Electronic Supporting Information (ESI) for

Dianthraceno[*a,e*]pentalenes: Synthesis, Crystallographic Structures and Applications for Organic Field-Effect Transistors

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1. Experimental section

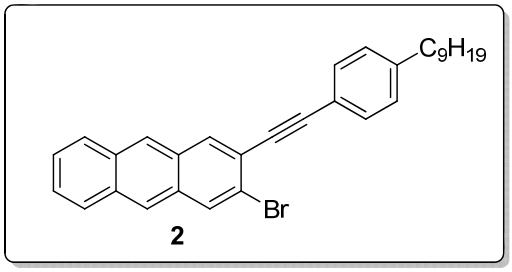
1.1. Materials

All reagents were purchased from commercial sources without further purification.Anhydrous dichloromethane (DCM)was distilled from CaH_2. Anhydrous 1,4-dioxane, toluene and THF were distilled from sodium-benzophenone immediately prior to use. 2,3-Dibromoanthracene **1**, 1,3-diphenylisobenzofuran **3** and 1-ethynyl-4-nonylbenzene were prepared by following literature procedures.

1.2. General characterization method

^1H and ^{13}C NMR spectra were recorded using Advance 500 MHz Bruker spectrometer in $CDCl_3$with tetramethylsilane (TMS) as the internal standard. The chemical shift was recorded in ppm and the following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t= triplet, m = multiplet, br = broad.Column chromatography was performed on silica gel 60 (Merck 40-60 nm, 230-400 mesh). EI mass spectra were recorded on Agilent 5975C DIP/MS mass spectrometer. UV-vis absorption and fluorescence spectra were recorded on a Shimadzu UV-1700 spectrophotometer and a RF-5301 fluorometer, respectively. Cyclic voltammetry and differential pulse voltammetry 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 mVs^{-1}. The potential was externally calibrated against the ferrocene/ferrocenium couple. The HOMO and LUMO energy levels were calculated using the following equations: HOMO = - [E_{ox}^{onset} + 4.8] eV, LUMO = - [E_{red}^{onset} + 4.8] eV, where E_{ox}^{onset} and E_{red}^{onset} are the onset of the first oxidation and reduction wave, respectively.Thermogravimetric analysis (TGA) was carried out on a TA instrument 2960 at a heating rate of 10 $^oCmin^{-1}$ under nitrogen flow. Differential scanning calorimetry (DSC) was performed on a TA instrument 2920 at a heating/cooling rate of 10 $^oCmin^{-1}$ under nitrogen flow. Tapping-mode Atomic Force Microscopy (TM-AFM) was performed on a Nanoscope V microscope (Veeco Inc.). X-ray diffraction (XRD) patterns of the thin film were measured on a Bruker-AXS D8 DISCOVER with GADDS X-ray diffractometer. Copper Kα line was used as a radiation source with λ = 1.5408 Å.

1.3. Synthetic procedures and characterization data



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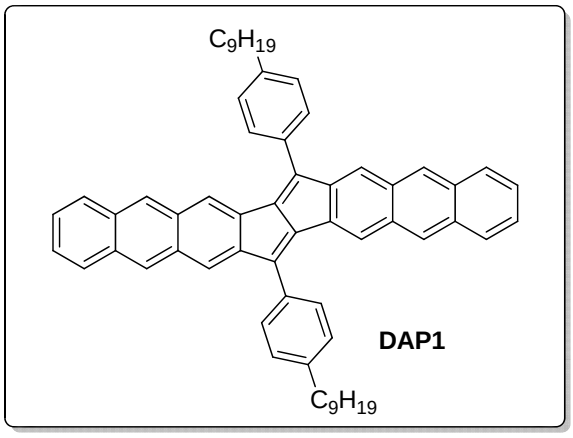
2-Bromo-3-((4-nonylphenyl)ethynyl)anthracene (compound **2**)

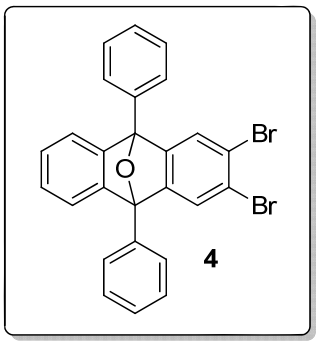
A mixture of compound **1** (1.80 g, 5.4 mmol), 1-ethynyl-4-nonylbenzene (1.29 g, 5.6 mmol), $Pd(PPh_3)_2Cl_2$ (190 mg, 5%) andCuI (31 mg, 3%) in anhydrous THF (15 mL) and

Et_3N (15 mL) was degassed by three freeze-pupm-thaw cycles. The mixture was stirred at 75 ^oC under argon for overnight. The mixture was extracted with EtOAc (50 mL ×2). The combined organic phase was washed with HCl (10%) solution (50 mL ×2) and brine (50 mL ×1). The organic phase was dried over anhydrous Na_2SO_4 and the organic solvent was removed under reduced pressure. The crude product was purified by column chromatography (DCM/Hexane = 10:1) to afford compound **2** (0.90 g) in 35% yield. ^1H NMR (500 MHz, $CDCl_3$, ppm): δ = 8.36 (s, 1H), 8.30 (s, 1H), 8.28 (s, 1H), 8.25 (s, 1H), 8.02-7.97 (m, 2H), 7.56 (d, *J* =8.0 Hz, 2H), 7.51-7.48 (m, 2H), 7.20 (d, *J* =8.0 Hz, 2H), 2.64 (t, *J* =7.75 Hz, 2H), 1.65-1.60 (m, 2H), 1.39-1.20 (m, 12H), 0.89 (t, *J* = 6.75 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ = 143.95, 133.18, 132.50, 132.15, 131.65, 131.23, 130.94, 129.74, 128.55, 128.35, 128.17, 126.39, 126.34, 126.05, 125.30, 122.28, 121.34, 120.13, 94.29, 88.06, 35.99, 31.89, 31.27, 29.54, 29.50, 29.32, 29.26, 22.67, 14.11. HRMS (EI): calcd for $C_{31}H_{31}Br$ (M^+), 482.1609; found, 482.1607 (error: -0.40 ppm).



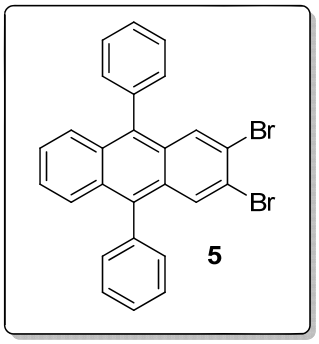
7,16-Bis(4-nonylphenyl) dianthraceno[a,e]pentalene(compound **DAP1**)

A reaction flask was charged with monomer **2**(0.270g, 0.56mmol), hydroquinone (0.125 g, 1.12 mmol), Cs_2CO_3 (0.370 g, 1.12 mmol), CsF (0.187 g, 1.23 mmol), P(2-furyl)$_3$ (30 mg, 0.13 mmol), and $Pd_2(dba)_3$ (30 mg, 0.033 mmol) and then purged with argon. Anhydrous 1,4-dioxane (15 mL) was injected into the reaction mixture and deoxygenated three freeze-pump-thaw cycles. The suspension was immediately heated to135^{o}C. After heating for 24 h the reaction mixture was cooled down and diluted with $CHCl_3$ (25 mL), filtered through celite, and then concentrated to yield raw solid. After purification by column chromatography (silica gel, DCM : Hexane=1 : 4), the product **3** was dissolved in $CHCl_3$, precipitated in methanol: acetone = 3:2 and filtered. This procedure was repeated for 3 times to give the pure product**3** (37 mg) in 16% yield. ^1H NMR (500 MHz, $CDCl_3$, ppm): δ = 8.16 (d, *J* = 6.5 Hz, 4H), 8.11 (s, 2H), 7.89-7.84 (m, 4H), 7.85 (s, 2H), 7.83 (s, 2H), 7.75 (s, 2H), 7.47 (d, *J* = 7.5 Hz, 4H), 7.41-7.37 (m, 4H), 2.81 (t, *J* = 8.0 Hz, 4H), 1.85-1.75 (m, 4H), 1.52-1.30 (m, 24H), 0.92 (t, *J* = 6.75 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ = 147.21, 144.70, 143.62, 136.11, 132.27, 131.98, 131.95, 131.72, 131.54, 131.30, 128.90, 128.89, 128.14, 128.11, 127.55, 127.15, 125.63, 125.43, 121.72, 120.45, 36.12, 31.97, 31.49, 29.67, 29.63, 29.60, 29.42, 22.73, 14.16. HRMS (EI): calcd for $C_{62}H_{62}$ (M^+), 806.4852; found, 806.4852 (error: 0.11 ppm).



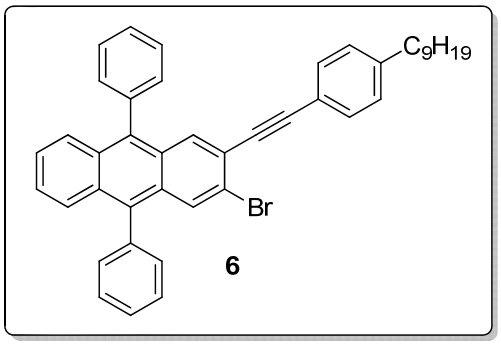
2,3-Dibromo-9,10-diphenyl-9,10-dihydro-9,10-epoxyanthracene(compound **4**)

A solution of compound **3** (11.10 g, 38.8 mmol) and 1,2,4,5-tetrabromobenzene (16.60 g, 42.0 mmol) in toluene (120 mL) was cooled to -50 ºC, then *n*-BuLi (1.6 M, 27 mL) was added dropwise. After addition, the mixture was warmed to room temperature naturally and stirred for overnight. The mixture was extracted with chloroform (80 mL ×2). The combined organic phase was washed with brine (60 mL ×2). The organic phase was dried over anhydrous Na_2SO_4 and organic solvent was removed under reduced pressure. The crude product was purified by column chromatography (CH_2Cl_2/Hexane = 1:4) to afford compound **4** (12.05 g) in 58% yield. ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ = 7.88 (d, *J* = 7.5 Hz, 4H), 7.62 (t, *J* = 7.75 Hz, 4H), 7.56 (s, 2H), 7.52 (t, *J* = 7.25 Hz, 2H), 7.41-7.37 (m, 2H), 7.11-7.07 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ = 151.61, 149.19, 133.95, 128.97, 128.65, 126.49, 126.36, 125.63, 121.77, 120.67, 90.22. HRMS (EI): calcd for $C_{26}H_{16}Br_2O$ (M^+), 503.9547; found, 503.9535 (error: -2.48 ppm).



