Supporting Information for

TCNQ-embedded heptacene and nonacene: synthesis, characterization and physical properties

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1. General Method

All reagents and starting materials were obtained from commercial sources and used without further purification. Dichloromethane was distilled over CaH_2 before use. Chlorobenzene was dried with KOH before use. ^{1}H and ^{13}C NMR spectra were recorded using Advance 300 MHz and 500 MHz Bruker spectrometer in $CDCl_3$. All chemical shifts are quoted in ppm, relative to tetramethylsilane, using the residual solvent peak as a reference standard. Column chromatography was performed on silica gel 60 (Merck 40-60 nm, 230-400 mesh). MALDI-TOF mass spectra were measured on a Bruker Autoflex MALDI-TOF instrument using 1,8,9-trihydroxyanthracene as the matrix. Atmosphere Pressure Chemical Ionization (APCI) MS analysis was carried out on a Bruker amaZonX instrument. High resolution electronic ionization (EI) MS was carried out on a Finnigan TSQ 7000 triple stage quadrupole mass spectrometer. UV-vis absorption and fluorescence spectra were recorded on a Shimadzu UV-1700 spectrophotometer and a RF- 5301 fluorometer, respectively. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) measurements were performed in dry dichloromethane on a CHI 620C electrochemical analyzer with a three-electrode cell, using 0.1 M Bu_4NPF_6 as supporting electrolyte, AgCl/Ag as reference electrode, gold disk as working electrode, Pt wire as counter electrode, and scan rate at 50 mV/s. The potential was externally calibrated against the ferrocene/ferrocenium couple. Room temperature XRD measurements were performed on a Bruker-AXS D8 DISCOVER with GADDS Powder X-ray diffractometer with Cu K_α radiation.

2. DFT calculations on 4 and 9

Density functional theory (DFT) calculations have been performed at the B3LYP/6-31G* level of theory, as implemented in the *Gaussian 09* program package.[1] The geometry of **4** and **9** was fully optimized in gas phase using the default convergence criteria without any constraints and confirmed by frequency calculations.

Reference:

1. Gaussian 09; Revision A.2; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.;

Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc., Wallingford CT, 2009.

3. Device fabrication details

Top-contact, bottom-gate TFT devices were prepared on the p+ silicon wafer, and 200 nm thermal SiO_2 layer serves as the gate dielectric. The SiO_2/Si substrate was cleaned with acetone and isopropanol, then immerse in a piranha solution for 8 minutes. Followed by rinsing with deionized water, and then treated with octadecyltrimethoxysilane (OTS) spin coated from 10 mM trichloroethylene solution. The semiconductor layer was deposited on top of the OTS-modified dielectric surface by spin-casting from the solution of **4** in chloroform (0.8 wt%). The thin films were then annealed at 100 ^{o}C for 30 minutes in the vacuum. Subsequently, gold source/drain electrodes (80nm) were deposited by thermal evaporation through a metal shadow mask to create a series of FETs with channel (W/L = 40). The FET devices were then characterized using a Keithley SCS-4200 semiconductor parameter analyzer in the N_2 glovebox. To minimize leakage currents, small trenches in the thin film around the electrodes were created with a needle. The FET mobility was extracted using the following equation in the saturation regime from the gate sweep: $I_D = W/(2L)C_i\mu(V_G - V_T)^2$, where I_D is the drain current, μ is the field-effect mobility, C_i is the capacitance per unit area of the gate dielectric layer (SiO_2, 200 nm, C_i = 17 nF cm^{-2}), and V_G and V_T are gate voltage and threshold voltage, respectively. W and L are respectively channel width and length.

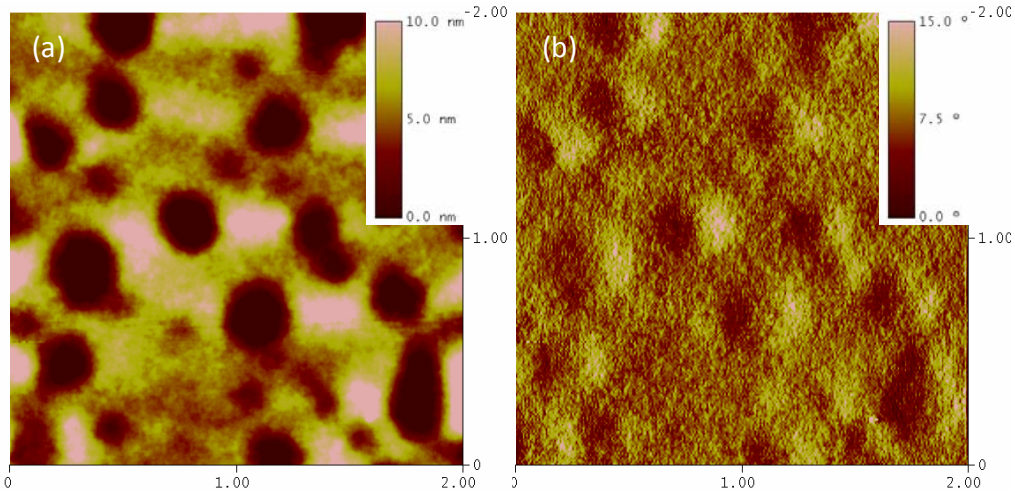

Figure S1. AFM images of the thin films of **4** on OTS modified SiO_2 substrates: height image (left) and phase image (right).

4. ^{1}H and ^{13}C NMR spectra of all new compounds

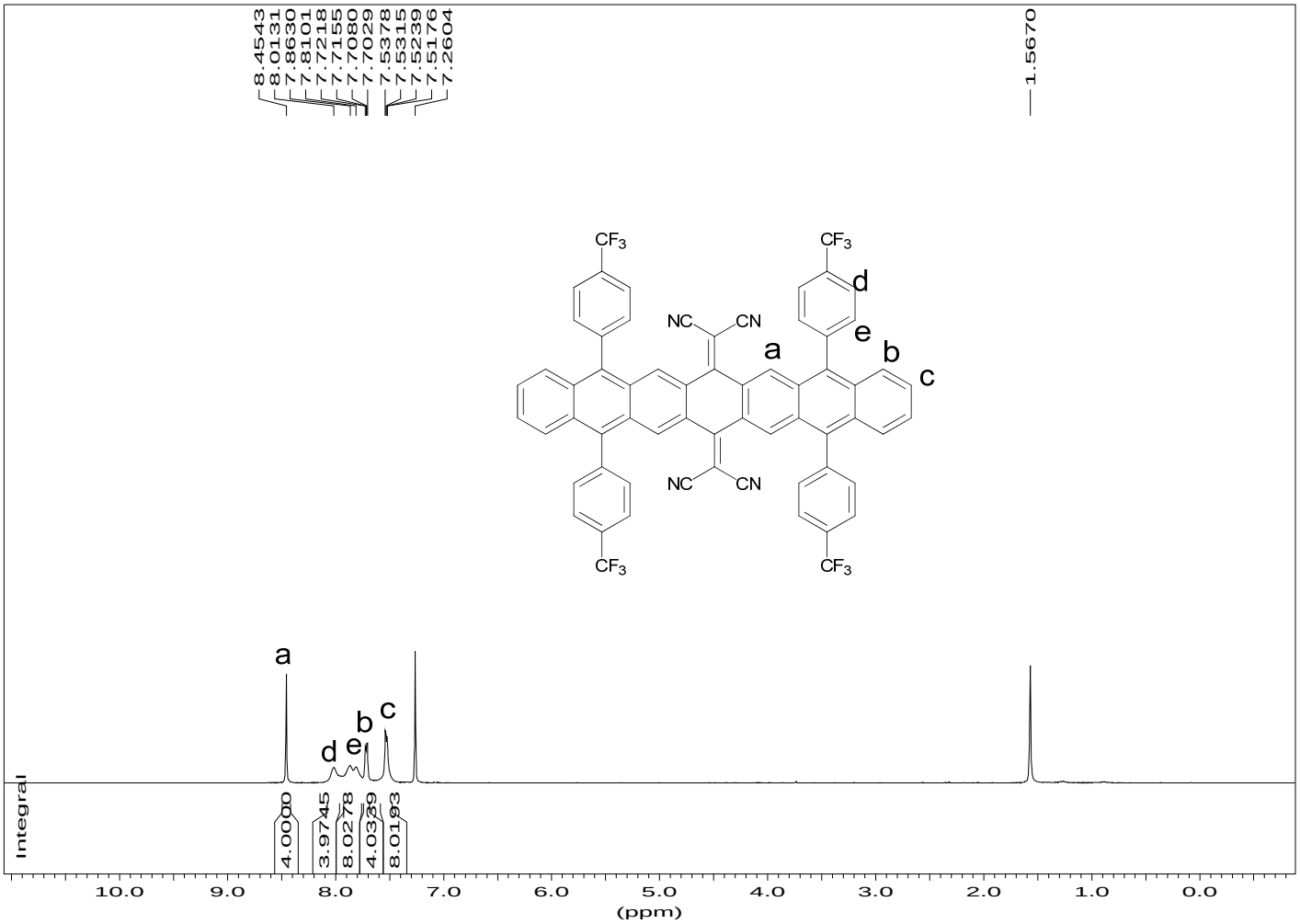

Figure S2. The ^{1}H NMR of compound **2** in $CDCl_3$.

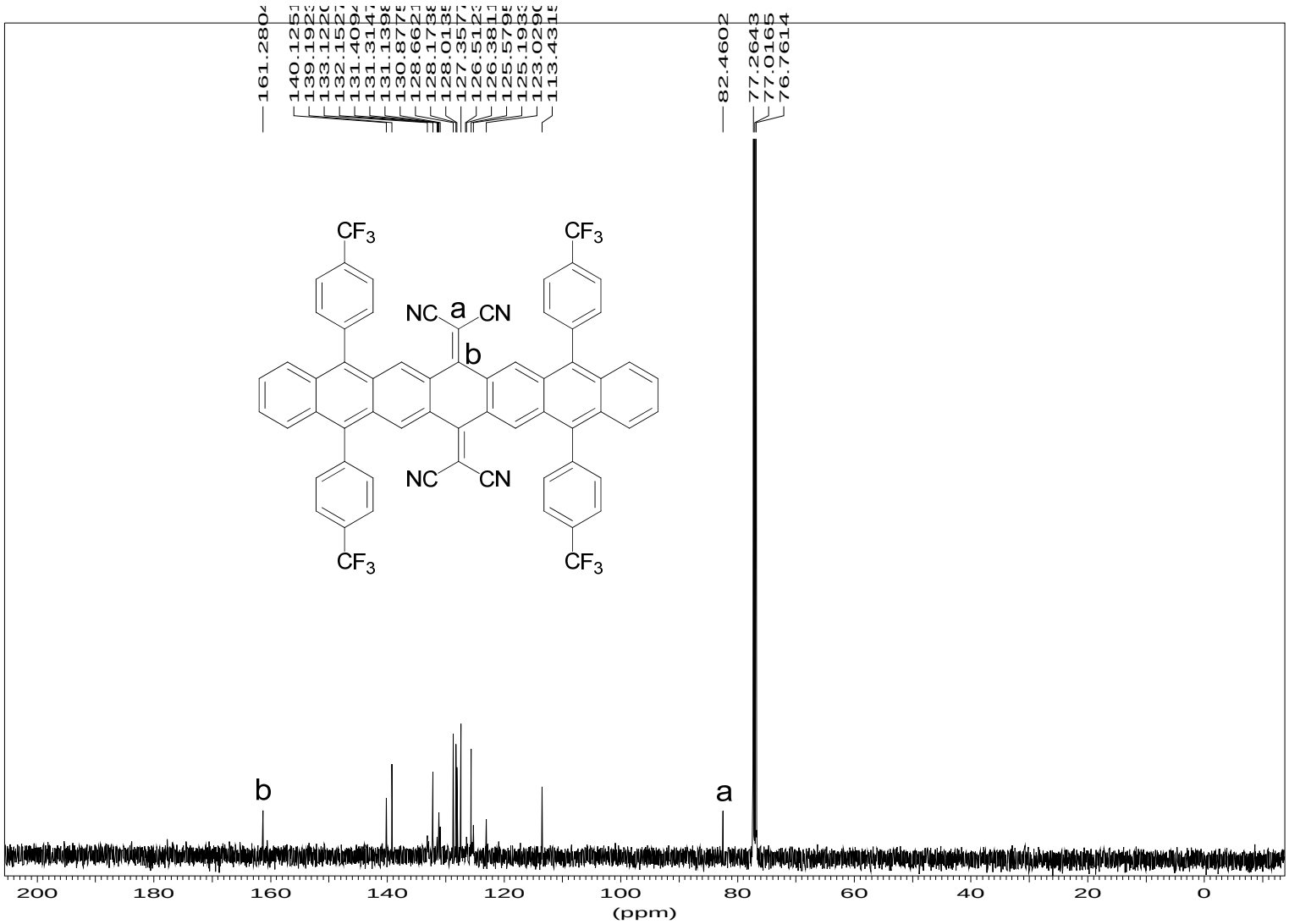

Figure S3. The ^{13}C NMR of compound **2** in $CDCl_3$.

