N10	20.0(9)	16.1(8)	19.6(8)	-1.3(6)	3.7(7)	-1.9(6)
C10A	21.0(10)	16.4(9)	16.5(10)	1.3(7)	0.9(8)	0.7(7)
C11	22.0(10)	17.0(9)	18.5(10)	-1.2(7)	2.2(8)	0.4(7)
C11B	19.2(10)	21.4(10)	16.0(9)	2.8(7)	2.9(8)	3.1(7)
C12	24.2(12)	27.6(11)	34.7(13)	-0.6(9)	6.7(10)	-5.0(9)
C13	29.3(13)	46.7(15)	32.1(14)	4.1(11)	9.0(11)	-7.1(11)
C14	29.6(13)	45.0(14)	36.1(14)	-0.7(11)	10.7(11)	-4.4(11)
C15	37.3(15)	56.1(17)	34.8(14)	0.9(12)	10.7(12)	-3.7(12)
C16	33.4(15)	63.0(19)	47.3(17)	15.3(14)	10.4(13)	-5.2(13)
C17	26.7(12)	24.5(10)	22.1(11)	-3.2(8)	8.4(9)	-0.2(8)
C18	30.7(14)	66.6(18)	27.6(13)	-10.0(12)	1.5(11)	13.1(13)
C19	33.9(14)	62.2(18)	34.2(14)	-3.8(13)	3.9(12)	20.3(13)
C20	29.9(14)	48.8(15)	43.5(16)	-2.2(12)	11.9(12)	10.4(11)
C21	43.9(18)	80(2)	56(2)	0.8(17)	24.7(16)	20.2(16)
C22	23.1(11)	14.1(8)	18.4(10)	-1.3(7)	2.0(8)	-1.6(7)
C23	28.4(12)	19.6(10)	20.4(11)	0.0(7)	-0.8(9)	-2.0(8)
C24	28.8(12)	24.6(10)	22.5(11)	1.5(8)	-1.3(9)	-6.3(9)
Si25	30.0(4)	28.5(3)	21.8(3)	3.1(2)	-2.3(3)	-10.8(3)
C26	37.6(17)	80(2)	41.6(17)	20.0(15)	9.0(13)	-12.4(15)
C27	163(5)	44.5(18)	32.1(17)	6.8(13)	-33(2)	-34(2)
C28	53(2)	85(2)	65(2)	44(2)	25.4(17)	25.9(18)

Table 4 Bond Lengths for A184.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Se1	C2	1.906(2)	C9	C9A	1.379(3)
Se1	C11B	1.885(2)	C9A	N10	1.397(3)
C2	C3	1.341(3)	N10	C10A	1.394(3)
C2	C12	1.497(3)	N10	C22	1.464(3)
C3	C3A	1.449(3)	C10A	C11	1.386(3)
C3A	C4	1.392(3)	C11	C11B	1.388(3)
C3A	C11B	1.426(3)	C12	C13	1.513(3)
C4	C4A	1.396(3)	C13	C14	1.524(3)
C4A	C4B	1.446(3)	C14	C15	1.505(4)
C4A	C10A	1.428(3)	C15	C16	1.517(4)
C4B	C5	1.390(3)	C17	C18	1.515(3)
C4B	C9A	1.425(3)	C18	C19	1.524(4)
C5	C5A	1.397(3)	C19	C20	1.511(4)
C5A	C6	1.449(3)	C20	C21	1.516(4)
C5A	C8A	1.421(3)	C22	C23	1.524(3)
C6	C7	1.345(3)	C23	C24	1.525(3)
C7	Se8	1.904(2)	C24	Si25	1.879(2)
C7	C17	1.495(3)	Si25	C26	1.846(3)
Se8	C8A	1.881(2)	Si25	C27	1.842(3)
C8A	C9	1.394(3)	Si25	C28	1.871(3)