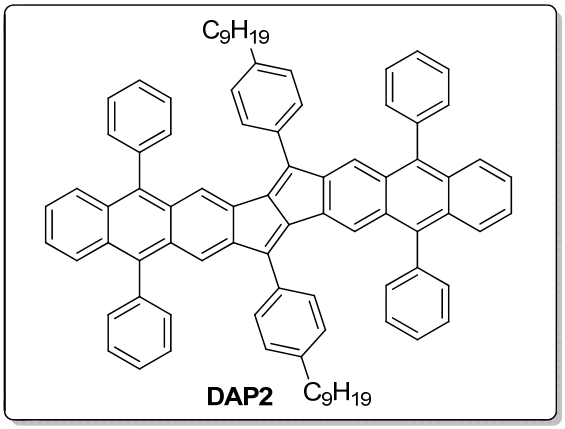
2,3-Dibromo-9,10-diphenylanthracene(compound **5**)

To a suspension of Zn dust (0.57 g, 8.8 mmol) in THF (10 mL) cooled in an ice-water bathwas carefully added $TiCl_4$ (1.2 mL, 11.0 mmol) under argon, and the reaction mixture was heated to reflux for 5 minutes. Then the mixture was cooled to 0 ºC and a solution of compound **4** (1.02 g, 2 mmol) in THF (10 mL) was added dropwise. After addition, the mixture was reflux overnight. After cooled down the reaction to room temperature, the mixture was poured into a cold 10% HCl solution (40 mL). The mixture was extracted with chloroform (60 mL ×2). The combined organic phase was washed with brine (50 mL ×2), dried over anhydrous Na_2SO_4 and the organic solvent was removed under reduced pressure. The crude product was purified by column chromatography (CH_2Cl_2/Hexane = 1:2) to afford compound **5** (0.80 g) in 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$, ppm): 7.99 (s, 2H), 7.68-7.56 (m, 8H), 7.46-7.43 (m, 4H), 7.38-7.34 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ = 137.81, 136.66, 131.24, 131.15, 130.59, 129.30, 128.68, 128.00, 127.06, 125.91, 121.67. HRMS (EI): calcd for $C_{26}H_{16}Br_2$ (M^+), 485.9619; found, 485.9595 (error: -4.84 ppm).



2-Bromo-3-((4-nonylphenyl)ethynyl)-9,10-diphenylanthracene(compound **6**)

A mixture of compound **5** (1.95 g, 4.0 mmol), 1-ethynyl-4-nonylbenzene (1.10 g, 4.8 mmol), CuI (38 mg, 3%) and catalyst $Pd(PPh_3)_2Cl_2$ (140 mg, 5%) in anhydrous THF (20 mL) and Et_3N (10 mL) was degassed by three freeze-pupm-thaw cycles. The mixture was stirred at 75 ^oC under argon for overnight. The mixture was extracted with chloroform (60 mL ×2). The combined organic phase was washed with HCl (10%) solution (50 mL ×2) and brine (50 mL ×1). The organic phase was dried over anhydrous Na_2SO_4 and organic solvent was removed under reduced pressure. The crude product was purified by column chromatography (DCM/Hexane = 10:1) to afford compound **6** (0.92 g) in 36% yield. ^1H NMR (500 MHz, $CDCl_3$, ppm): δ = 7.97 (s, 1H), 7.94 (s, 1H), 7.69-7.57 (m, 8H), 7.50-7.45 (m, 6H), 7.37-7.33 (m, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 2.61 (t, *J* = 7.75 Hz, 2H), 1.75-1.65 (m, 2H), 1.35-1.20 (m, 12H), 0.89 (t, *J* = 6.75 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ = 143.86, 138.08, 138.01, 137.43, 136.36, 132.06, 131.58, 131.28, 131.19, 130.91, 130.48, 129.78, 129.60, 128.64, 128.62, 128.45, 128.18, 127.89, 127.85, 127.18, 127.04, 125.93, 125.64, 121.90, 121.65, 120.02, 94.30, 88.37, 35.94, 31.87, 31.22, 29.52, 29.47, 29.29, 29.21, 22.66, 14.10. HRMS (EI): calcd for $C_{43}H_{39}Br$ (M^+), 634.2235; found, 634.2233 (error: -0.27 ppm).



7,16-Bis(4-nonylphenyl)-5,9,14,18-tetraphenyl dianthraceno[*a,e*]pentalene (compound **DAP2**)

A reaction flask was charged with monomer **6**(0.53g, 0.83mmol), hydroquinone (0.185 g, 1.68 mmol), Cs_2CO_3 (0.547 g, 1.68 mmol), CsF (0.277 g, 1.82 mmol), P(2-furyl)$_3$ (38 mg, 0.16 mmol), and $Pd_2(dba)_3$ (38 mg, 0.04 mmol) and then purged with argon. Anhydrous 1,4-dioxane (18 mL) was injected into the reaction mixture and deoxygenated three freeze-pump-thaw cycles. The suspension was immediately heated to135^oC. After heating for 24 h the reaction mixture was diluted with $CHCl_3$ (25 mL), filtered through celite, and

then concentrated to yield raw solid. After purification by column chromatography (silica gel, DCM/Hexane = 1:4), the product was dissolved in $CHCl_3$, precipitated in methanol: acetone = 3:2 and filtered. This procedure was repeated for 3 times to give the pure product**DAP2** (70 mg) in 15% yield.^{1}H NMR (500 MHz, CD_2Cl_2, ppm): δ =7.96 (s, 2H),7.62-7.55 (m, 14H), 7.54-7.48 (m, 4H), 7.46-7.39 (m, 12H), 7.31-7.25 (m, 4H), 7.02 (d, *J* = 8.0 Hz, 4H), 2.65 (t, *J* = 8.0 Hz, 4H), 1.70 (t, *J* = 7.0 Hz, 4H), 1.50-1.40 (m, 24H), 0.95 (m, 6H);^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ = 146.03, 144.83, 142.94, 138.99, 138.82, 138.33, 137.93, 135.97, 131.28, 131.16, 131.07, 131.05, 130.63, 130.45, 130.00, 129.44, 128.37, 128.28, 127.38, 127.22, 127.11, 127.06, 125.29, 125.08, 120.77, 119.56, 36.02, 32.00, 31.49, 29.72, 29.61, 29.47, 22.75, 14.16. HR-APCI: calcd for $C_{86}H_{79}$ ($M+H^+$), 1111.6182; found, 1111.6176 (error: -0.54 ppm).

2. DFT calculation details

DFT calculations have been performed both at the B3LYP/6-31G**[1-5] level of theory, as implemented in the Gaussian 09 program package.[6]

Table S1DFT (B3LYP/6-31G**) calculated energies levels of **DAP1** and **DAP2** (eV)

	DAP1(eV)	**DAP2**(eV)
LUMO+5	-0.08	-0.11
LUMO+4	-0.16	-0.18
LUMO+3	-0.30	-0.30
LUMO+2	-1.32	-1.29
LUMO+1	-1.87	-1.82
LUMO	-2.14	-2.03
HOMO	-4.68	-4.56
HOMO-1	-5.29	-5.16
HOMO-2	-5.61	-5.50
HOMO-3	-5.90	-5.74
HOMO-4	-6.52	-6.41
HOMO-5	-6.55	-6.41
HOMO-6	-6.78	-6.58

Table S2 Selected TD-DFT (B3LYP/6-31G**) calculated wavelngth, oscillator strength and compositions of major electronic transitions of **DAP1**.

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
547.3	0.5057	H-0->L+0 (+92%)
398.2	0.3988	H-1->L+1(+92%)
374.7	0.5235	H-3->L+0(+69%) H-2->L+1(24%)
363.6	1.2983	H-2->L+1(+61%)H-3->L+0(+26%)
307.4	0.4202	H-0->L+4(+56%) H-3->L+2(10%) H-6->L+0(8%) H-5->L+1(+8%)
297.6	0.6847	H-0->L+5(+39%)H-6->L+0(+30%) H-0->L+4(+21%)

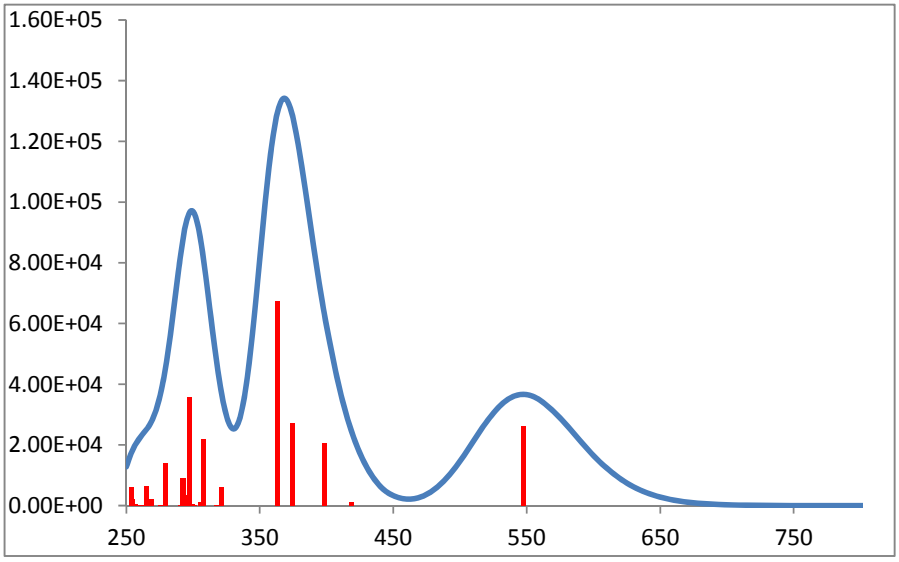


Fig. S1 Calculated (B3LYP/6-31G**) absorption spectrum of **DAP1**.