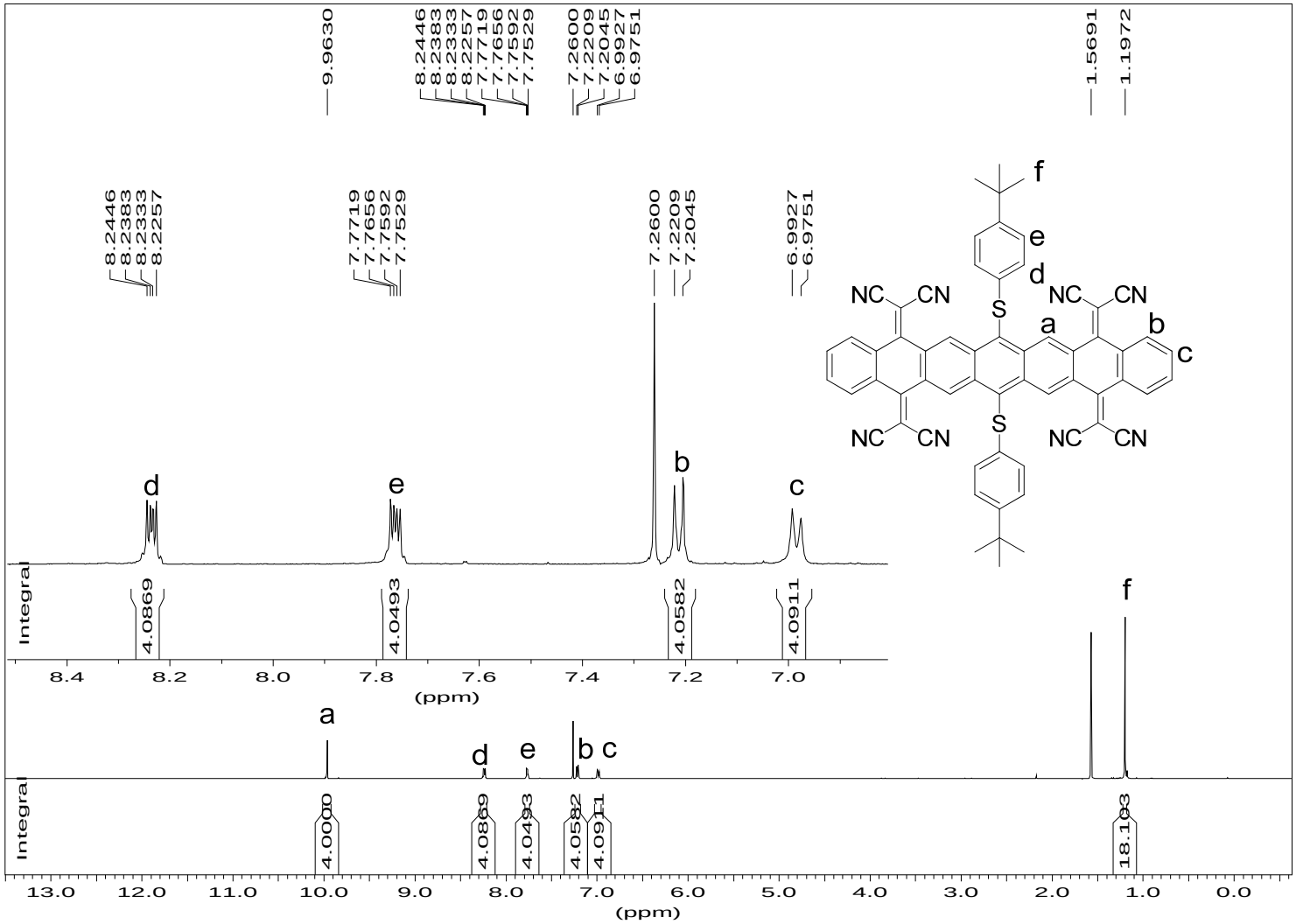

Figure S4. The ^{1}H NMR of compound **4** in $CDCl_3$.

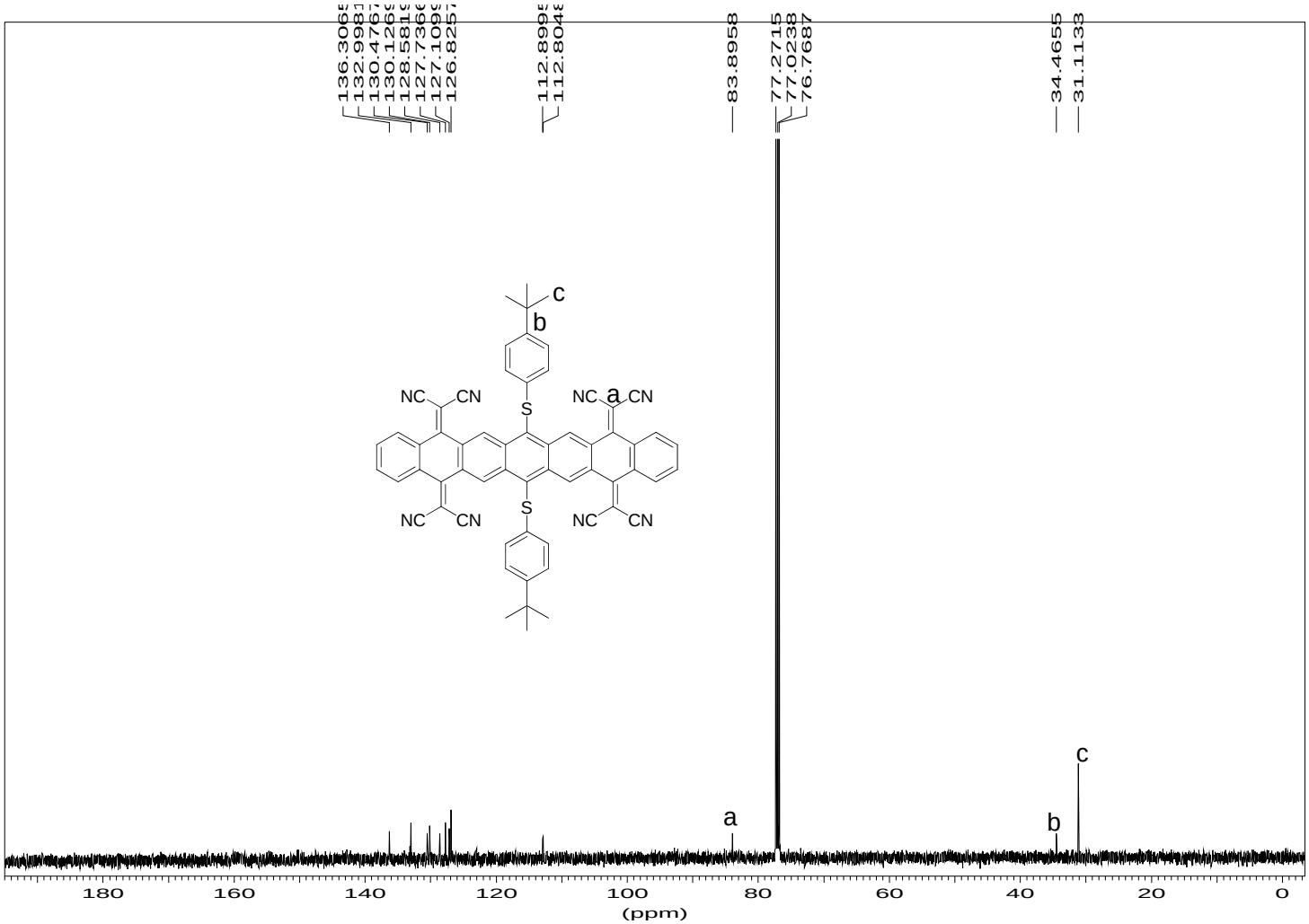

Figure S5. The ^{13}C NMR of compound **4** in $CDCl_3$.

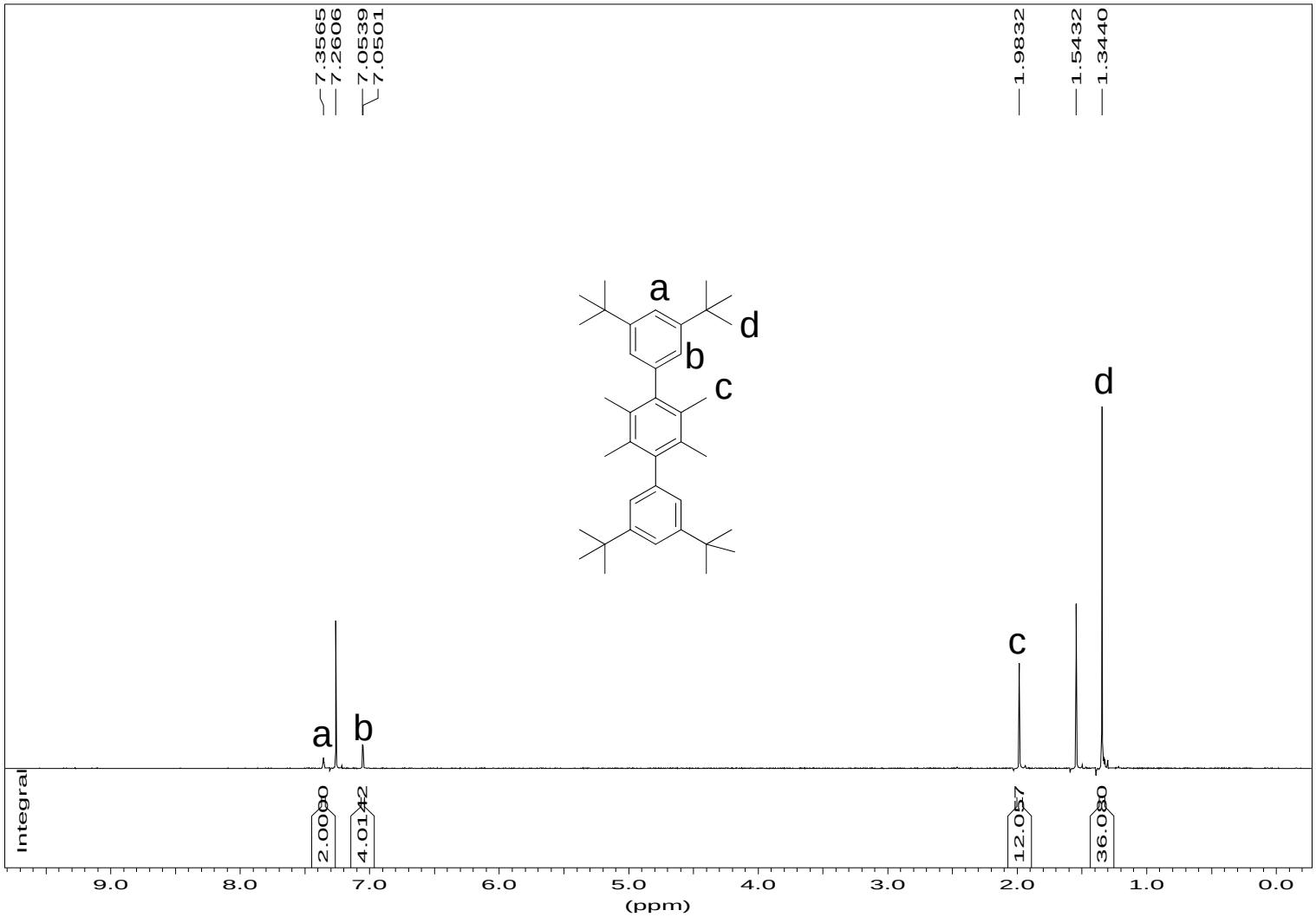

Figure S6. The ^{1}H NMR of compound **6** in $CDCl_3$.