Table 5 Bond Angles for A184.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11B	Se1	C2	87.35(9)	C9	C9A	N10	128.08(18)
C3	C2	Se1	111.71(16)	N10	C9A	C4B	109.45(18)
C3	C2	C12	127.5(2)	C9A	N10	C22	122.66(17)
C12	C2	Se1	120.77(17)	C10A	N10	C9A	108.08(16)
C2	C3	C3A	116.71(19)	C10A	N10	C22	122.95(17)
C4	C3A	C3	127.22(19)	N10	C10A	C4A	109.28(18)
C4	C3A	C11B	119.46(18)	C11	C10A	C4A	122.46(19)
C11B	C3A	C3	113.33(19)	C11	C10A	N10	128.26(18)
C3A	C4	C4A	119.17(18)	C10A	C11	C11B	116.55(18)
C4	C4A	C4B	133.70(18)	C3A	C11B	Se1	110.89(15)
C4	C4A	C10A	119.59(19)	C11	C11B	Se1	126.33(15)
C10A	C4A	C4B	106.66(17)	C11	C11B	C3A	122.77(19)
C5	C4B	C4A	133.66(18)	C2	C12	C13	116.1(2)
C5	C4B	C9A	119.84(19)	C12	C13	C14	111.6(2)
C9A	C4B	C4A	106.45(17)	C15	C14	C13	114.7(2)
C4B	C5	C5A	118.95(18)	C14	C15	C16	111.9(2)
C5	C5A	C6	127.32(18)	C7	C17	C18	115.14(19)
C5	C5A	C8A	119.61(18)	C17	C18	C19	114.2(2)

C8A	C5A	C6	113.06(19)	C20	C19	C18	114.9(2)
C7	C6	C5A	116.75(18)	C19	C20	C21	113.4(2)
C6	C7	Se8	111.57(15)	N10	C22	C23	111.92(16)
C6	C7	C17	128.63(19)	C22	C23	C24	113.33(17)
C17	C7	Se8	119.76(16)	C23	C24	Si25	114.36(15)
C8A	Se8	C7	87.30(9)	C26	Si25	C24	110.36(12)
C5A	C8A	Se8	111.31(15)	C26	Si25	C28	107.69(16)
C9	C8A	C5A	122.37(19)	C27	Si25	C24	110.27(12)
C9	C8A	Se8	126.29(15)	C27	Si25	C26	110.7(2)
C9A	C9	C8A	116.74(18)	C27	Si25	C28	108.4(2)
C9	C9A	C4B	122.47(19)	C28	Si25	C24	109.32(13)

Table 6 Torsion Angles for A184.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
Se1	C2	C3	C3A	1.1(2)	C6	C5A	C8A	Se8	0.3(2)
Se1	C2	C12	C13	42.1(3)	C6	C5A	C8A	C9	178.47(19)
C2	Se1	C11B	C3A	0.66(15)	C6	C7	C17	C18	134.2(3)
C2	Se1	C11B	C11	179.67(19)	C7	Se8	C8A	C5A	0.10(15)
C2	C3	C3A	C4	179.0(2)	C7	Se8	C8A	C9	-177.98(19)
C2	C3	C3A	C11B	-0.6(3)	C7	C17	C18	C19	-178.3(2)
C2	C12	C13	C14	165.4(2)	Se8	C7	C17	C18	-48.3(3)
C3	C2	C12	C13	-140.6(2)	Se8	C8A	C9	C9A	176.89(15)
C3	C3A	C4	C4A	179.91(19)	C8A	C5A	C6	C7	-0.7(3)
C3	C3A	C11B	Se1	-0.2(2)	C8A	C9	C9A	C4B	0.9(3)
C3	C3A	C11B	C11	-179.29(18)	C8A	C9	C9A	N10	-178.30(19)
C3A	C4	C4A	C4B	-177.1(2)	C9	C9A	N10	C10A	176.5(2)
C3A	C4	C4A	C10A	-0.3(3)	C9	C9A	N10	C22	23.8(3)
C4	C3A	C11B	Se1	-179.87(15)	C9A	C4B	C5	C5A	-1.3(3)
C4	C3A	C11B	C11	1.1(3)	C9A	N10	C10A	C4A	2.7(2)
C4	C4A	C4B	C5	-0.4(4)	C9A	N10	C10A	C11	-177.18(19)
C4	C4A	C4B	C9A	177.0(2)	C9A	N10	C22	C23	80.2(2)
C4	C4A	C10A	N10	-179.22(17)	N10	C10A	C11	C11B	179.73(19)
C4	C4A	C10A	C11	0.7(3)	N10	C22	C23	C24	-178.88(19)
C4A	C4B	C5	C5A	175.8(2)	C10A	C4A	C4B	C5	-177.5(2)
C4A	C4B	C9A	C9	-177.59(18)	C10A	C4A	C4B	C9A	-0.1(2)
C4A	C4B	C9A	N10	1.7(2)	C10A	N10	C22	C23	-68.5(3)
C4A	C10A	C11	C11B	-0.2(3)	C10A	C11	C11B	Se1	-179.62(15)
C4B	C4A	C10A	N10	-1.6(2)	C10A	C11	C11B	C3A	-0.7(3)
C4B	C4A	C10A	C11	178.29(18)	C11B	C3A	C4	C4A	-0.5(3)
C4B	C5	C5A	C6	-177.07(19)	C12	C2	C3	C3A	-176.4(2)
C4B	C5	C5A	C8A	1.2(3)	C12	C13	C14	C15	179.4(2)
C4B	C9A	N10	C10A	-2.8(2)	C13	C14	C15	C16	173.8(2)
C4B	C9A	N10	C22	-155.50(17)	C17	C18	C19	C20	-60.5(4)