Table S3 Selected TD-DFT (B3LYP/6-31G**) calculated wavelength, oscillator strength and compositions of major electronic transitions of **DAP2**.

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
557.3	0.5459	H-0->L+0 (+94%)
410.7	0.3974	H-1->L+1(+94%)
381.3	0.5565	H-3->L+0(+61%) H-2->L+1(33%)
371.5	1.1488	H-2->L+1(+57%)H-3->L+0(+34%)
315.8	0.4270	H-0->L+4(+57%) H-4->L+0(21%) H-3->L+2(12%)
306.8	0.2764	H-3->L+2(+38%) H-6->L+0(+18%) H-0->L+9(+13%) H-0->L+8(11%) H-0->L+4(9%)

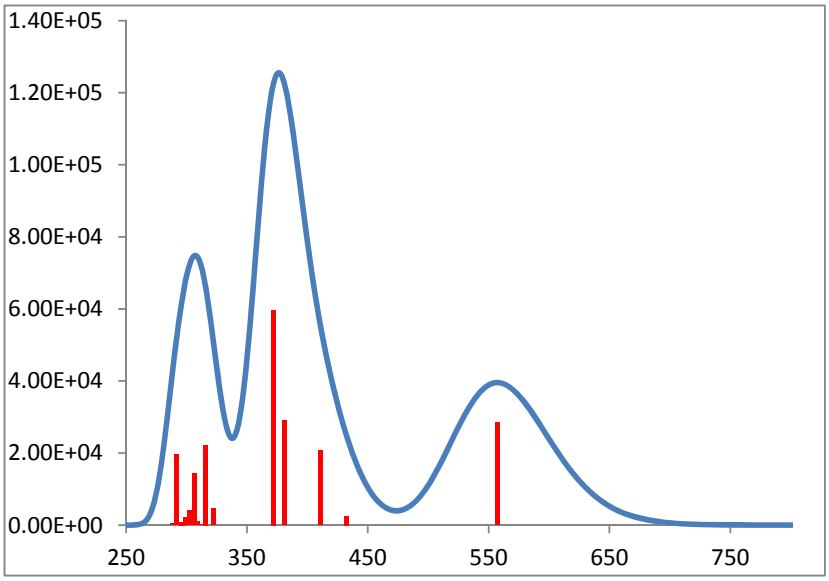


Fig. S2 Calculated (B3LYP/6-31G**) absorption spectrum of **DAP2**.

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2. Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter***1988**, *37*, 785.
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6. *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. Differential pulse voltammograms

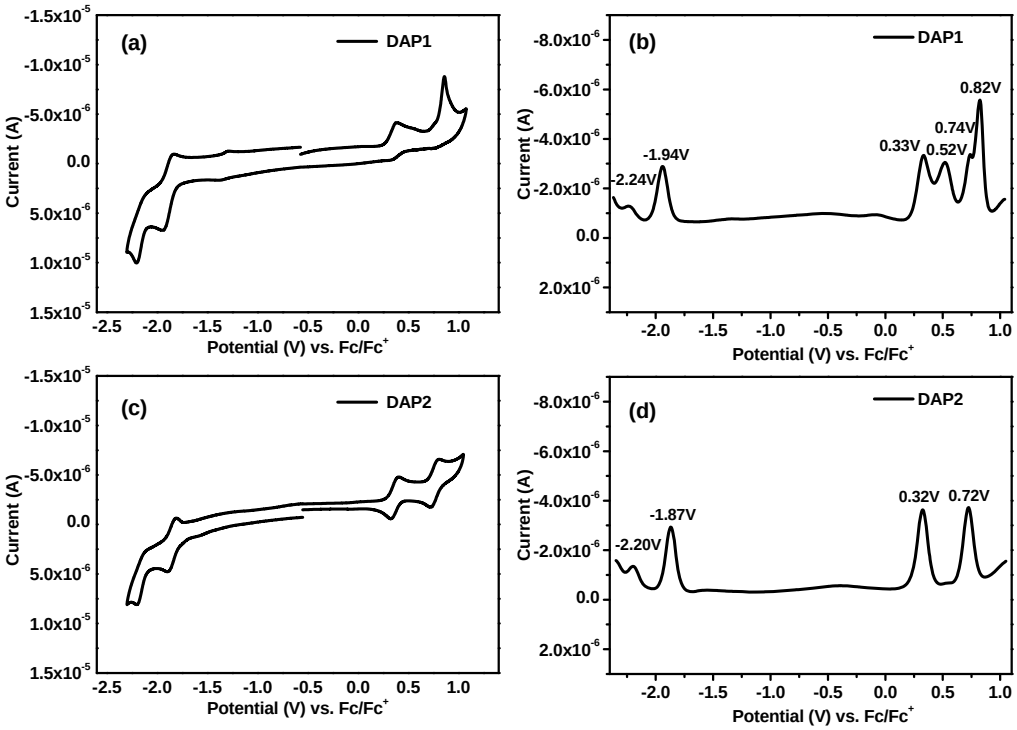
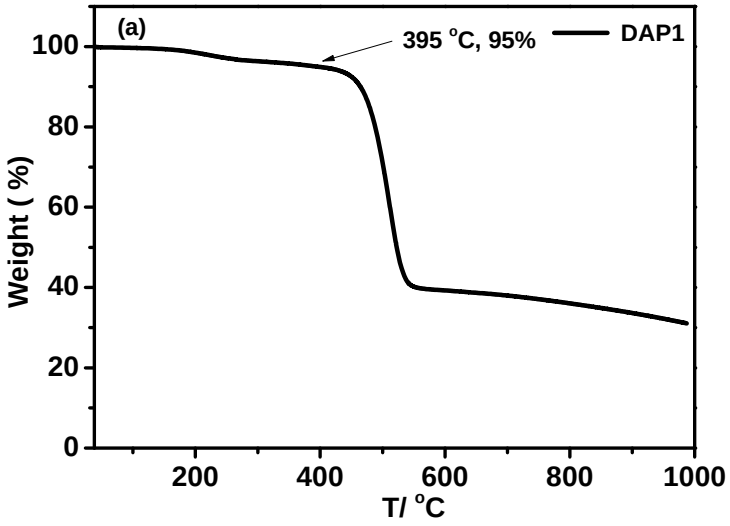
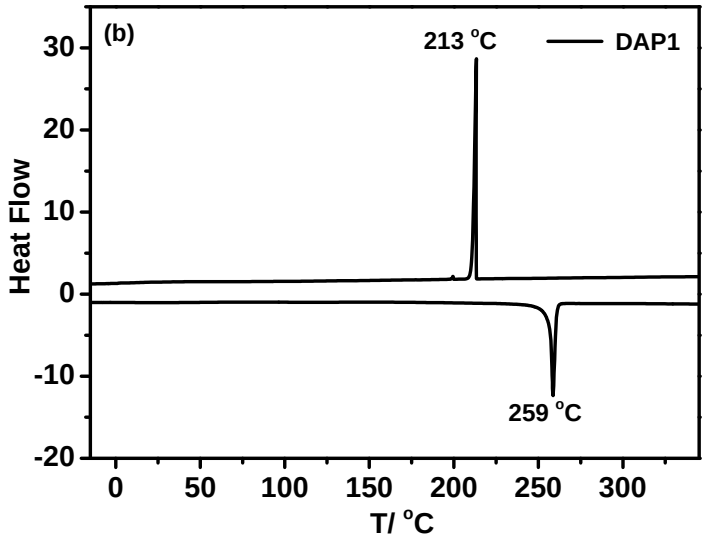


Fig. S3 Cyclic voltammograms (1×10^{-3} M) of **DAP1** (a) and **DAP2** (c) recorded in dry dichloromethane; Differential pulse voltammograms (1×10^{-3} M) of compounds **DAP1** (b) and **DAP2** (d) in dry dichloromethane with 0.1 M Bu_4NPF_6 as the supporting electrolyte, AgCl/Ag as reference electrode, Au as working electrode (surface area = 12.6 mm^2), Pt wire as counter electrode. The DPV measurements were performed in the oxidation mode, potential step = 0.004 V, pulse amplitude = 0.05 V, pulse width = 0.05 s.