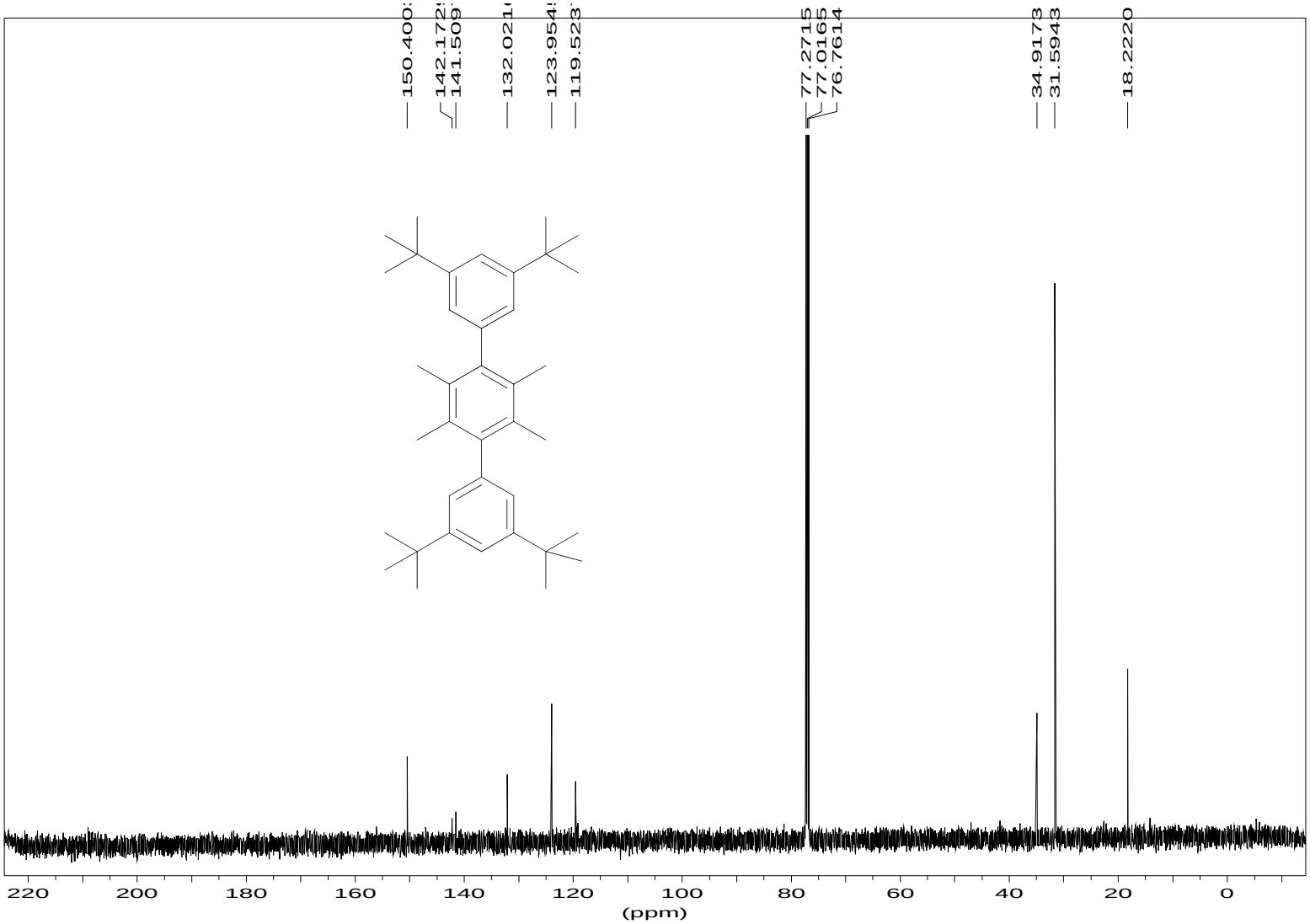

Figure S7. The ^{13}C NMR of compound **6** in $CDCl_3$.

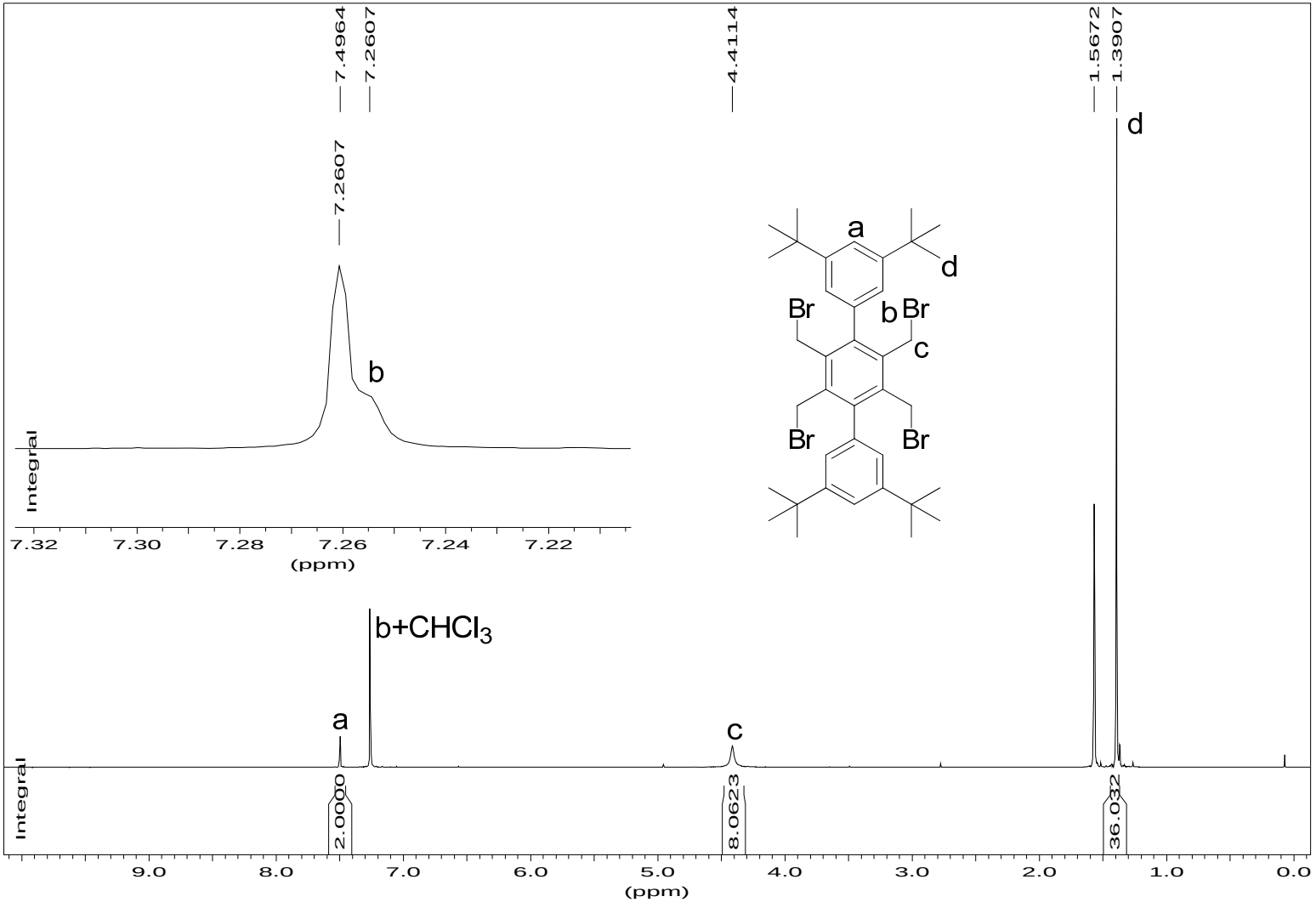

Figure S8. The ^{1}H NMR of compound **7** in $CDCl_3$.

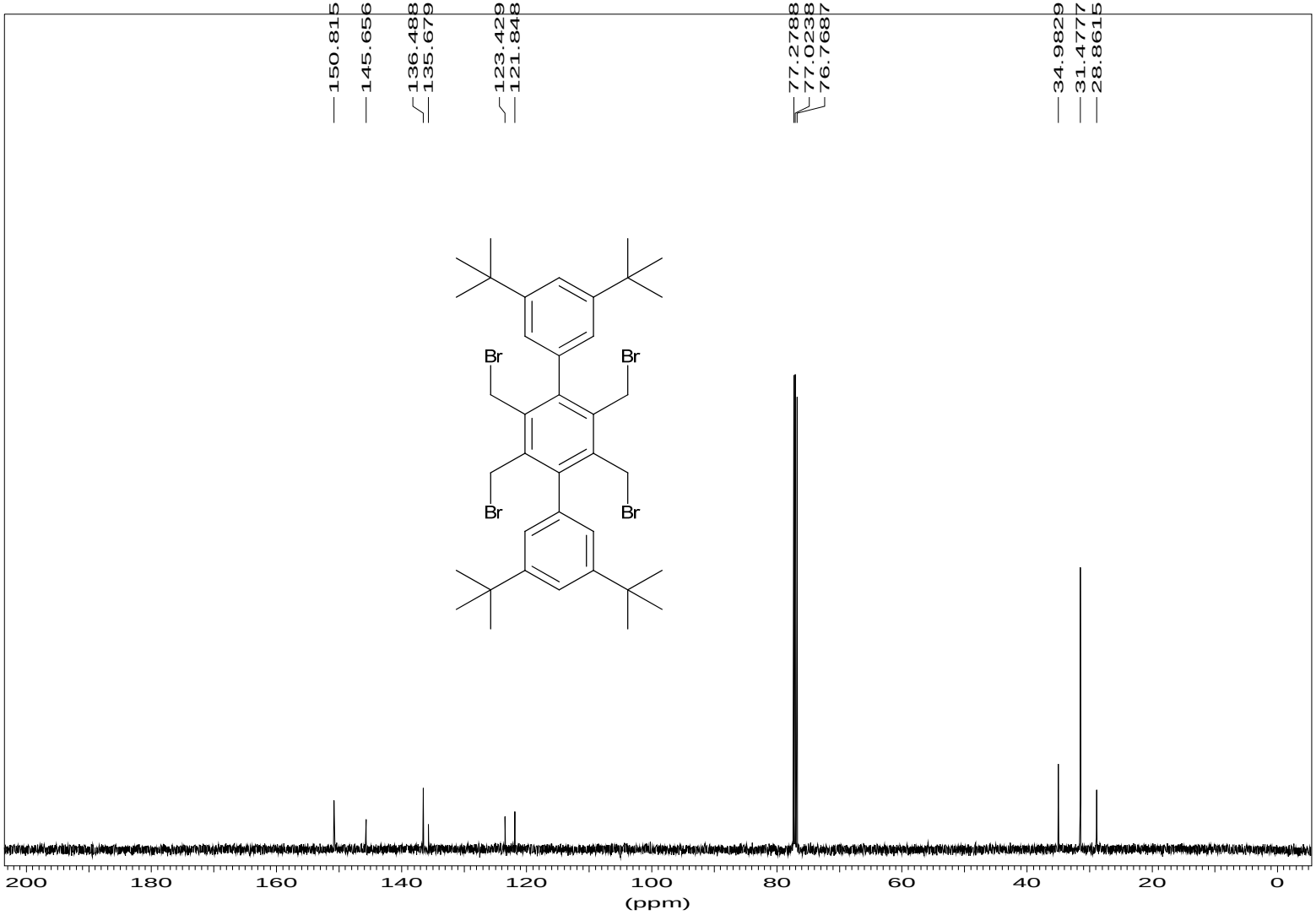

Figure S9. The ^{13}C NMR of compound **7** in $CDCl_3$.