C5	C4B	C9A	C9	0.2(3)	C18	C19	C20	C21	-173.3(3)
C5	C4B	C9A	N10	179.56(17)	C22	N10	C10A	C4A	155.35(17)
C5	C5A	C6	C7	177.6(2)	C22	N10	C10A	C11	-24.6(3)
C5	C5A	C8A	Se8	-178.22(15)	C22	C23	C24	Si25	-172.65(16)
C5	C5A	C8A	C9	0.0(3)	C23	C24	Si25	C26	53.4(2)
C5A	C6	C7	Se8	0.8(2)	C23	C24	Si25	C27	176.0(2)
C5A	C6	C7	C17	178.4(2)	C23	C24	Si25	C28	-64.9(2)
C5A	C8A	C9	C9A	-1.0(3)					

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for A184.

Atom	***x***	***y***	***z***	***U*(eq)**
H3	9465.11	9927.08	6590.65	26
H4	8276.41	8915.05	6860.77	22
H5	7037.69	8836.94	7230.67	23
H6	5912.38	9813.08	7594.95	25
H9	5892.84	1953.06	6600.69	24
H11	8254.04	2044.59	5920.4	23
H12A	10890.06	8002.25	6377.18	35
H12B	10516.48	10348.72	6218.56	35
H13A	10286.76	8938.36	5347.91	43
H13B	10825.48	6991.2	5555.75	43
H14A	11143.86	11747.33	5625.75	44
H14B	11681.71	9814.71	5839.29	44
H15A	11080.49	10304.57	4792.47	51
H15B	11677.97	8583.67	5026.29	51
H16A	12136.02	11810.63	4705.4	72
H16B	11827.4	13419.1	5063.78	72
H16C	12424.49	11699.34	5297.44	72
H17A	4734.92	10230.43	7810.45	29
H17B	4608.24	7822.11	8032.6	29
H18A	3720.44	7083.37	7317.69	51
H18B	3854.39	9457.23	7082.47	51
H19A	3475.23	11398.77	7724.98	53
H19B	2893.44	9779.86	7423.13	53
H20A	3713.75	8877.63	8402.53	48
H20B	3200.57	7054.24	8096.04	48
H21A	2687.31	8922.26	8677.6	87
H21B	2782.3	11306.56	8429.74	87
H21C	2268.84	9482.15	8123.08	87
H22A	6503(13)	40(40)	6108(9)	19(6)
H22B	7207(12)	-90(40)	5928(9)	16(6)
H23A	6881.37	2988.08	5349.9	29

H23B	6178.42	3217.68	5514.12	29
H24A	5798.36	-273.22	5137.53	32
H24B	6521.85	-763.66	5023.46	32
H26A	6773.23	4542.7	4475.86	80
H26B	6973.47	2347.06	4203.78	80
H26C	6440.54	4116.71	3896.9	80
H27A	5186.98	-1265.72	4012.64	134
H27B	5387.68	262.23	3589.75	134
H27C	5920.61	-1507.42	3896.62	134
H28A	5347.59	5051.03	4655.02	98
H28B	5028.36	4566.04	4076.42	98
H28C	4801.28	3081.21	4495.04	98