4. TGA and DSC curves





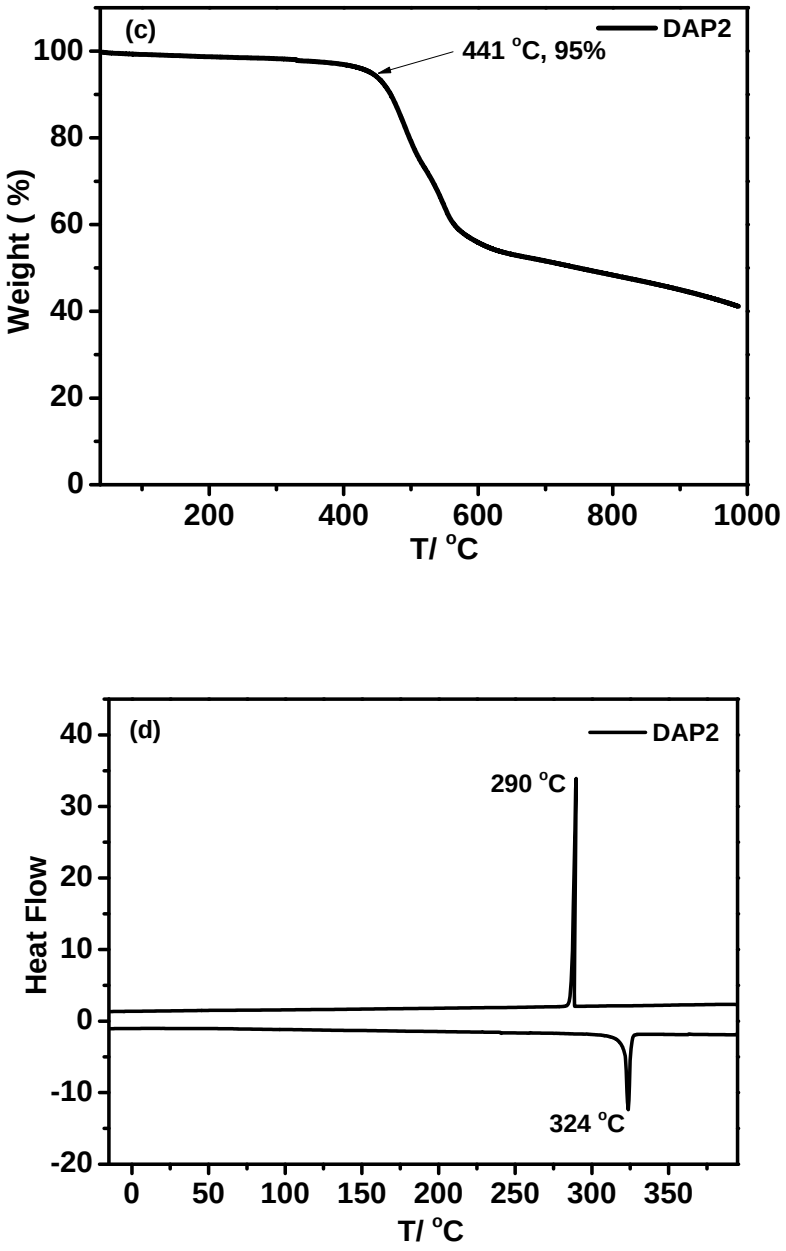


Fig. S4 Thermogravimetric analysis (TGA) of compounds **DAP1** (a) and **DAP2** (c); Differential scanning calorimetry (DSC) of compounds **DAP1** (b) and **DAP2** (d) in N_2 at a heating rate of 10 ^{o}C min^{-1}.

5. Details of device fabrication and additional characterization data

Organic field effect transistors (OFETs) of **DAP1**and **DAP2** were fabricated on n^+-Si/SiO_2 substrates using a bottom-gate top-contact device structure. The SiO_2dielectric was treated with octadecyltrichlorosilane (ODTS) or hexamethyldisilazane (HMDS), and the thin film was spin-coated from $CHCl_3$ solution onto the substrates, then thermal annealed at selective temperatures for 20 min. Finally, Au source/drain electrodes (80 nm) were patterned onto the organic layer through a shadow mask to afford the devices. All devices were characterized in N_2 atmosphere.

Table S4 The device characteristics of thin film **DAP1** and **DAP2**.

Compound	Surface treatment	Annealing Temp [^{o}C]	μ[$cm^2V^{-1}s^{-1}$]	V_T [V]	On/off
DAP1	HMDS	As-spun	6.2×10^{-4}	0	1.6×10^4
	HMDS	120	2.8×10^{-4}	-2	3.5×10^4
	HMDS	150	6.4×10^{-5}	0	1.4×10^4
	HMDS	180	2.0×10^{-5}	-5	1.7×10^4
	ODTS	As-spun	0.001	0	1.5×10^4
	ODTS	120	7.4×10^{-4}	0	1.1×10^4
	ODTS	150	1.8×10^{-4}	0	1.7×10^4
DAP2	HMDS	As-spun	2.4×10^{-4}	-5	4.2×10^5
	HMDS	150	0.012	-13	1.1×10^6
	ODTS	As-spun	0.027	-10	8.3×10^5
	ODTS	120	0.45	-2	7.8×10^4
	ODTS	150	0.65(0.86)	-2	2.2×10^5
	ODTS	180	0.36	0	3.6×10^4

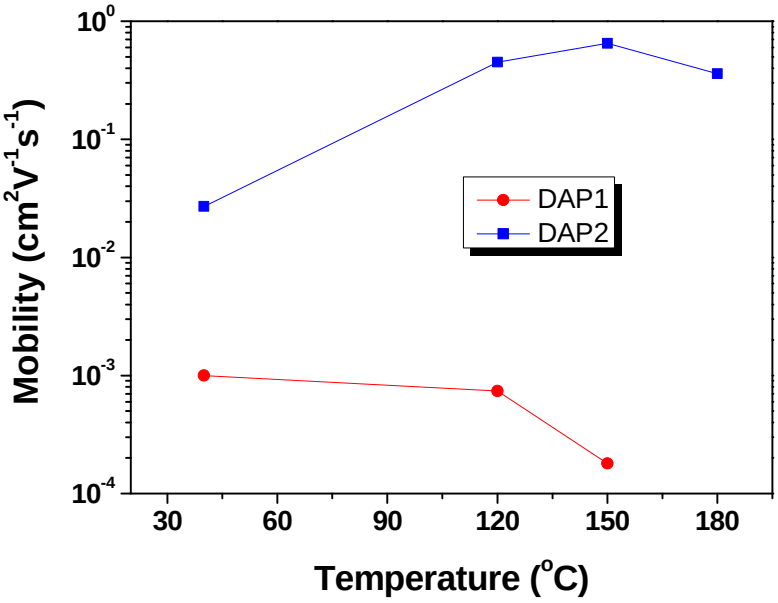


Fig. S5 The charge carrier mobilities of **DAP1** and **DAP2** with respect to the annealing temperatures.

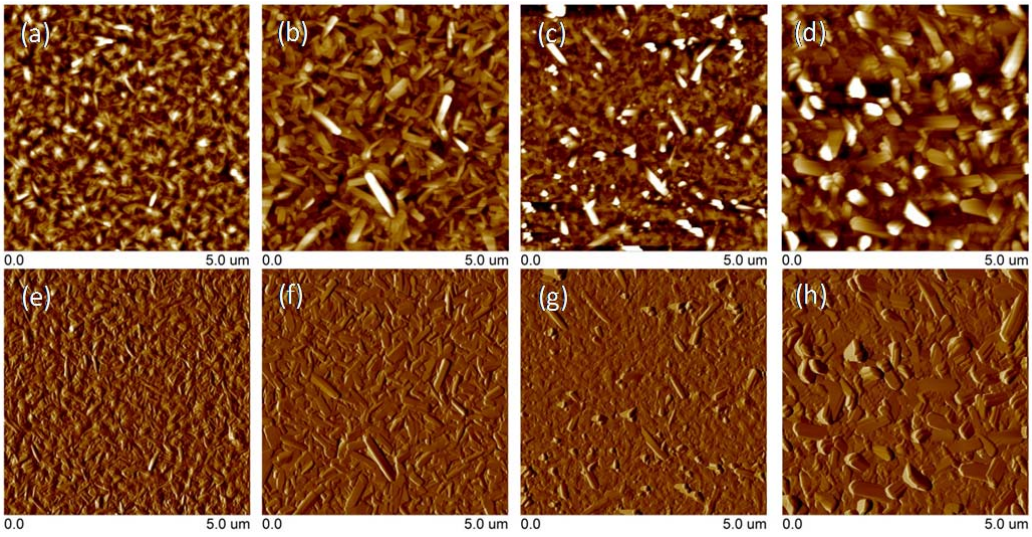


Fig. S6 The AFM images of the thin film **DAP1** spin coated from $CHCl_3$ solution onto ODTS (a: before annealing; b: annealing at 150 ^oC) and HMDS (c: before annealing; d: annealing at 150 ^oC) treated substrates. (e-h) are the corresponding phase images.

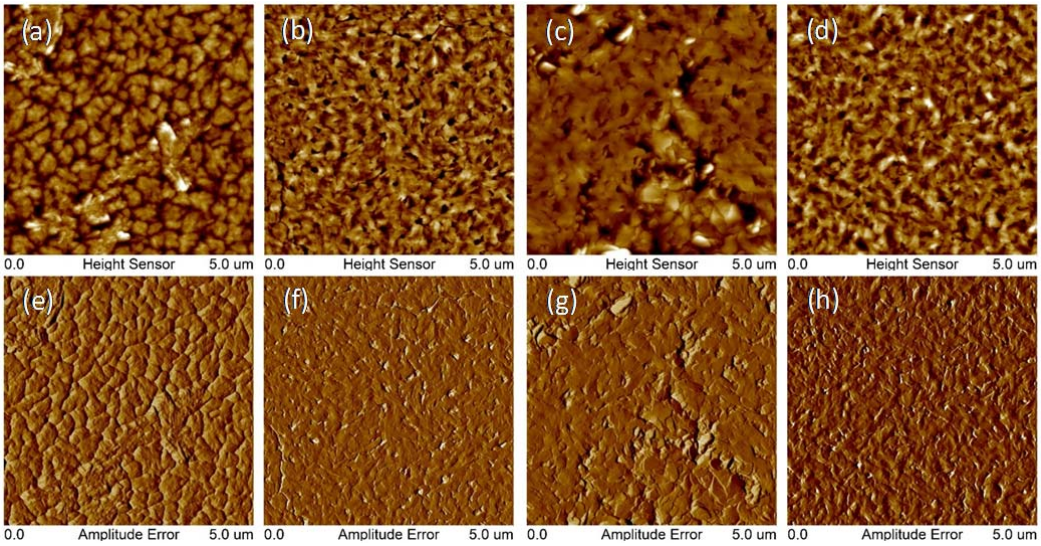


Fig. S7 The AFM images of thin film **DAP2** spin coated from $CHCl_3$ solution on the ODTS-treated substrates annealing at 120 ^oC (a), 150 ^oC (b), and 180 ^oC (c), and on the HMDS -treated substrates annealing at 150 ^oC (d). (e-h) are the corresponding phase images.