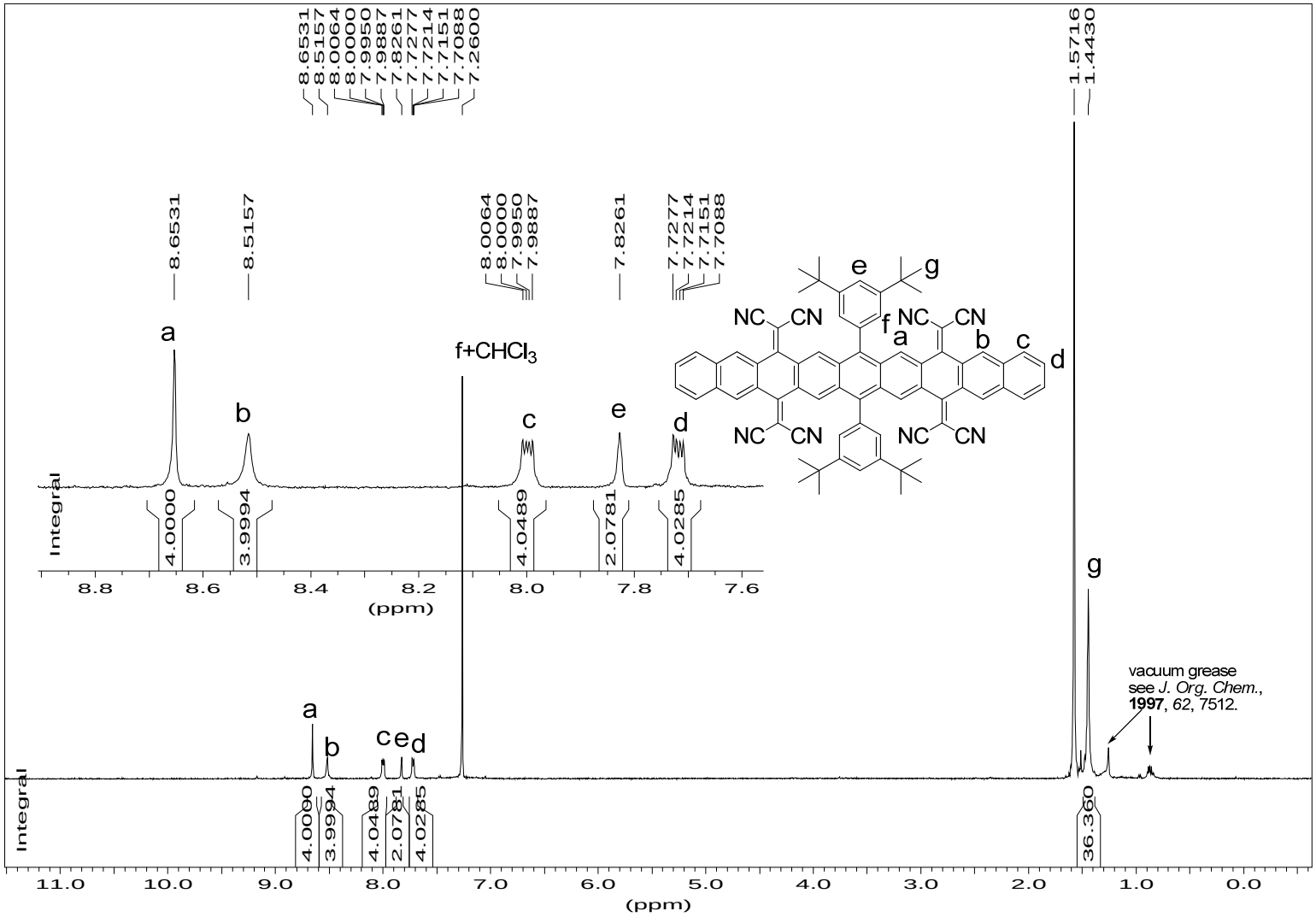

Figure S10. The ^{1}H NMR of compound **9** in $CDCl_3$.

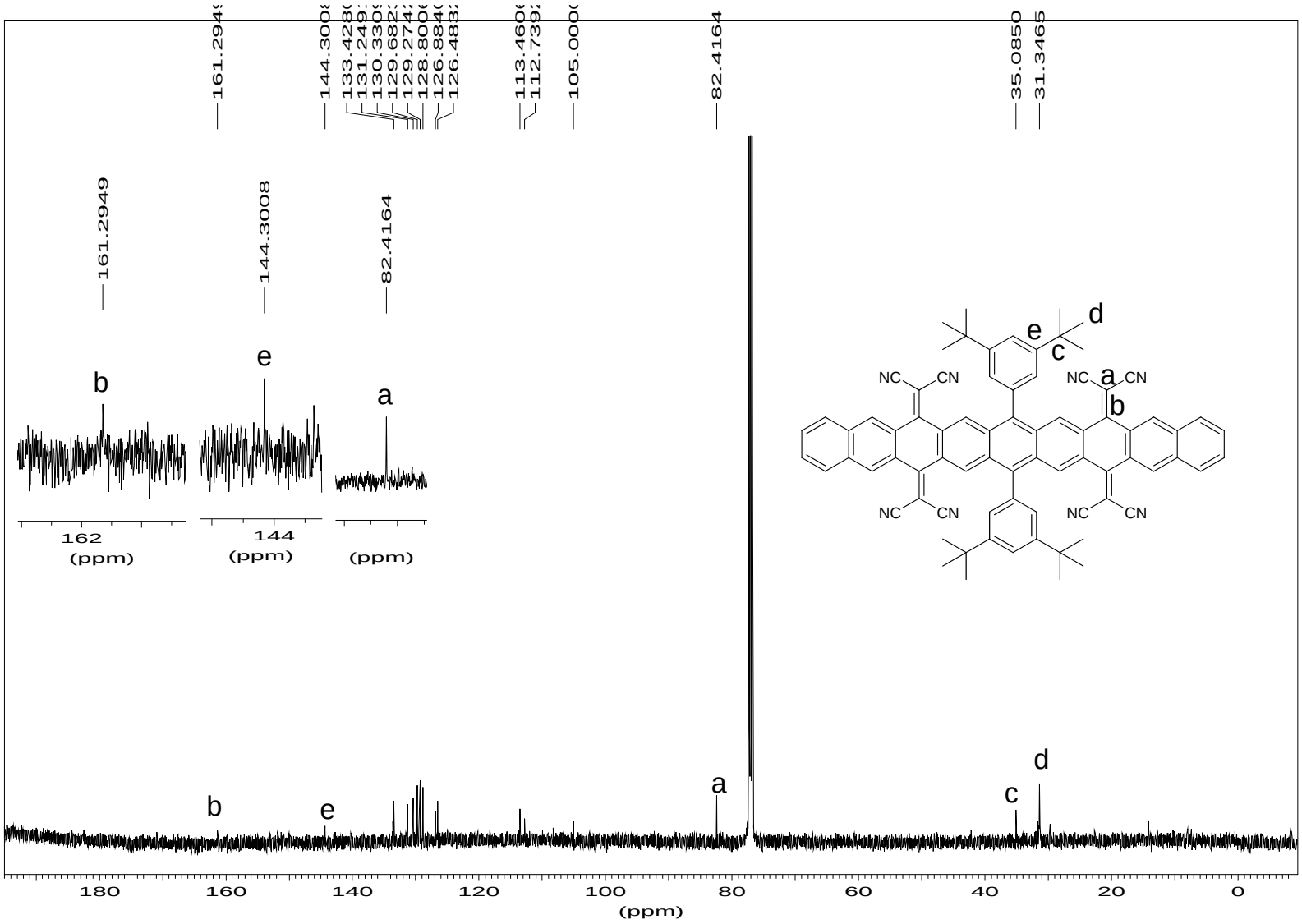

Figure S11. The ^{13}C NMR of compound **9** in $CDCl_3$.

5. Crystallographic data for 2 and 4

Table S1: Crystallographic data and structure refinement for compound 2.

Identification code	c436	
Empirical formula	C66.50 H30.50 Cl7.50 F12 N4	
Formula weight	1379.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 13.0937(14) Å	α= 90°.
	b = 15.1874(17) Å	β= 98.319(3)°.
	c = 30.448(3) Å	γ = 90°.
Volume	5991.1(11) Å^3	
Z	4	
Density (calculated)	1.529 Mg/m^3	
Absorption coefficient	0.438 mm^{-1}	
F(000)	2772	
Crystal size	0.34 x 0.10 x 0.08 mm^3	
Theta range for data collection	2.10 to 25.00°.	
Index ranges	-15<=h<=15, -18<=k<=18, -36<=l<=29	
Reflections collected	34762	
Independent reflections	10551 [R(int) = 0.0561]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.6468 and 0.5500
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10551 / 339 / 958
Goodness-of-fit on F^2	1.084
Final R indices [I>2sigma(I)]	R1 = 0.0633, wR2 = 0.1644
R indices (all data)	R1 = 0.0973, wR2 = 0.1850
Largest diff. peak and hole	1.433 and -0.889 e.Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound 2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	14626(4)	3439(4)	5671(2)	57(1)
F(2)	14234(4)	4719(4)	5428(2)	55(1)
F(3)	14578(3)	3734(4)	4976(2)	56(1)
F(1A)	14393(5)	3794(5)	5823(2)	56(1)
F(2A)	14380(5)	4585(5)	5261(3)	56(1)
F(3A)	14661(4)	3139(4)	5264(2)	56(1)
C(44)	3487(8)	1160(8)	4504(4)	39(1)
F(4)	2800(7)	1824(5)	4510(3)	39(1)
F(5)	3308(5)	568(5)	4809(2)	39(1)
F(6)	3236(5)	764(5)	4101(2)	40(1)
C(44A)	3495(8)	1148(7)	4535(4)	39(1)
F(4A)	2759(6)	1742(5)	4396(2)	39(1)
F(5A)	3251(4)	840(5)	4930(2)	39(1)
F(6A)	3338(4)	471(5)	4250(2)	40(1)
F(7)	16035(2)	200(2)	3869(1)	47(1)
F(8)	16441(2)	-1085(2)	4098(1)	76(1)
F(9)	16455(2)	-744(2)	3422(1)	62(1)
F(10)	4802(2)	-3335(2)	3097(1)	49(1)
F(11)	4662(2)	-2277(2)	2623(1)	61(1)
F(12)	5014(2)	-3579(2)	2421(1)	36(1)

N(1)	11679(3)	3479(2)	3733(1)	34(1)
N(2)	12655(3)	1272(2)	3035(1)	39(1)
N(3)	6082(3)	1961(2)	3217(1)	26(1)
N(4)	7229(3)	28(2)	2420(1)	30(1)
C(1)	10560(3)	1351(2)	3650(1)	19(1)
C(2)	9819(3)	1702(2)	3929(1)	18(1)
C(3)	10124(3)	2218(2)	4291(1)	19(1)
C(4)	9418(3)	2513(2)	4573(1)	18(1)
C(5)	9751(3)	3023(2)	4950(1)	19(1)
C(6)	9033(3)	3309(2)	5224(1)	19(1)
C(7)	9328(3)	3857(2)	5603(1)	22(1)
C(8)	8618(3)	4140(3)	5858(1)	23(1)
C(9)	7567(3)	3916(2)	5745(1)	22(1)
C(10)	7250(3)	3397(2)	5388(1)	22(1)
C(11)	7963(3)	3063(2)	5116(1)	18(1)
C(12)	7644(3)	2506(2)	4751(1)	19(1)
C(13)	8363(3)	2243(2)	4476(1)	19(1)
C(14)	8067(3)	1690(2)	4099(1)	19(1)
C(15)	8756(3)	1428(2)	3828(1)	18(1)
C(16)	8493(3)	834(2)	3447(1)	17(1)
C(17)	9288(3)	175(2)	3398(1)	18(1)
C(18)	9049(3)	-679(2)	3289(1)	20(1)
C(19)	9819(3)	-1330(2)	3260(1)	19(1)
C(20)	9560(3)	-2203(2)	3145(1)	19(1)
C(21)	10340(3)	-2825(2)	3109(1)	19(1)