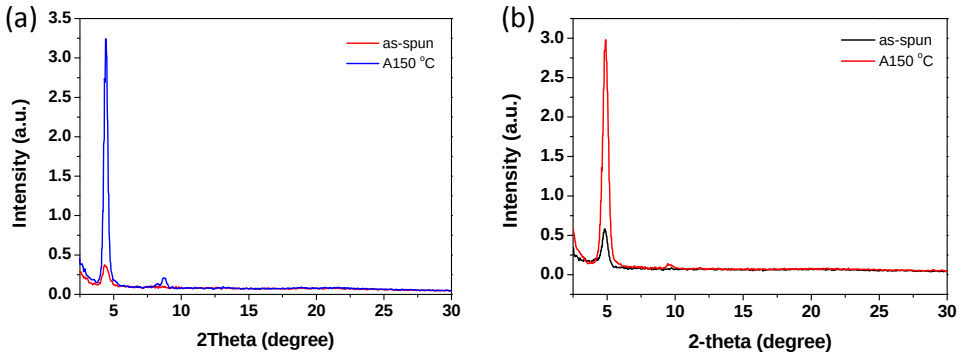


Fig. S8 XRD patterns of **DAP1** (a) and **DAP2** (b) thin films on ODTS-modified substrates.

6. X-ray crystallographic analysis of DAP1 and DAP2

Measurements were made on aBruker Apex II X-ray diffractometer by using graphite monochromated Cu Kα (λ = 1.54178 Å) radiation. The data were corrected for Lorentz and polarization effects with the SMART suite of programs and for absorption effects with SADABS.[1] Both crystal structures were solved by direct methods and refined on F^2 by full-matrix least-squares techniques with SHELXTL–97 program.[2]

For **DAP1**, the pendant $–PhC_9H_{19}$ moiety is disordered with the relative ratios of 0.49/0.51 refined for the two components. For **DAP2**, a small amount of spatially delocalized electron density (50 electrons per cell) in the lattice was found due to the uncharacterizable disordered solvent. The solvent contribution was thus modeled using SQUEEZE in the Platon program suite.[3] Whereas relevant, the formulae presented in the context for **DAP2** are those after SQUEEZE. **DAP1** and **DAP2** were crystallized as very thin platelets and were weakly diffracted, particularly in the high resolution region. The weak diffractions of **DAP1** and **DAP2** may be the cause of their relatively high R_1 (0.1023 for **DAP1**; 0.1286 for **DAP2**) and wR_2 (0.2577 for **DAP1**; 0.3259 for **DAP2**) values. A summary of the relevant crystallographic data for **DAP1** and **DAP2** are listed in Table S5 – Table S16.

References

1. Sheldrick, G. M. SADABS. Program for empirical absorption correction of area detector data; University of Göttingen: Germany 2008.

2. Sheldrick, G. M. Acta Cryst. 2008, A64, 112-122.

3. Spek, A. J. Appl. Crystallogr. 2003, 36, 7.

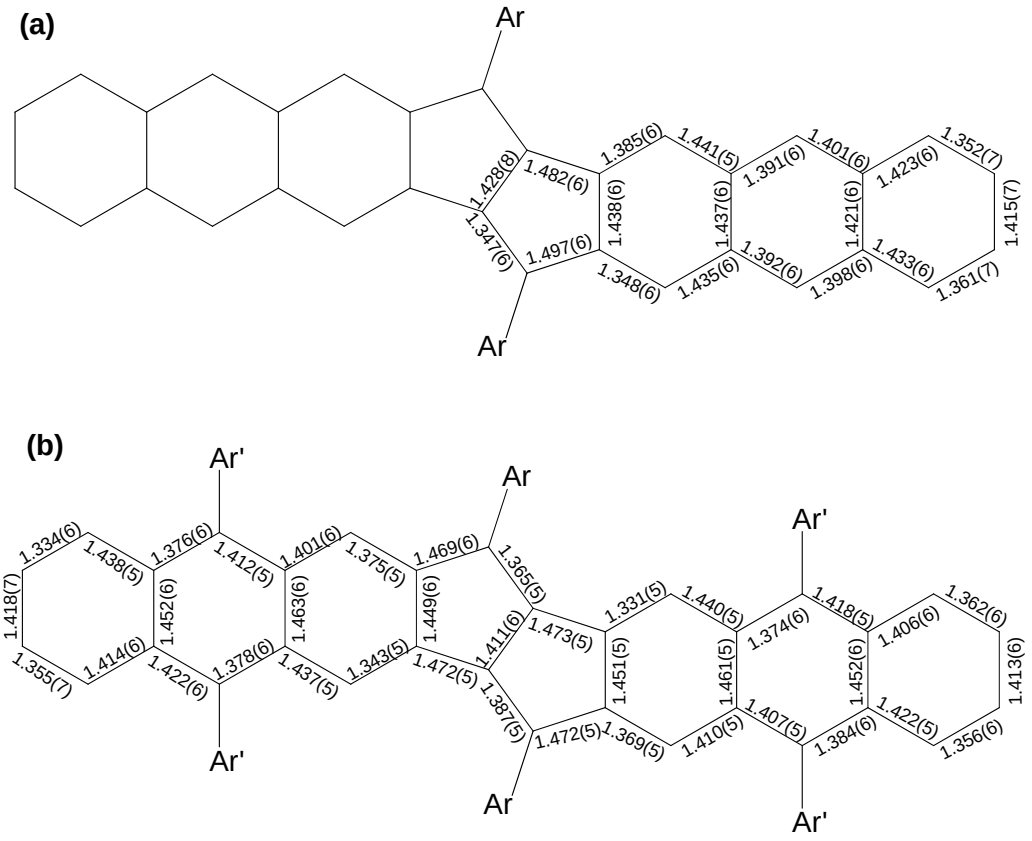


Fig. S9 Selected bond lengths of **DAP1** and **DAP2** (based on X-ray crystallographic structures).

Table S5. Crystallographic data and structure refinement for **DAP1**

Identification code	DAP1
Empirical formula	C62 H60
Formula weight	805.20
Temperature	100(2) K
Wavelength	1.54178 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 4.9784(3) A alpha = 95.603(4) deg.
	b = 11.3963(7) A beta = 92.746(4) deg.
	c = 19.9225(11) A gamma = 93.200(4) deg.
Volume	1121.54(11) A^3
Z, Calculated density	1, 1.1920(1) Mg/m^3
Absorption coefficient	0.501 mm^-1

F(000)	432.1
Crystal size	1.00 x 0.10 x 0.06 mm
Theta range for data collection	2.23 to 61.28 deg.
Limiting indices	-5<=h<=4, -12<=k<=12, -22<=l<=22
Reflections collected / unique	22106 / 3426 [R(int) = 0.0564]
Completeness to theta =	61.28 98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9664 and 0.5979
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3426 / 169 / 362
Goodness-of-fit on F^2	0.941
Final R indices [I>2sigma(I)]	R1 = 0.1023, wR2 = 0.2577
R indices (all data)	R1 = 0.1090, wR2 = 0.2621
Largest diff. peak and hole	0.550 and -0.336 e.A^-3

Table S6. Atomic coordinates (x 10^4) and equivalent isotropicdisplacement parameters (A^2 x 10^3) for **DAP1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	-152(8)	115(3)	10354(2)	27(1)
C(2)	1527(7)	1001(3)	10653(2)	25(1)
C(3)	3239(8)	1392(3)	10108(2)	28(1)
C(4)	5289(8)	2223(4)	10139(2)	29(1)
C(5)	6594(8)	2460(3)	9535(2)	25(1)
C(6)	8772(7)	3286(3)	9552(2)	25(1)
C(7)	10000(7)	3568(3)	8968(2)	25(1)
C(8)	12233(8)	4420(3)	8977(2)	34(1)
C(9)	13309(9)	4694(4)	8393(3)	44(1)

C(10)	12272(10)	4125(4)	7763(2)	45(1)
C(11)	10203(9)	3297(4)	7734(2)	36(1)
C(12)	9004(8)	2994(3)	8332(2)	26(1)
C(13)	6863(8)	2137(3)	8313(2)	30(1)
C(14)	5649(8)	1850(3)	8895(2)	25(1)
C(15)	3469(8)	961(3)	8881(2)	30(1)
C(16)	2351(7)	722(3)	9480(2)	27(1)
C(17)	1683(8)	1532(4)	11361(2)	29(1)
C(20)	2040(14)	2664(4)	12690(2)	61(2)
C(18)	4221(19)	1852(8)	11702(4)	37(2)
C(19)	4370(20)	2372(9)	12348(5)	53(2)
C(21)	-400(30)	2298(8)	12359(5)	52(2)
C(22)	-564(18)	1759(7)	11701(4)	33(2)
C(18A)	1559(14)	2774(7)	11473(4)	28(2)
C(19A)	1759(17)	3325(7)	12123(4)	35(2)
C(21A)	1950(20)	1485(8)	12589(5)	49(3)
C(22A)	1762(15)	916(7)	11931(4)	31(2)
C(23)	1205(19)	3350(7)	13375(4)	30(1)
C(23A)	3091(18)	3216(7)	13409(4)	30(1)
C(24)	2530(40)	4601(15)	13506(11)	30(1)
C(25)	1750(20)	5249(9)	14161(5)	30(1)
C(26)	2970(20)	6493(10)	14321(6)	30(1)
C(27)	2000(20)	7159(10)	14944(5)	30(1)
C(28)	1830(20)	8138(8)	15189(5)	30(1)
C(29)	2270(30)	9013(14)	15732(8)	29(3)
C(30)	1920(30)	9989(10)	16015(5)	40(3)
C(31)	3570(40)	10687(18)	16656(10)	55(5)
C(24A)	1990(30)	4421(12)	13529(9)	28(3)
C(25A)	3110(20)	5094(8)	14198(4)	31(2)
C(26A)	1850(20)	6294(8)	14344(5)	31(2)
C(27A)	3220(20)	7000(8)	14981(5)	35(2)

C(28A)	3280(20)	8356(8)	15140(4)	36(2)
C(29A)	3350(40)	8880(17)	15817(9)	48(5)
C(30A)	3460(30)	10236(9)	15960(5)	44(3)
C(31A)	2510(30)	10879(15)	16552(9)	44(4)

Table S7. Bond lengths [A] and angles [deg] for **DAP1**.

C(1)-C(2)	1.347(6)
C(1)-C(1)#1	1.428(8)
C(1)-C(16)#1	1.482(6)
C(2)-C(17)	1.477(5)
C(2)-C(3)	1.497(6)
C(3)-C(4)	1.348(6)
C(3)-C(16)	1.438(6)
C(4)-C(5)	1.435(6)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.392(6)
C(5)-C(14)	1.437(5)
C(6)-C(7)	1.398(6)
C(6)-H(6A)	0.9500
C(7)-C(12)	1.421(6)
C(7)-C(8)	1.433(6)
C(8)-C(9)	1.361(7)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.415(7)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.352(7)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.423(6)
C(11)-H(11A)	0.9500

C(12)-C(13)	1.401(6)
C(13)-C(14)	1.391(6)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.441(5)
C(15)-C(16)	1.385(6)
C(15)-H(15A)	0.9500
C(16)-C(1)#1	1.482(6)
C(17)-C(22)	1.360(9)
C(17)-C(22A)	1.392(10)
C(17)-C(18A)	1.416(9)
C(17)-C(18)	1.417(10)
C(20)-C(21A)	1.337(11)
C(20)-C(21)	1.380(14)
C(20)-C(19)	1.411(14)
C(20)-C(19A)	1.422(10)
C(20)-C(23A)	1.561(9)
C(20)-C(23)	1.591(9)
C(18)-C(19)	1.360(13)
C(18)-H(18A)	0.9500
C(19)-H(19A)	0.9500
C(21)-C(22)	1.388(13)
C(21)-H(21A)	0.9500
C(22)-H(22A)	0.9500
C(18A)-C(19A)	1.381(11)
C(18A)-H(18B)	0.9500
C(19A)-H(19B)	0.9500
C(21A)-C(22A)	1.402(12)
C(21A)-H(21B)	0.9500
C(22A)-H(22B)	0.9500
C(23)-C(24)	1.530(15)
C(23)-H(23A)	0.9900

C(23)-H(23B)	0.9900
C(23A)-C(24A)	1.508(19)
C(23A)-H(23C)	0.9900
C(23A)-H(23D)	0.9900
C(24)-C(25)	1.51(2)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.510(15)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.505(15)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.182(14)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.399(19)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.22(2)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.60(2)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(24A)-C(25A)	1.534(19)
C(24A)-H(24C)	0.9900
C(24A)-H(24D)	0.9900
C(25A)-C(26A)	1.545(14)
C(25A)-H(25C)	0.9900

C(25A)-H(25D)	0.9900
C(26A)-C(27A)	1.544(14)
C(26A)-H(26C)	0.9900
C(26A)-H(26D)	0.9900
C(27A)-C(28A)	1.545(13)
C(27A)-H(27C)	0.9900
C(27A)-H(27D)	0.9900
C(28A)-C(29A)	1.42(2)
C(28A)-H(28B)	0.9900
C(28A)-H(28C)	0.9900
C(29A)-C(30A)	1.54(2)
C(29A)-H(29B)	0.9900
C(29A)-H(29C)	0.9900
C(30A)-C(31A)	1.44(2)
C(30A)-H(30C)	0.9900
C(30A)-H(30D)	0.9900
C(31A)-H(31D)	0.9800
C(31A)-H(31E)	0.9800
C(31A)-H(31F)	0.9800

C(2)-C(1)-C(1)#1	113.5(5)
C(2)-C(1)-C(16)#1	140.3(4)
C(1)#1-C(1)-C(16)#1	106.2(4)
C(1)-C(2)-C(17)	128.9(4)
C(1)-C(2)-C(3)	105.8(3)
C(17)-C(2)-C(3)	125.3(3)
C(4)-C(3)-C(16)	121.1(4)
C(4)-C(3)-C(2)	130.2(4)
C(16)-C(3)-C(2)	108.7(3)
C(3)-C(4)-C(5)	119.8(4)
C(3)-C(4)-H(4A)	120.1

C(5)-C(4)-H(4A)	120.1
C(6)-C(5)-C(14)	118.5(3)
C(6)-C(5)-C(4)	121.3(4)
C(14)-C(5)-C(4)	120.2(4)
C(5)-C(6)-C(7)	122.3(4)
C(5)-C(6)-H(6A)	118.8
C(7)-C(6)-H(6A)	118.8
C(6)-C(7)-C(12)	119.1(4)
C(6)-C(7)-C(8)	122.9(4)
C(12)-C(7)-C(8)	118.0(4)
C(9)-C(8)-C(7)	120.8(4)
C(9)-C(8)-H(8A)	119.6
C(7)-C(8)-H(8A)	119.6
C(8)-C(9)-C(10)	120.5(4)
C(8)-C(9)-H(9A)	119.7
C(10)-C(9)-H(9A)	119.7
C(11)-C(10)-C(9)	120.5(4)
C(11)-C(10)-H(10A)	119.8
C(9)-C(10)-H(10A)	119.8
C(10)-C(11)-C(12)	120.8(4)
C(10)-C(11)-H(11A)	119.6
C(12)-C(11)-H(11A)	119.6
C(13)-C(12)-C(7)	118.9(4)
C(13)-C(12)-C(11)	121.7(4)
C(7)-C(12)-C(11)	119.4(4)
C(14)-C(13)-C(12)	122.0(4)
C(14)-C(13)-H(13A)	119.0
C(12)-C(13)-H(13A)	119.0
C(13)-C(14)-C(5)	119.2(4)
C(13)-C(14)-C(15)	122.4(4)
C(5)-C(14)-C(15)	118.4(4)

C(16)-C(15)-C(14)	119.4(4)
C(16)-C(15)-H(15A)	120.3
C(14)-C(15)-H(15A)	120.3
C(15)-C(16)-C(3)	120.9(4)
C(15)-C(16)-C(1)#1	133.3(4)
C(3)-C(16)-C(1)#1	105.7(3)
C(22)-C(17)-C(22A)	72.3(5)
C(22)-C(17)-C(18A)	72.2(5)
C(22A)-C(17)-C(18A)	116.8(5)
C(22)-C(17)-C(18)	117.8(6)
C(22A)-C(17)-C(18)	73.8(5)
C(18A)-C(17)-C(18)	79.2(5)
C(22)-C(17)-C(2)	121.9(5)
C(22A)-C(17)-C(2)	125.9(4)
C(18A)-C(17)-C(2)	117.2(5)
C(18)-C(17)-C(2)	120.3(5)
C(21A)-C(20)-C(21)	72.7(7)
C(21A)-C(20)-C(19)	73.7(7)
C(21)-C(20)-C(19)	116.5(6)
C(21A)-C(20)-C(19A)	119.1(6)
C(21)-C(20)-C(19A)	72.8(6)
C(19)-C(20)-C(19A)	79.2(6)
C(21A)-C(20)-C(23A)	115.8(6)
C(21)-C(20)-C(23A)	137.6(7)
C(19)-C(20)-C(23A)	105.4(7)
C(19A)-C(20)-C(23A)	123.7(5)
C(21A)-C(20)-C(23)	122.4(6)
C(21)-C(20)-C(23)	103.3(7)
C(19)-C(20)-C(23)	140.1(7)
C(19A)-C(20)-C(23)	113.4(6)
C(23A)-C(20)-C(23)	35.4(4)

C(19)-C(18)-C(17)	120.3(9)
C(19)-C(18)-H(18A)	119.8
C(17)-C(18)-H(18A)	119.8
C(18)-C(19)-C(20)	121.9(9)
C(18)-C(19)-H(19A)	119.0
C(20)-C(19)-H(19A)	119.0
C(20)-C(21)-C(22)	121.5(9)
C(20)-C(21)-H(21A)	119.2
C(22)-C(21)-H(21A)	119.2
C(17)-C(22)-C(21)	121.6(9)
C(17)-C(22)-H(22A)	119.2
C(21)-C(22)-H(22A)	119.2
C(19A)-C(18A)-C(17)	119.9(7)
C(19A)-C(18A)-H(18B)	120.0
C(17)-C(18A)-H(18B)	120.0
C(18A)-C(19A)-C(20)	121.1(7)
C(18A)-C(19A)-H(19B)	119.5
C(20)-C(19A)-H(19B)	119.5
C(20)-C(21A)-C(22A)	120.1(8)
C(20)-C(21A)-H(21B)	119.9
C(22A)-C(21A)-H(21B)	119.9
C(17)-C(22A)-C(21A)	122.6(7)
C(17)-C(22A)-H(22B)	118.7
C(21A)-C(22A)-H(22B)	118.7
C(24)-C(23)-C(20)	113.0(10)
C(24)-C(23)-H(23A)	109.0
C(20)-C(23)-H(23A)	109.0
C(24)-C(23)-H(23B)	109.0
C(20)-C(23)-H(23B)	109.0
H(23A)-C(23)-H(23B)	107.8
C(24A)-C(23A)-C(20)	107.9(9)

C(24A)-C(23A)-H(23C)	110.1
C(20)-C(23A)-H(23C)	110.1
C(24A)-C(23A)-H(23D)	110.1
C(20)-C(23A)-H(23D)	110.1
H(23C)-C(23A)-H(23D)	108.4
C(25)-C(24)-C(23)	113.0(13)
C(25)-C(24)-H(24A)	109.0
C(23)-C(24)-H(24A)	109.0
C(25)-C(24)-H(24B)	109.0
C(23)-C(24)-H(24B)	109.0
H(24A)-C(24)-H(24B)	107.8
C(26)-C(25)-C(24)	115.9(10)
C(26)-C(25)-H(25A)	108.3
C(24)-C(25)-H(25A)	108.3
C(26)-C(25)-H(25B)	108.3
C(24)-C(25)-H(25B)	108.3
H(25A)-C(25)-H(25B)	107.4
C(25)-C(26)-C(27)	115.2(10)
C(25)-C(26)-H(26A)	108.5
C(27)-C(26)-H(26A)	108.5
C(25)-C(26)-H(26B)	108.5
C(27)-C(26)-H(26B)	108.5
H(26A)-C(26)-H(26B)	107.5
C(28)-C(27)-C(26)	140.4(11)
C(28)-C(27)-H(27A)	101.9
C(26)-C(27)-H(27A)	101.9
C(28)-C(27)-H(27B)	101.9
C(26)-C(27)-H(27B)	101.9
H(27A)-C(27)-H(27B)	104.7
C(27)-C(28)-C(29)	151.0(11)
C(27)-C(28)-H(28A)	104.5