C(22)	10104(3)	-3705(2)	2966(1)	21(1)
C(23)	10864(3)	-4295(3)	2919(1)	25(1)
C(24)	11922(3)	-4036(3)	2998(1)	25(1)
C(25)	12176(3)	-3198(3)	3134(1)	23(1)
C(26)	11410(3)	-2566(2)	3197(1)	18(1)
C(27)	11668(3)	-1689(2)	3324(1)	20(1)
C(28)	10886(3)	-1070(2)	3354(1)	18(1)
C(29)	11114(3)	-177(2)	3483(1)	18(1)
C(30)	10359(3)	438(2)	3502(1)	18(1)
C(31)	10868(3)	3247(2)	5064(1)	19(1)
C(32)	11499(3)	2794(3)	5394(1)	26(1)
C(33)	12544(3)	2976(3)	5485(1)	28(1)
C(34)	12967(3)	3622(3)	5244(1)	25(1)
C(35)	12351(3)	4082(3)	4914(1)	28(1)
C(36)	11305(3)	3890(3)	4822(1)	23(1)
C(37)	14078(4)	3826(4)	5344(2)	56(1)
C(38)	6567(3)	2164(2)	4679(1)	18(1)
C(39)	6285(3)	1528(3)	4968(1)	25(1)
C(40)	5291(3)	1202(3)	4919(1)	28(1)
C(41)	4562(3)	1500(3)	4576(1)	25(1)
C(42)	4833(3)	2128(3)	4284(1)	31(1)
C(43)	5828(3)	2457(3)	4337(1)	28(1)
C(45)	12775(3)	-1425(2)	3430(1)	20(1)
C(46)	13403(3)	-1796(3)	3791(1)	25(1)
C(47)	14422(3)	-1555(3)	3898(1)	27(1)

C(48)	14831(3)	-927(3)	3650(1)	24(1)
C(49)	14219(3)	-532(3)	3291(1)	25(1)
C(50)	13200(3)	-788(3)	3180(1)	23(1)
C(51)	15931(3)	-641(3)	3762(2)	33(1)
C(52)	8445(3)	-2451(2)	3044(1)	21(1)
C(53)	7969(3)	-2978(3)	3328(1)	24(1)
C(54)	6924(3)	-3155(3)	3244(1)	26(1)
C(55)	6336(3)	-2813(3)	2867(1)	24(1)
C(56)	6807(3)	-2293(3)	2575(1)	26(1)
C(57)	7844(3)	-2117(3)	2664(1)	23(1)
C(58)	5209(3)	-3000(3)	2756(2)	32(1)
C(59)	11344(3)	1841(3)	3530(1)	21(1)
C(60)	11512(3)	2753(3)	3651(1)	24(1)
C(61)	12065(3)	1506(3)	3252(1)	26(1)
C(62)	7604(3)	894(2)	3155(1)	19(1)
C(63)	6771(3)	1502(2)	3199(1)	19(1)
C(64)	7416(3)	389(3)	2751(1)	22(1)
C(1S)	447(3)	8790(3)	1853(1)	43(1)
Cl(1)	1577(14)	8320(20)	2109(4)	75(4)
Cl(2)	17(15)	9499(7)	2226(5)	82(4)
Cl(3)	529(12)	9326(10)	1349(3)	51(3)
Cl(1A)	1727(6)	8541(6)	2105(3)	60(2)
Cl(2A)	-137(8)	9524(3)	2192(3)	37(2)
Cl(3A)	564(11)	9240(10)	1339(3)	62(3)
C(2S)	1830(3)	5506(3)	6390(1)	25(1)

Cl(4)	1997(1)	5088(1)	5866(1)	45(1)
Cl(5)	536(1)	5786(1)	6399(1)	36(1)
Cl(6)	2617(1)	6437(1)	6514(1)	31(1)
C(3S)	-4(17)	10060(20)	4834(8)	138(2)
Cl(7)	525(8)	10317(8)	5376(4)	138(2)
Cl(8)	798(15)	9340(30)	4602(11)	96(4)
Cl(9)	-1221(8)	9600(13)	4823(5)	137(2)
C(3SA)	82(16)	10080(20)	4851(8)	138(2)
Cl(7A)	500(16)	9230(30)	4546(11)	96(4)
Cl(8A)	1037(10)	10331(11)	5303(4)	138(2)
Cl(9A)	-1067(10)	9872(10)	5023(5)	138(2)

Table S3. Bond lengths [Å] and angles [°] for compound 2.

F(1)-C(37)	1.283(7)
F(2)-C(37)	1.389(7)
F(3)-C(37)	1.384(7)
F(1A)-C(37)	1.459(8)
F(2A)-C(37)	1.256(8)
F(3A)-C(37)	1.337(7)
C(44)-F(5)	1.337(11)
C(44)-F(4)	1.353(11)
C(44)-F(6)	1.363(11)
C(44)-C(41)	1.486(11)

C(44A)-F(6A)	1.341(10)
C(44A)-F(4A)	1.342(10)
C(44A)-F(5A)	1.372(10)
C(44A)-C(41)	1.485(10)
F(7)-C(51)	1.320(5)
F(8)-C(51)	1.323(5)
F(9)-C(51)	1.330(5)
F(10)-C(58)	1.333(5)
F(11)-C(58)	1.341(5)
F(12)-C(58)	1.344(5)
N(1)-C(60)	1.145(5)
N(2)-C(61)	1.143(5)
N(3)-C(63)	1.148(5)
N(4)-C(64)	1.143(5)
C(1)-C(59)	1.360(5)
C(1)-C(30)	1.471(5)
C(1)-C(2)	1.477(5)
C(2)-C(3)	1.365(5)
C(2)-C(15)	1.443(5)
C(3)-C(4)	1.421(5)
C(4)-C(5)	1.401(5)
C(4)-C(13)	1.431(5)
C(5)-C(6)	1.413(5)
C(5)-C(31)	1.493(5)
C(6)-C(7)	1.430(5)

C(6)-C(11)	1.441(5)
C(7)-C(8)	1.364(5)
C(8)-C(9)	1.412(5)
C(9)-C(10)	1.358(5)
C(10)-C(11)	1.427(5)
C(11)-C(12)	1.411(5)
C(12)-C(13)	1.405(5)
C(12)-C(38)	1.489(5)
C(13)-C(14)	1.429(5)
C(14)-C(15)	1.366(5)
C(15)-C(16)	1.472(5)
C(16)-C(62)	1.361(5)
C(16)-C(17)	1.467(5)
C(17)-C(18)	1.364(5)
C(17)-C(30)	1.449(5)
C(18)-C(19)	1.424(5)
C(19)-C(20)	1.400(5)
C(19)-C(28)	1.440(5)
C(20)-C(21)	1.408(5)
C(20)-C(52)	1.495(5)
C(21)-C(22)	1.425(5)
C(21)-C(26)	1.442(5)
C(22)-C(23)	1.363(5)
C(23)-C(24)	1.427(6)
C(24)-C(25)	1.364(5)

C(25)-C(26)	1.422(5)
C(26)-C(27)	1.414(5)
C(27)-C(28)	1.402(5)
C(27)-C(45)	1.493(5)
C(28)-C(29)	1.431(5)
C(29)-C(30)	1.366(5)
C(31)-C(32)	1.388(5)
C(31)-C(36)	1.394(5)
C(32)-C(33)	1.384(5)
C(33)-C(34)	1.389(6)
C(34)-C(35)	1.383(6)
C(34)-C(37)	1.476(6)
C(35)-C(36)	1.389(5)
C(38)-C(43)	1.388(5)
C(38)-C(39)	1.391(5)
C(39)-C(40)	1.381(5)
C(40)-C(41)	1.384(6)
C(41)-C(42)	1.385(6)
C(42)-C(43)	1.383(6)
C(45)-C(46)	1.394(5)
C(45)-C(50)	1.396(5)
C(46)-C(47)	1.376(5)
C(47)-C(48)	1.373(5)
C(48)-C(49)	1.396(6)
C(48)-C(51)	1.495(6)

C(49)-C(50)	1.384(5)
C(52)-C(53)	1.391(5)
C(52)-C(57)	1.396(5)
C(53)-C(54)	1.381(5)
C(54)-C(55)	1.386(6)
C(55)-C(56)	1.397(6)
C(55)-C(58)	1.494(5)
C(56)-C(57)	1.372(5)
C(59)-C(60)	1.442(6)
C(59)-C(61)	1.449(5)
C(62)-C(64)	1.439(5)
C(62)-C(63)	1.450(5)
C(1S)-Cl(2)	1.718(8)
C(1S)-Cl(1)	1.724(8)
C(1S)-Cl(3A)	1.737(8)
C(1S)-Cl(3)	1.754(7)
C(1S)-Cl(2A)	1.768(6)
C(1S)-Cl(1A)	1.779(8)
C(2S)-Cl(5)	1.750(4)
C(2S)-Cl(4)	1.759(4)
C(2S)-Cl(6)	1.759(4)
C(3S)-Cl(9)	1.74(2)
C(3S)-Cl(7)	1.74(2)
C(3S)-Cl(8)	1.74(2)
C(3SA)-Cl(9A)	1.693(19)

C(3SA)-Cl(7A)	1.72(2)
C(3SA)-Cl(8A)	1.76(2)
F(5)-C(44)-F(4)	108.0(9)
F(5)-C(44)-F(6)	106.5(8)
F(4)-C(44)-F(6)	105.5(8)
F(5)-C(44)-C(41)	112.9(8)
F(4)-C(44)-C(41)	110.8(9)
F(6)-C(44)-C(41)	112.7(8)
F(6A)-C(44A)-F(4A)	106.0(8)
F(6A)-C(44A)-F(5A)	105.8(8)
F(4A)-C(44A)-F(5A)	104.9(8)
F(6A)-C(44A)-C(41)	112.7(8)
F(4A)-C(44A)-C(41)	114.1(9)
F(5A)-C(44A)-C(41)	112.5(7)
C(59)-C(1)-C(30)	122.8(3)
C(59)-C(1)-C(2)	122.8(3)
C(30)-C(1)-C(2)	114.4(3)
C(3)-C(2)-C(15)	119.7(3)
C(3)-C(2)-C(1)	122.2(3)
C(15)-C(2)-C(1)	117.9(3)
C(2)-C(3)-C(4)	122.0(3)
C(5)-C(4)-C(3)	121.1(3)
C(5)-C(4)-C(13)	120.3(3)
C(3)-C(4)-C(13)	118.6(3)
C(4)-C(5)-C(6)	119.9(3)

C(4)-C(5)-C(31)	119.6(3)
C(6)-C(5)-C(31)	120.4(3)
C(5)-C(6)-C(7)	122.0(3)
C(5)-C(6)-C(11)	119.6(3)
C(7)-C(6)-C(11)	118.4(3)
C(8)-C(7)-C(6)	121.1(4)
C(7)-C(8)-C(9)	120.4(3)
C(10)-C(9)-C(8)	120.6(4)
C(9)-C(10)-C(11)	121.4(4)
C(12)-C(11)-C(10)	121.7(3)
C(12)-C(11)-C(6)	120.2(3)
C(10)-C(11)-C(6)	118.1(3)
C(13)-C(12)-C(11)	119.5(3)
C(13)-C(12)-C(38)	121.0(3)
C(11)-C(12)-C(38)	119.4(3)
C(12)-C(13)-C(14)	121.3(3)
C(12)-C(13)-C(4)	120.4(3)
C(14)-C(13)-C(4)	118.3(3)
C(15)-C(14)-C(13)	122.0(3)
C(14)-C(15)-C(2)	119.3(3)
C(14)-C(15)-C(16)	123.7(3)
C(2)-C(15)-C(16)	116.9(3)
C(62)-C(16)-C(17)	122.1(3)
C(62)-C(16)-C(15)	123.8(3)
C(17)-C(16)-C(15)	114.1(3)

C(18)-C(17)-C(30)	119.7(3)
C(18)-C(17)-C(16)	122.2(3)
C(30)-C(17)-C(16)	118.0(3)
C(17)-C(18)-C(19)	122.4(3)
C(20)-C(19)-C(18)	121.6(3)
C(20)-C(19)-C(28)	120.2(3)
C(18)-C(19)-C(28)	118.2(3)
C(19)-C(20)-C(21)	120.2(3)
C(19)-C(20)-C(52)	118.9(3)
C(21)-C(20)-C(52)	120.8(3)
C(20)-C(21)-C(22)	121.7(3)
C(20)-C(21)-C(26)	119.9(3)
C(22)-C(21)-C(26)	118.4(3)
C(23)-C(22)-C(21)	121.3(4)
C(22)-C(23)-C(24)	120.4(4)
C(25)-C(24)-C(23)	119.8(4)
C(24)-C(25)-C(26)	121.7(4)
C(27)-C(26)-C(25)	121.8(3)
C(27)-C(26)-C(21)	119.7(3)
C(25)-C(26)-C(21)	118.4(3)
C(28)-C(27)-C(26)	120.1(3)
C(28)-C(27)-C(45)	120.1(3)
C(26)-C(27)-C(45)	119.9(3)
C(27)-C(28)-C(29)	121.9(3)
C(27)-C(28)-C(19)	120.0(3)

C(29)-C(28)-C(19)	118.1(3)
C(30)-C(29)-C(28)	122.4(3)
C(29)-C(30)-C(17)	119.1(3)
C(29)-C(30)-C(1)	124.1(3)
C(17)-C(30)-C(1)	116.8(3)
C(32)-C(31)-C(36)	118.8(3)
C(32)-C(31)-C(5)	121.1(3)
C(36)-C(31)-C(5)	120.0(3)
C(33)-C(32)-C(31)	120.9(4)
C(32)-C(33)-C(34)	119.6(4)
C(35)-C(34)-C(33)	120.4(4)
C(35)-C(34)-C(37)	119.9(4)
C(33)-C(34)-C(37)	119.7(4)
C(34)-C(35)-C(36)	119.6(4)
C(35)-C(36)-C(31)	120.6(4)
F(2A)-C(37)-F(1)	114.9(6)
F(2A)-C(37)-F(3A)	118.4(5)
F(1)-C(37)-F(3A)	60.9(4)
F(2A)-C(37)-F(3)	74.3(5)
F(1)-C(37)-F(3)	107.8(5)
F(3A)-C(37)-F(3)	54.8(4)
F(2A)-C(37)-F(2)	25.8(4)
F(1)-C(37)-F(2)	104.7(5)
F(3A)-C(37)-F(2)	136.4(5)
F(3)-C(37)-F(2)	100.0(5)

F(2A)-C(37)-F(1A)	100.5(5)
F(1)-C(37)-F(1A)	33.2(3)
F(3A)-C(37)-F(1A)	94.1(5)
F(3)-C(37)-F(1A)	135.1(5)
F(2)-C(37)-F(1A)	80.6(5)
F(2A)-C(37)-C(34)	118.7(5)
F(1)-C(37)-C(34)	119.3(5)
F(3A)-C(37)-C(34)	111.7(5)
F(3)-C(37)-C(34)	112.2(4)
F(2)-C(37)-C(34)	110.9(4)
F(1A)-C(37)-C(34)	109.1(4)
C(43)-C(38)-C(39)	118.5(3)
C(43)-C(38)-C(12)	122.7(3)
C(39)-C(38)-C(12)	118.8(3)
C(40)-C(39)-C(38)	120.9(4)
C(39)-C(40)-C(41)	120.0(4)
C(40)-C(41)-C(42)	119.8(4)
C(40)-C(41)-C(44A)	119.0(5)
C(42)-C(41)-C(44A)	121.2(5)
C(40)-C(41)-C(44)	122.2(6)
C(42)-C(41)-C(44)	118.1(6)
C(44A)-C(41)-C(44)	3.6(8)
C(43)-C(42)-C(41)	119.9(4)
C(42)-C(43)-C(38)	120.9(4)
C(46)-C(45)-C(50)	118.3(3)

C(46)-C(45)-C(27)	120.4(3)
C(50)-C(45)-C(27)	121.3(3)
C(47)-C(46)-C(45)	121.4(4)
C(48)-C(47)-C(46)	119.8(4)
C(47)-C(48)-C(49)	120.3(4)
C(47)-C(48)-C(51)	121.1(4)
C(49)-C(48)-C(51)	118.6(4)
C(50)-C(49)-C(48)	119.6(4)
C(49)-C(50)-C(45)	120.6(4)
F(7)-C(51)-F(8)	106.3(4)
F(7)-C(51)-F(9)	105.0(3)
F(8)-C(51)-F(9)	106.4(4)
F(7)-C(51)-C(48)	113.5(3)
F(8)-C(51)-C(48)	112.9(4)
F(9)-C(51)-C(48)	112.1(4)
C(53)-C(52)-C(57)	118.3(3)
C(53)-C(52)-C(20)	122.0(3)
C(57)-C(52)-C(20)	119.7(3)
C(54)-C(53)-C(52)	121.2(4)
C(53)-C(54)-C(55)	119.8(4)
C(54)-C(55)-C(56)	119.7(4)
C(54)-C(55)-C(58)	121.8(4)
C(56)-C(55)-C(58)	118.5(4)
C(57)-C(56)-C(55)	119.9(4)
C(56)-C(57)-C(52)	121.1(4)

F(10)-C(58)-F(11)	107.0(4)
F(10)-C(58)-F(12)	106.7(3)
F(11)-C(58)-F(12)	105.8(3)
F(10)-C(58)-C(55)	113.0(4)
F(11)-C(58)-C(55)	112.3(4)
F(12)-C(58)-C(55)	111.6(3)
C(1)-C(59)-C(60)	123.4(3)
C(1)-C(59)-C(61)	123.1(3)
C(60)-C(59)-C(61)	113.5(3)
N(1)-C(60)-C(59)	176.7(4)
N(2)-C(61)-C(59)	177.3(4)
C(16)-C(62)-C(64)	123.2(3)
C(16)-C(62)-C(63)	124.3(3)
C(64)-C(62)-C(63)	112.4(3)
N(3)-C(63)-C(62)	176.5(4)
N(4)-C(64)-C(62)	175.9(4)
Cl(2)-C(1S)-Cl(1)	107.6(7)
Cl(2)-C(1S)-Cl(3A)	115.5(7)
Cl(1)-C(1S)-Cl(3A)	112.9(10)
Cl(2)-C(1S)-Cl(3)	110.8(7)
Cl(1)-C(1S)-Cl(3)	115.5(10)
Cl(3A)-C(1S)-Cl(3)	4.7(11)
Cl(2)-C(1S)-Cl(2A)	6.9(8)
Cl(1)-C(1S)-Cl(2A)	114.4(6)
Cl(3A)-C(1S)-Cl(2A)	112.4(6)

Cl(3)-C(1S)-Cl(2A)	107.7(6)
Cl(2)-C(1S)-Cl(1A)	103.1(8)
Cl(1)-C(1S)-Cl(1A)	12.7(10)
Cl(3A)-C(1S)-Cl(1A)	105.8(7)
Cl(3)-C(1S)-Cl(1A)	107.6(7)
Cl(2A)-C(1S)-Cl(1A)	110.0(5)
Cl(5)-C(2S)-Cl(4)	110.5(2)
Cl(5)-C(2S)-Cl(6)	109.8(2)
Cl(4)-C(2S)-Cl(6)	109.9(2)
Cl(9)-C(3S)-Cl(7)	110.3(13)
Cl(9)-C(3S)-Cl(8)	110.0(13)
Cl(7)-C(3S)-Cl(8)	110.2(13)
Cl(9A)-C(3SA)-Cl(7A)	113.0(13)
Cl(9A)-C(3SA)-Cl(8A)	111.1(13)
Cl(7A)-C(3SA)-Cl(8A)	109.7(13)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 2. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	21(1)	72(2)	78(2)	-17(1)	6(1)	-6(1)
F(2)	20(1)	70(2)	76(2)	-20(2)	9(1)	-8(1)

F(3)	19(1)	72(2)	76(2)	-20(1)	9(1)	-8(1)
F(1A)	21(1)	72(2)	76(2)	-19(2)	6(1)	-6(1)
F(2A)	20(1)	71(2)	77(2)	-18(1)	8(1)	-9(1)
F(3A)	19(1)	72(2)	78(2)	-20(1)	7(1)	-6(1)
C(44)	24(1)	46(2)	46(2)	-5(1)	0(1)	-8(1)
F(4)	23(1)	47(2)	46(2)	-5(1)	-1(1)	-7(1)
F(5)	24(1)	46(2)	47(2)	-4(1)	0(1)	-8(1)
F(6)	25(1)	46(2)	46(2)	-5(1)	-1(1)	-8(1)
C(44A)	24(1)	46(2)	46(2)	-5(1)	0(1)	-8(1)
F(4A)	23(1)	47(2)	46(2)	-5(1)	-1(1)	-7(1)
F(5A)	24(1)	46(2)	46(2)	-4(1)	1(1)	-8(1)
F(6A)	25(1)	46(2)	47(2)	-5(1)	-1(1)	-8(1)
F(7)	32(1)	36(2)	71(2)	-12(1)	4(1)	-12(1)
F(8)	33(2)	72(2)	112(3)	53(2)	-27(2)	-16(2)
F(9)	28(2)	80(2)	85(2)	-33(2)	29(2)	-18(2)
F(10)	25(1)	81(2)	44(2)	-13(2)	13(1)	-14(1)
F(11)	22(1)	42(2)	115(3)	-2(2)	-6(2)	7(1)
F(12)	28(1)	44(2)	34(1)	-9(1)	-3(1)	-12(1)
N(1)	33(2)	28(2)	45(2)	-6(2)	17(2)	-4(2)
N(2)	45(2)	28(2)	49(2)	3(2)	28(2)	1(2)
N(3)	22(2)	28(2)	27(2)	-3(1)	1(1)	2(2)
N(4)	33(2)	30(2)	26(2)	-6(2)	-2(2)	7(2)
C(1)	16(2)	20(2)	20(2)	-2(2)	0(2)	1(2)
C(2)	18(2)	15(2)	21(2)	2(2)	2(2)	0(2)
C(3)	17(2)	19(2)	21(2)	3(2)	1(2)	-3(2)