C(29)-C(28)-H(28A)	104.5
C(30)-C(29)-C(28)	151.9(13)
C(30)-C(29)-H(29A)	104.0
C(28)-C(29)-H(29A)	104.0
C(29)-C(30)-C(31)	128.8(13)
C(29)-C(30)-H(30A)	105.1
C(31)-C(30)-H(30A)	105.1
C(29)-C(30)-H(30B)	105.1
C(31)-C(30)-H(30B)	105.1
H(30A)-C(30)-H(30B)	105.9
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(23A)-C(24A)-C(25A)	112.4(12)
C(23A)-C(24A)-H(24C)	109.1
C(25A)-C(24A)-H(24C)	109.1
C(23A)-C(24A)-H(24D)	109.1
C(25A)-C(24A)-H(24D)	109.1
H(24C)-C(24A)-H(24D)	107.9
C(26A)-C(25A)-C(24A)	112.4(10)
C(26A)-C(25A)-H(25C)	109.1
C(24A)-C(25A)-H(25C)	109.1
C(26A)-C(25A)-H(25D)	109.1
C(24A)-C(25A)-H(25D)	109.1
H(25C)-C(25A)-H(25D)	107.9
C(27A)-C(26A)-C(25A)	111.0(8)
C(27A)-C(26A)-H(26C)	109.4
C(25A)-C(26A)-H(26C)	109.4

C(27A)-C(26A)-H(26D)	109.5
C(25A)-C(26A)-H(26D)	109.4
H(26C)-C(26A)-H(26D)	108.0
C(28A)-C(27A)-C(26A)	125.3(8)
C(28A)-C(27A)-H(27C)	106.0
C(26A)-C(27A)-H(27C)	106.0
C(28A)-C(27A)-H(27D)	106.0
C(26A)-C(27A)-H(27D)	106.0
H(27C)-C(27A)-H(27D)	106.3
C(29A)-C(28A)-C(27A)	120.8(10)
C(29A)-C(28A)-H(28B)	107.1
C(27A)-C(28A)-H(28B)	107.1
C(29A)-C(28A)-H(28C)	107.1
C(27A)-C(28A)-H(28C)	107.1
H(28B)-C(28A)-H(28C)	106.8
C(28A)-C(29A)-C(30A)	119.5(13)
C(28A)-C(29A)-H(29B)	107.4
C(30A)-C(29A)-H(29B)	107.4
C(28A)-C(29A)-H(29C)	107.4
C(30A)-C(29A)-H(29C)	107.4
H(29B)-C(29A)-H(29C)	107.0
C(31A)-C(30A)-C(29A)	125.3(14)
C(31A)-C(30A)-H(30C)	106.0
C(29A)-C(30A)-H(30C)	106.0
C(31A)-C(30A)-H(30D)	106.0
C(29A)-C(30A)-H(30D)	106.0
H(30C)-C(30A)-H(30D)	106.3
C(30A)-C(31A)-H(31D)	109.5
C(30A)-C(31A)-H(31E)	109.5
H(31D)-C(31A)-H(31E)	109.5
C(30A)-C(31A)-H(31F)	109.5

H(31D)-C(31A)-H(31F)	109.5
H(31E)-C(31A)-H(31F)	109.5

Symmetry transformations used to generate equivalent atoms:

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

Table S8. Anisotropic displacement parameters (A^2 x 10^3) for **DAP1**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	26(2)	25(2)	29(2)	-8(2)	-8(2)	15(2)
C(2)	15(2)	28(2)	33(2)	2(2)	-1(2)	10(2)
C(3)	23(2)	25(2)	35(2)	4(2)	2(2)	10(2)
C(4)	26(2)	30(2)	32(2)	3(2)	2(2)	11(2)
C(5)	24(2)	23(2)	28(2)	3(2)	0(2)	10(2)
C(6)	22(2)	24(2)	30(2)	-6(2)	-1(2)	8(2)
C(7)	17(2)	18(2)	40(2)	1(2)	-1(2)	10(2)
C(8)	26(2)	20(2)	54(3)	-3(2)	-2(2)	6(2)
C(9)	32(2)	27(2)	74(3)	13(2)	12(2)	1(2)
C(10)	46(3)	43(3)	48(3)	20(2)	6(2)	8(2)
C(11)	34(2)	41(2)	35(2)	11(2)	1(2)	10(2)
C(12)	26(2)	23(2)	31(2)	5(2)	1(2)	9(2)
C(13)	34(2)	26(2)	28(2)	-3(2)	-5(2)	7(2)
C(14)	23(2)	19(2)	34(2)	2(2)	-2(2)	2(2)
C(15)	25(2)	21(2)	41(2)	-5(2)	-5(2)	8(2)
C(16)	15(2)	22(2)	48(2)	9(2)	6(2)	11(2)
C(17)	25(2)	30(2)	30(2)	-6(2)	-4(2)	5(2)
C(20)	124(5)	30(2)	24(2)	-6(2)	12(3)	-32(3)
C(18)	38(4)	40(5)	32(4)	17(4)	-7(3)	-8(4)

C(19)	82(6)	42(5)	31(4)	17(4)	-31(4)	-32(5)
C(21)	97(6)	20(4)	40(5)	-3(4)	35(5)	-9(5)
C(22)	39(4)	21(4)	37(4)	-3(3)	10(3)	-2(4)
C(18A)	15(4)	38(4)	30(4)	-4(3)	2(3)	5(3)
C(19A)	38(5)	28(4)	37(4)	-8(3)	11(4)	-11(4)
C(21A)	83(7)	28(4)	32(4)	-3(3)	15(5)	-26(5)
C(22A)	22(4)	26(4)	44(4)	-11(3)	8(3)	-2(3)
C(23)	36(2)	29(2)	25(2)	0(1)	2(2)	2(2)
C(23A)	36(2)	29(2)	25(2)	0(1)	2(2)	2(2)
C(24)	36(2)	29(2)	25(2)	0(1)	2(2)	2(2)
C(25)	36(2)	29(2)	25(2)	0(1)	2(2)	2(2)
C(26)	36(2)	29(2)	25(2)	0(1)	2(2)	2(2)
C(27)	36(2)	29(2)	25(2)	0(1)	2(2)	2(2)
C(28)	36(2)	29(2)	25(2)	0(1)	2(2)	2(2)
C(29)	46(9)	26(7)	14(6)	7(5)	-7(6)	-12(6)
C(30)	47(7)	39(7)	33(5)	-6(5)	7(5)	-5(6)
C(31)	68(12)	50(8)	42(8)	-15(6)	-25(8)	5(9)
C(24A)	32(8)	27(6)	23(4)	1(5)	3(5)	0(4)
C(25A)	32(5)	29(4)	31(5)	1(3)	-2(4)	5(4)
C(26A)	36(6)	28(5)	28(4)	-2(4)	1(4)	-6(4)
C(27A)	49(6)	27(5)	28(5)	0(3)	-4(5)	10(5)
C(28A)	42(6)	31(5)	36(5)	2(4)	12(4)	0(4)
C(29A)	77(13)	36(7)	27(6)	2(5)	-35(8)	-3(8)
C(30A)	59(8)	29(6)	42(6)	-6(4)	5(6)	-2(5)
C(31A)	50(9)	40(7)	37(8)	-7(5)	-6(7)	-10(7)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **DAP1**.

	x	y	z	U(eq)

H(4A)	5868	2651	10559	35
H(6A)	9447	3671	9976	30
H(8A)	12972	4799	9397	41
H(9A)	14768	5272	8408	52
H(10A)	13036	4326	7359	53
H(11A)	9542	2915	7308	43
H(13A)	6220	1740	7889	36
H(15A)	2805	542	8465	35
H(18A)	5829	1703	11479	44
H(19A)	6085	2544	12575	64
H(21A)	-2016	2417	12586	63
H(22A)	-2285	1544	11484	39
H(18B)	1338	3227	11100	33
H(19B)	1708	4160	12194	42
H(21B)	2008	1031	12965	59
H(22B)	1687	77	11871	38
H(23A)	-777	3396	13360	36
H(23B)	1715	2896	13756	36
H(23C)	2475	2709	13754	36
H(23D)	5086	3285	13438	36
H(24A)	4512	4557	13518	36
H(24B)	2009	5057	13128	36
H(25A)	-233	5276	14147	36
H(25B)	2278	4784	14535	36
H(26A)	2580	6942	13930	36
H(26B)	4953	6462	14376	36
H(27A)	120	6828	14949	36
H(27B)	2984	6802	15309	36
H(28A)	958	8523	14844	36
H(29A)	3442	8673	16040	35

H(30A)	23	9948	16141	48
H(30B)	2012	10530	15656	48
H(31A)	2804	11452	16764	83
H(31B)	5462	10812	16553	83
H(31C)	3449	10223	17044	83
H(24C)	6	4333	13532	33
H(24D)	2460	4888	13152	33
H(25C)	2754	4603	14571	37
H(25D)	5088	5229	14182	37
H(26C)	2044	6757	13952	37
H(26D)	-101	6158	14408	37
H(27C)	2408	6666	15370	42
H(27D)	5122	6792	14993	42
H(28B)	4878	8689	14930	44
H(28C)	1676	8630	14904	44
H(29B)	4943	8600	16058	58
H(29C)	1740	8562	16027	58
H(30C)	5375	10508	15938	53
H(30D)	2490	10525	15569	53
H(31D)	2950	11725	16541	66
H(31E)	3378	10612	16958	66
H(31F)	552	10736	16561	66

Table S10. Torsion angles [deg] for **DAP1**.