C(4)	19(2)	14(2)	21(2)	3(1)	2(2)	2(2)
C(5)	19(2)	17(2)	21(2)	1(2)	2(2)	-1(2)
C(6)	21(2)	18(2)	17(2)	2(2)	3(2)	0(2)
C(7)	21(2)	22(2)	22(2)	-1(2)	3(2)	-3(2)
C(8)	28(2)	23(2)	18(2)	-5(2)	2(2)	-7(2)
C(9)	28(2)	20(2)	20(2)	-1(2)	8(2)	-1(2)
C(10)	19(2)	23(2)	24(2)	2(2)	5(2)	-1(2)
C(11)	20(2)	15(2)	19(2)	1(1)	1(2)	0(2)
C(12)	19(2)	20(2)	19(2)	1(2)	4(2)	0(2)
C(13)	20(2)	18(2)	20(2)	-2(2)	3(2)	1(2)
C(14)	15(2)	19(2)	22(2)	3(2)	-1(2)	-1(2)
C(15)	18(2)	15(2)	20(2)	-1(2)	0(2)	1(2)
C(16)	18(2)	16(2)	19(2)	2(2)	6(2)	-4(2)
C(17)	20(2)	20(2)	13(2)	-2(1)	4(2)	-2(2)
C(18)	16(2)	27(2)	15(2)	-3(2)	2(2)	-1(2)
C(19)	21(2)	21(2)	16(2)	-4(2)	5(2)	0(2)
C(20)	20(2)	21(2)	15(2)	0(2)	2(2)	1(2)
C(21)	23(2)	20(2)	14(2)	1(2)	4(2)	0(2)
C(22)	21(2)	21(2)	21(2)	2(2)	2(2)	-2(2)
C(23)	34(2)	19(2)	21(2)	-3(2)	3(2)	-2(2)
C(24)	28(2)	24(2)	23(2)	-2(2)	5(2)	4(2)
C(25)	21(2)	28(2)	20(2)	2(2)	4(2)	3(2)
C(26)	22(2)	19(2)	13(2)	1(1)	3(2)	3(2)
C(27)	20(2)	21(2)	18(2)	-2(2)	5(2)	-1(2)
C(28)	18(2)	21(2)	14(2)	-2(2)	3(1)	-1(2)

C(29)	14(2)	21(2)	20(2)	-2(2)	4(2)	-2(2)
C(30)	19(2)	21(2)	15(2)	-1(2)	2(2)	-2(2)
C(31)	22(2)	17(2)	16(2)	-6(2)	2(2)	0(2)
C(32)	28(2)	22(2)	26(2)	0(2)	3(2)	-4(2)
C(33)	26(2)	25(2)	31(2)	-1(2)	-4(2)	4(2)
C(34)	20(2)	21(2)	35(2)	-8(2)	3(2)	2(2)
C(35)	23(2)	29(2)	32(2)	-1(2)	6(2)	-7(2)
C(36)	24(2)	21(2)	23(2)	1(2)	-2(2)	0(2)
C(37)	20(1)	71(2)	76(2)	-19(1)	8(1)	-7(1)
C(38)	17(2)	20(2)	19(2)	-6(2)	4(2)	0(2)
C(39)	22(2)	27(2)	24(2)	1(2)	-1(2)	-2(2)
C(40)	28(2)	26(2)	31(2)	-3(2)	7(2)	-4(2)
C(41)	19(2)	29(2)	29(2)	-7(2)	5(2)	-1(2)
C(42)	19(2)	38(3)	33(2)	6(2)	-1(2)	0(2)
C(43)	28(2)	36(2)	22(2)	2(2)	6(2)	0(2)
C(45)	19(2)	18(2)	23(2)	-4(2)	7(2)	1(2)
C(46)	26(2)	24(2)	26(2)	2(2)	7(2)	-2(2)
C(47)	24(2)	23(2)	32(2)	7(2)	0(2)	3(2)
C(48)	21(2)	20(2)	32(2)	-2(2)	8(2)	2(2)
C(49)	20(2)	26(2)	30(2)	2(2)	8(2)	0(2)
C(50)	24(2)	23(2)	23(2)	0(2)	5(2)	-1(2)
C(51)	24(2)	30(3)	45(3)	2(2)	5(2)	-3(2)
C(52)	18(2)	18(2)	25(2)	-9(2)	2(2)	3(2)
C(53)	26(2)	22(2)	24(2)	-2(2)	3(2)	0(2)
C(54)	25(2)	26(2)	27(2)	-4(2)	6(2)	-5(2)

C(55)	20(2)	22(2)	31(2)	-11(2)	6(2)	-2(2)
C(56)	23(2)	27(2)	26(2)	-5(2)	-3(2)	2(2)
C(57)	25(2)	24(2)	21(2)	-4(2)	6(2)	0(2)
C(58)	23(2)	32(3)	41(3)	-5(2)	2(2)	-1(2)
C(59)	19(2)	24(2)	21(2)	-2(2)	3(2)	0(2)
C(60)	20(2)	26(2)	28(2)	-1(2)	10(2)	-3(2)
C(61)	28(2)	18(2)	34(2)	3(2)	9(2)	-1(2)
C(62)	21(2)	18(2)	19(2)	-3(2)	4(2)	-1(2)
C(63)	19(2)	19(2)	17(2)	-4(2)	-2(2)	-5(2)
C(64)	20(2)	20(2)	25(2)	2(2)	0(2)	1(2)
C(1S)	55(3)	38(3)	39(3)	-10(2)	16(2)	-16(2)
Cl(1)	90(5)	82(8)	57(4)	31(4)	28(3)	57(5)
Cl(2)	86(6)	111(8)	51(4)	0(3)	16(4)	17(4)
Cl(3)	81(6)	47(4)	24(4)	14(4)	8(4)	-10(3)
Cl(1A)	97(3)	39(3)	48(3)	-1(3)	27(2)	2(4)
Cl(2A)	52(3)	25(3)	36(3)	-11(2)	19(2)	0(2)
Cl(3A)	70(5)	81(6)	37(4)	-18(3)	16(3)	-30(4)
C(2S)	29(2)	22(2)	26(2)	-4(2)	5(2)	-1(2)
Cl(4)	55(1)	46(1)	39(1)	-21(1)	17(1)	-11(1)
Cl(5)	27(1)	41(1)	41(1)	-2(1)	7(1)	-2(1)
Cl(6)	35(1)	29(1)	28(1)	-5(1)	3(1)	-11(1)
C(3S)	86(4)	122(4)	200(7)	45(5)	4(5)	-28(4)
Cl(7)	88(4)	122(4)	199(7)	45(4)	4(5)	-28(4)
Cl(8)	87(11)	128(9)	71(7)	40(4)	8(9)	-2(11)
Cl(9)	86(4)	122(5)	199(7)	45(5)	4(5)	-28(4)

C(3SA)	87(4)	122(4)	200(7)	45(5)	4(5)	-28(4)
Cl(7A)	88(11)	128(9)	71(7)	40(4)	8(9)	-3(11)
Cl(8A)	87(4)	122(4)	199(7)	44(5)	4(5)	-28(4)
Cl(9A)	86(3)	122(4)	200(7)	45(5)	4(5)	-28(4)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound 2.

	x	y	z	U(eq)
H(3)	10829	2384	4358	23
H(7)	10030	4026	5679	26
H(8)	8833	4489	6113	28
H(9)	7076	4130	5920	26
H(10)	6540	3252	5317	26
H(14)	7371	1499	4035	23
H(18)	8343	-846	3230	23
H(22)	9403	-3884	2903	25
H(23)	10688	-4884	2833	30
H(24)	12448	-4445	2956	30
H(25)	12883	-3033	3189	28
H(29)	11815	-6	3558	22
H(32)	11210	2354	5560	31
H(33)	12969	2659	5710	34

H(35)	12642	4528	4751	34
H(36)	10883	4199	4592	28
H(39)	6783	1316	5202	30
H(40)	5107	772	5121	34
H(42)	4336	2332	4048	37
H(43)	6009	2889	4136	34
H(46)	13123	-2224	3968	30
H(47)	14841	-1824	4142	32
H(49)	14500	-89	3123	30
H(50)	12786	-527	2932	28
H(53)	8370	-3222	3584	28
H(54)	6609	-3509	3443	31
H(56)	6409	-2063	2314	31
H(57)	8158	-1761	2465	28
H(1S)	-75	8309	1792	51
H(2S)	2036	5043	6619	31
H(3S)	-71	10617	4655	165
H(3SA)	-8	10612	4655	165

Table S6. Crystallographic data and structure refinement for compound 4.

Identification code	c526
Empirical formula	C66 H42 Cl12 N8 S2
Formula weight	1436.60
Temperature	100(2) K

Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.1259(11) Å	α= 102.087(2)°.
	b = 11.1866(13) Å	β= 91.163(2)°.
	c = 15.4918(17) Å	γ = 105.935(2)°.
Volume	1644.3(3) $Å^3$	
Z	1	
Density (calculated)	1.451 Mg/m^3	
Absorption coefficient	0.617 mm^{-1}	
F(000)	730	
Crystal size	0.56 x 0.36 x 0.20 mm^3	
Theta range for data collection	1.35 to 27.50°.	
Index ranges	-13<=h<=13, -14<=k<=14, -20<=l<=20	
Reflections collected	21459	
Independent reflections	7560 [R(int) = 0.0391]	
Completeness to theta = 27.50°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8866 and 0.7239	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7560 / 0 / 397	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0535, wR2 = 0.1501	
R indices (all data)	R1 = 0.0735, wR2 = 0.1632	
Largest diff. peak and hole	1.810 and -0.463 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound 4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	11232(1)	660(1)	3218(1)	16(1)
N(1)	5182(3)	4505(3)	7522(2)	29(1)
N(2)	8735(3)	3258(3)	7893(2)	28(1)
N(3)	11310(2)	4366(2)	3777(2)	22(1)
N(4)	8282(3)	6342(2)	3661(2)	25(1)
C(1)	10531(3)	280(2)	4199(2)	14(1)
C(2)	9618(3)	915(2)	4621(2)	14(1)
C(3)	9206(3)	1843(2)	4268(2)	14(1)
C(4)	8348(3)	2483(2)	4687(2)	14(1)
C(5)	7901(3)	3454(2)	4346(2)	14(1)
C(6)	6454(3)	3426(2)	4470(2)	15(1)
C(7)	5631(3)	3662(3)	3834(2)	17(1)
C(8)	4244(3)	3520(3)	3944(2)	20(1)
C(9)	3685(3)	3172(3)	4690(2)	20(1)
C(10)	4496(3)	2962(2)	5343(2)	17(1)
C(11)	5888(3)	3083(2)	5237(2)	15(1)
C(12)	6816(3)	2859(2)	5890(2)	15(1)
C(13)	7807(3)	2202(2)	5496(2)	15(1)

C(14)	8165(3)	1298(2)	5844(2)	14(1)
C(15)	9084(3)	634(2)	5430(2)	14(1)
C(16)	9868(3)	-231(3)	2396(2)	18(1)
C(17)	9850(3)	192(3)	1618(2)	30(1)
C(18)	8832(4)	-482(3)	944(2)	35(1)
C(19)	7824(3)	-1574(3)	1010(2)	26(1)
C(20)	7884(3)	-1976(3)	1796(2)	29(1)
C(21)	8893(3)	-1325(3)	2483(2)	26(1)
C(22)	6737(4)	-2307(3)	245(2)	34(1)
C(24)	7385(5)	-3123(5)	-427(3)	56(1)
C(25)	5486(4)	-3174(4)	556(2)	40(1)
C(23)	6225(5)	-1384(5)	-190(3)	60(1)
C(26)	6818(3)	3272(2)	6774(2)	17(1)
C(27)	5888(3)	3953(3)	7174(2)	20(1)
C(28)	7888(3)	3233(3)	7391(2)	20(1)
C(29)	8778(3)	4331(3)	3980(2)	15(1)
C(30)	8453(3)	5422(3)	3777(2)	18(1)
C(31)	10185(3)	4338(2)	3865(2)	17(1)
C(1S)	5665(4)	9879(4)	2513(3)	45(1)
Cl(1)	5628(1)	9926(1)	3661(1)	49(1)
Cl(2)	6689(1)	11281(1)	2306(1)	41(1)
Cl(3)	9518(1)	3405(1)	1672(1)	46(1)
C(2S)	8757(3)	4254(3)	1077(2)	31(1)
Cl(4)	7202(1)	4387(1)	1509(1)	34(1)
Cl(5)	8515(1)	3538(1)	-53(1)	45(1)

Cl(6)	3969(1)	9486(1)	2026(1)	50(1)

Table S8. Bond lengths [Å] and angles [°] for compound 4.

S(1)-C(1)	1.772(3)
S(1)-C(16)	1.779(3)
N(1)-C(27)	1.141(4)
N(2)-C(28)	1.135(4)
N(3)-C(31)	1.143(4)
N(4)-C(30)	1.138(4)
C(1)-C(2)	1.407(3)
C(1)-C(15)#1	1.408(4)
C(2)-C(3)	1.421(3)
C(2)-C(15)	1.435(4)
C(3)-C(4)	1.362(4)
C(3)-H(3A)	0.9500
C(4)-C(13)	1.438(4)
C(4)-C(5)	1.471(3)
C(5)-C(29)	1.360(4)
C(5)-C(6)	1.474(3)
C(6)-C(7)	1.390(4)
C(6)-C(11)	1.409(4)
C(7)-C(8)	1.388(4)
C(7)-H(7A)	0.9500

C(8)-C(9)	1.380(4)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.387(4)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.395(4)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.472(4)
C(12)-C(26)	1.350(4)
C(12)-C(13)	1.471(3)
C(13)-C(14)	1.365(4)
C(14)-C(15)	1.426(3)
C(14)-H(14A)	0.9500
C(15)-C(1)#1	1.408(4)
C(16)-C(21)	1.379(4)
C(16)-C(17)	1.384(4)
C(17)-C(18)	1.386(5)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.384(5)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.388(4)
C(19)-C(22)	1.528(4)
C(20)-C(21)	1.390(4)
C(20)-H(20A)	0.9500
C(21)-H(21A)	0.9500
C(22)-C(24)	1.518(5)

C(22)-C(25)	1.524(5)
C(22)-C(23)	1.536(5)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(26)-C(27)	1.440(4)
C(26)-C(28)	1.446(4)
C(29)-C(31)	1.437(4)
C(29)-C(30)	1.441(4)
C(1S)-Cl(2)	1.722(4)
C(1S)-Cl(6)	1.762(4)
C(1S)-Cl(1)	1.769(4)
C(1S)-H(1SA)	1.0000
Cl(3)-C(2S)	1.756(3)
C(2S)-Cl(5)	1.748(3)
C(2S)-Cl(4)	1.754(3)
C(2S)-H(2SA)	1.0000
C(1)-S(1)-C(16)	102.07(12)
C(2)-C(1)-C(15)#1	119.8(2)

C(2)-C(1)-S(1)	120.10(19)
C(15)#1-C(1)-S(1)	120.06(19)
C(1)-C(2)-C(3)	121.5(2)
C(1)-C(2)-C(15)	120.0(2)
C(3)-C(2)-C(15)	118.5(2)
C(4)-C(3)-C(2)	121.7(2)
C(4)-C(3)-H(3A)	119.2
C(2)-C(3)-H(3A)	119.2
C(3)-C(4)-C(13)	120.0(2)
C(3)-C(4)-C(5)	123.5(2)
C(13)-C(4)-C(5)	116.5(2)
C(29)-C(5)-C(4)	122.0(2)
C(29)-C(5)-C(6)	123.4(2)
C(4)-C(5)-C(6)	114.5(2)
C(7)-C(6)-C(11)	120.0(2)
C(7)-C(6)-C(5)	121.8(2)
C(11)-C(6)-C(5)	118.2(2)
C(8)-C(7)-C(6)	119.8(3)
C(8)-C(7)-H(7A)	120.1
C(6)-C(7)-H(7A)	120.1
C(9)-C(8)-C(7)	120.3(2)
C(9)-C(8)-H(8A)	119.8
C(7)-C(8)-H(8A)	119.8
C(8)-C(9)-C(10)	120.8(2)
C(8)-C(9)-H(9A)	119.6

C(10)-C(9)-H(9A)	119.6
C(9)-C(10)-C(11)	119.7(2)
C(9)-C(10)-H(10A)	120.2
C(11)-C(10)-H(10A)	120.2
C(10)-C(11)-C(6)	119.5(2)
C(10)-C(11)-C(12)	123.2(2)
C(6)-C(11)-C(12)	117.3(2)
C(26)-C(12)-C(13)	122.2(2)
C(26)-C(12)-C(11)	123.7(2)
C(13)-C(12)-C(11)	114.1(2)
C(14)-C(13)-C(4)	119.7(2)
C(14)-C(13)-C(12)	122.4(2)
C(4)-C(13)-C(12)	117.8(2)
C(13)-C(14)-C(15)	121.5(2)
C(13)-C(14)-H(14A)	119.2
C(15)-C(14)-H(14A)	119.2
C(1)#1-C(15)-C(14)	121.2(2)
C(1)#1-C(15)-C(2)	120.2(2)
C(14)-C(15)-C(2)	118.6(2)
C(21)-C(16)-C(17)	119.7(3)
C(21)-C(16)-S(1)	123.6(2)
C(17)-C(16)-S(1)	116.6(2)
C(16)-C(17)-C(18)	119.3(3)
C(16)-C(17)-H(17A)	120.4
C(18)-C(17)-H(17A)	120.4

C(19)-C(18)-C(17)	122.7(3)
C(19)-C(18)-H(18A)	118.6
C(17)-C(18)-H(18A)	118.6
C(18)-C(19)-C(20)	116.4(3)
C(18)-C(19)-C(22)	121.2(3)
C(20)-C(19)-C(22)	122.4(3)
C(19)-C(20)-C(21)	122.3(3)
C(19)-C(20)-H(20A)	118.8
C(21)-C(20)-H(20A)	118.8
C(16)-C(21)-C(20)	119.5(3)
C(16)-C(21)-H(21A)	120.2
C(20)-C(21)-H(21A)	120.2
C(24)-C(22)-C(25)	108.7(3)
C(24)-C(22)-C(19)	108.0(3)
C(25)-C(22)-C(19)	111.7(3)
C(24)-C(22)-C(23)	110.1(4)
C(25)-C(22)-C(23)	107.5(3)
C(19)-C(22)-C(23)	110.7(3)
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22)-C(25)-H(25A)	109.5

C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(12)-C(26)-C(27)	123.2(2)
C(12)-C(26)-C(28)	122.3(2)
C(27)-C(26)-C(28)	113.8(2)
N(1)-C(27)-C(26)	177.3(3)
N(2)-C(28)-C(26)	176.9(3)
C(5)-C(29)-C(31)	122.4(2)
C(5)-C(29)-C(30)	123.7(2)
C(31)-C(29)-C(30)	113.5(2)
N(4)-C(30)-C(29)	174.7(3)
N(3)-C(31)-C(29)	178.8(3)
Cl(2)-C(1S)-Cl(6)	112.1(2)
Cl(2)-C(1S)-Cl(1)	112.0(2)
Cl(6)-C(1S)-Cl(1)	109.6(2)
Cl(2)-C(1S)-H(1SA)	107.6

Cl(6)-C(1S)-H(1SA)	107.6
Cl(1)-C(1S)-H(1SA)	107.6
Cl(5)-C(2S)-Cl(4)	111.53(18)
Cl(5)-C(2S)-Cl(3)	111.0(2)
Cl(4)-C(2S)-Cl(3)	110.05(17)
Cl(5)-C(2S)-H(2SA)	108.1
Cl(4)-C(2S)-H(2SA)	108.1
Cl(3)-C(2S)-H(2SA)	108.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 4. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	14(1)	17(1)	19(1)	6(1)	4(1)	6(1)
N(1)	30(1)	36(2)	27(1)	6(1)	6(1)	19(1)
N(2)	27(1)	34(2)	24(1)	3(1)	-2(1)	13(1)
N(3)	15(1)	20(1)	32(1)	10(1)	4(1)	5(1)
N(4)	25(1)	24(1)	32(1)	13(1)	8(1)	11(1)
C(1)	11(1)	13(1)	17(1)	5(1)	2(1)	3(1)
C(2)	11(1)	12(1)	18(1)	3(1)	0(1)	3(1)
C(3)	12(1)	14(1)	16(1)	3(1)	1(1)	4(1)
C(4)	11(1)	12(1)	18(1)	3(1)	-1(1)	3(1)
C(5)	12(1)	13(1)	16(1)	2(1)	0(1)	5(1)
C(6)	13(1)	13(1)	19(1)	2(1)	1(1)	6(1)
C(7)	16(1)	16(1)	22(1)	4(1)	2(1)	6(1)
C(8)	16(1)	22(1)	25(1)	6(1)	-2(1)	9(1)
C(9)	11(1)	19(1)	29(2)	3(1)	1(1)	6(1)
C(10)	15(1)	14(1)	23(1)	4(1)	4(1)	6(1)
C(11)	16(1)	12(1)	20(1)	3(1)	1(1)	7(1)
C(12)	11(1)	12(1)	22(1)	6(1)	4(1)	4(1)
C(13)	11(1)	14(1)	19(1)	1(1)	1(1)	4(1)
C(14)	12(1)	14(1)	17(1)	3(1)	2(1)	3(1)
C(15)	11(1)	14(1)	17(1)	3(1)	1(1)	3(1)

C(16)	18(1)	19(1)	19(1)	3(1)	2(1)	8(1)
C(17)	32(2)	32(2)	25(2)	14(1)	0(1)	2(1)
C(18)	40(2)	40(2)	23(2)	11(1)	-1(1)	6(2)
C(19)	26(2)	31(2)	23(2)	4(1)	0(1)	12(1)
C(20)	31(2)	24(2)	29(2)	8(1)	-5(1)	3(1)
C(21)	30(2)	23(2)	24(2)	9(1)	-3(1)	6(1)
C(22)	38(2)	36(2)	24(2)	3(1)	-6(1)	8(2)
C(24)	50(2)	68(3)	34(2)	-17(2)	-3(2)	11(2)
C(25)	32(2)	46(2)	34(2)	0(2)	-8(1)	3(2)
C(23)	58(3)	58(3)	59(3)	24(2)	-29(2)	2(2)
C(26)	14(1)	14(1)	23(1)	7(1)	3(1)	6(1)
C(27)	21(1)	22(1)	20(1)	5(1)	2(1)	8(1)
C(28)	20(1)	18(1)	22(1)	4(1)	6(1)	8(1)
C(29)	14(1)	16(1)	17(1)	4(1)	1(1)	6(1)
C(30)	14(1)	20(1)	20(1)	7(1)	4(1)	5(1)
C(31)	20(1)	13(1)	20(1)	6(1)	1(1)	4(1)
C(1S)	38(2)	37(2)	55(2)	4(2)	3(2)	5(2)
Cl(1)	53(1)	36(1)	43(1)	11(1)	-2(1)	-13(1)
Cl(2)	43(1)	33(1)	39(1)	5(1)	13(1)	-2(1)
Cl(3)	43(1)	70(1)	40(1)	23(1)	10(1)	30(1)
C(2S)	29(2)	40(2)	21(2)	6(1)	3(1)	7(1)
Cl(4)	31(1)	45(1)	28(1)	7(1)	3(1)	13(1)
Cl(5)	42(1)	63(1)	23(1)	2(1)	4(1)	8(1)
Cl(6)	27(1)	64(1)	56(1)	18(1)	4(1)	7(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound 4.

	x	y	z	U(eq)
H(3A)	9537	2023	3726	17
H(7A)	6017	3919	3325	21
H(8A)	3676	3665	3504	24
H(9A)	2733	3074	4758	23
H(10A)	4105	2737	5859	20
H(14A)	7793	1108	6374	17
H(17A)	10527	935	1548	36
H(18A)	8827	-183	414	42
H(20A)	7211	-2723	1865	35
H(21A)	8910	-1631	3010	31
H(24A)	7705	-3710	-143	85
H(24B)	8169	-2572	-650	85
H(24C)	6701	-3613	-921	85
H(25A)	5778	-3781	833	61
H(25B)	4821	-3642	47	61
H(25C)	5054	-2658	987	61
H(23A)	7008	-810	-397	90
H(23B)	5782	-882	243	90

H(23C)	5559	-1871	-695	90
H(1SA)	6070	9182	2242	54
H(2SA)	9398	5134	1154	37