C(1)#1-C(1)-C(2)-C(17)	175.9(4)
C(16)#1-C(1)-C(2)-C(17)	-2.1(8)
C(1)#1-C(1)-C(2)-C(3)	-2.6(5)
C(16)#1-C(1)-C(2)-C(3)	179.4(4)

C(1)-C(2)-C(3)-C(4)	-177.8(4)
C(17)-C(2)-C(3)-C(4)	3.7(6)
C(1)-C(2)-C(3)-C(16)	2.9(4)
C(17)-C(2)-C(3)-C(16)	-175.7(3)
C(16)-C(3)-C(4)-C(5)	0.8(6)
C(2)-C(3)-C(4)-C(5)	-178.5(3)
C(3)-C(4)-C(5)-C(6)	-177.9(4)
C(3)-C(4)-C(5)-C(14)	2.7(5)
C(14)-C(5)-C(6)-C(7)	2.3(5)
C(4)-C(5)-C(6)-C(7)	-177.1(3)
C(5)-C(6)-C(7)-C(12)	-0.2(5)
C(5)-C(6)-C(7)-C(8)	179.7(3)
C(6)-C(7)-C(8)-C(9)	-177.9(4)
C(12)-C(7)-C(8)-C(9)	1.9(6)
C(7)-C(8)-C(9)-C(10)	-1.2(6)
C(8)-C(9)-C(10)-C(11)	-0.2(7)
C(9)-C(10)-C(11)-C(12)	0.8(7)
C(6)-C(7)-C(12)-C(13)	-1.7(5)
C(8)-C(7)-C(12)-C(13)	178.5(3)
C(6)-C(7)-C(12)-C(11)	178.5(3)
C(8)-C(7)-C(12)-C(11)	-1.3(5)
C(10)-C(11)-C(12)-C(13)	-179.8(4)
C(10)-C(11)-C(12)-C(7)	0.0(6)
C(7)-C(12)-C(13)-C(14)	1.3(6)
C(11)-C(12)-C(13)-C(14)	-178.8(4)
C(12)-C(13)-C(14)-C(5)	0.8(6)
C(12)-C(13)-C(14)-C(15)	-179.2(4)
C(6)-C(5)-C(14)-C(13)	-2.5(5)
C(4)-C(5)-C(14)-C(13)	176.9(3)
C(6)-C(5)-C(14)-C(15)	177.4(3)
C(4)-C(5)-C(14)-C(15)	-3.2(5)

C(13)-C(14)-C(15)-C(16)	-179.9(4)
C(5)-C(14)-C(15)-C(16)	0.1(5)
C(14)-C(15)-C(16)-C(3)	3.3(5)
C(14)-C(15)-C(16)-C(1)#1	-179.9(4)
C(4)-C(3)-C(16)-C(15)	-3.9(6)
C(2)-C(3)-C(16)-C(15)	175.5(3)
C(4)-C(3)-C(16)-C(1)#1	178.5(3)
C(2)-C(3)-C(16)-C(1)#1	-2.1(4)
C(1)-C(2)-C(17)-C(22)	-41.6(7)
C(3)-C(2)-C(17)-C(22)	136.6(5)
C(1)-C(2)-C(17)-C(22A)	48.7(7)
C(3)-C(2)-C(17)-C(22A)	-133.0(5)
C(1)-C(2)-C(17)-C(18A)	-126.7(5)
C(3)-C(2)-C(17)-C(18A)	51.5(6)
C(1)-C(2)-C(17)-C(18)	140.2(5)
C(3)-C(2)-C(17)-C(18)	-41.6(7)
C(22)-C(17)-C(18)-C(19)	-0.2(11)
C(22A)-C(17)-C(18)-C(19)	-59.4(8)
C(18A)-C(17)-C(18)-C(19)	62.8(8)
C(2)-C(17)-C(18)-C(19)	178.1(7)
C(17)-C(18)-C(19)-C(20)	-3.1(13)
C(21A)-C(20)-C(19)-C(18)	66.2(9)
C(21)-C(20)-C(19)-C(18)	5.8(12)
C(19A)-C(20)-C(19)-C(18)	-58.7(9)
C(23A)-C(20)-C(19)-C(18)	179.1(8)
C(23)-C(20)-C(19)-C(18)	-172.3(8)
C(21A)-C(20)-C(21)-C(22)	-66.3(9)
C(19)-C(20)-C(21)-C(22)	-5.3(12)
C(19A)-C(20)-C(21)-C(22)	62.8(9)
C(23A)-C(20)-C(21)-C(22)	-175.8(8)
C(23)-C(20)-C(21)-C(22)	173.5(8)

C(22A)-C(17)-C(22)-C(21)	60.7(8)
C(18A)-C(17)-C(22)-C(21)	-66.2(8)
C(18)-C(17)-C(22)-C(21)	0.7(11)
C(2)-C(17)-C(22)-C(21)	-177.6(7)
C(20)-C(21)-C(22)-C(17)	2.2(13)
C(22)-C(17)-C(18A)-C(19A)	64.3(8)
C(22A)-C(17)-C(18A)-C(19A)	5.7(9)
C(18)-C(17)-C(18A)-C(19A)	-59.9(8)
C(2)-C(17)-C(18A)-C(19A)	-178.5(6)
C(17)-C(18A)-C(19A)-C(20)	-1.2(11)
C(21A)-C(20)-C(19A)-C(18A)	-4.0(13)
C(21)-C(20)-C(19A)-C(18A)	-62.0(9)
C(19)-C(20)-C(19A)-C(18A)	60.3(8)
C(23A)-C(20)-C(19A)-C(18A)	161.7(8)
C(23)-C(20)-C(19A)-C(18A)	-159.4(7)
C(21)-C(20)-C(21A)-C(22A)	62.5(10)
C(19)-C(20)-C(21A)-C(22A)	-62.9(10)
C(19A)-C(20)-C(21A)-C(22A)	4.3(14)
C(23A)-C(20)-C(21A)-C(22A)	-162.4(8)
C(23)-C(20)-C(21A)-C(22A)	157.5(8)
C(22)-C(17)-C(22A)-C(21A)	-64.0(9)
C(18A)-C(17)-C(22A)-C(21A)	-5.4(10)
C(18)-C(17)-C(22A)-C(21A)	63.1(9)
C(2)-C(17)-C(22A)-C(21A)	179.1(7)
C(20)-C(21A)-C(22A)-C(17)	0.4(14)
C(21A)-C(20)-C(23)-C(24)	155.6(13)
C(21)-C(20)-C(23)-C(24)	-126.7(12)
C(19)-C(20)-C(23)-C(24)	51.5(15)
C(19A)-C(20)-C(23)-C(24)	-49.9(13)
C(23A)-C(20)-C(23)-C(24)	65.8(13)
C(21A)-C(20)-C(23A)-C(24A)	-156.4(9)

C(21)-C(20)-C(23A)-C(24A)	-64.2(11)
C(19)-C(20)-C(23A)-C(24A)	124.6(8)
C(19A)-C(20)-C(23A)-C(24A)	37.5(11)
C(23)-C(20)-C(23A)-C(24A)	-45.9(8)
C(20)-C(23)-C(24)-C(25)	-179.5(12)
C(23)-C(24)-C(25)-C(26)	-179.6(12)
C(24)-C(25)-C(26)-C(27)	175.2(13)
C(25)-C(26)-C(27)-C(28)	-158.1(15)
C(26)-C(27)-C(28)-C(29)	-128(2)
C(27)-C(28)-C(29)-C(30)	-169(3)
C(28)-C(29)-C(30)-C(31)	-166(3)
C(20)-C(23A)-C(24A)-C(25A)	-174.8(8)
C(23A)-C(24A)-C(25A)-C(26A)	-176.2(8)
C(24A)-C(25A)-C(26A)-C(27A)	-174.3(8)
C(25A)-C(26A)-C(27A)-C(28A)	156.4(9)
C(26A)-C(27A)-C(28A)-C(29A)	149.2(13)
C(27A)-C(28A)-C(29A)-C(30A)	179.1(12)
C(28A)-C(29A)-C(30A)-C(31A)	154.2(15)

Symmetry transformations used to generate equivalent atoms:

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

Table S11. Crystal data and structure refinement for **DAP2**.

Empirical formula	C86 H78	
Formula weight	1111.48	
Temperature	153(2) K	
Wavelength	1.54178 A	
Crystal system, space group	Triclinic, P-1	
Unit cell dimensions	a = 9.7359(19) A	alpha = 99.203(10) deg.
	b = 16.193(3) A	beta = 101.335(12) deg.
	c = 22.166(5) A	gamma = 101.921(9) deg.

Volume	3278.4(11) A^3
Z, Calculated density	2, 1.126 Mg/m^3
Absorption coefficient	0.475 mm^-1
F(000)	1188
Crystal size	0.40 x 0.20 x 0.04 mm
Theta range for data collection	2.85 to 63.68 deg.
Limiting indices	-11<=h<=11, -18<=k<=14, -25<=l<=25
Reflections collected / unique	28760 / 10632 [R(int) = 0.0857]
Completeness to theta =	63.68 98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9813 and 0.8328
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10632 / 0 / 775
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.1286, wR2 = 0.3259
R indices (all data)	R1 = 0.1791, wR2 = 0.3691
Largest diff. peak and hole	0.396 and -0.236 e.A^-3

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **DAP2**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	8196(5)	3680(3)	6385(2)	84(1)
C(2)	8029(5)	4431(3)	6703(2)	77(1)
C(3)	7954(4)	4560(2)	7337(2)	74(1)
C(4)	7784(4)	5343(2)	7667(2)	71(1)
C(5)	7713(4)	5440(2)	8287(2)	69(1)
C(6)	7567(4)	6236(2)	8633(2)	72(1)
C(7)	7476(4)	6322(2)	9230(2)	68(1)

C(8)	7327(4)	7036(2)	9696(2)	66(1)
C(9)	7361(4)	7893(2)	9758(2)	69(1)
C(10)	7328(4)	8201(2)	10414(2)	69(1)
C(11)	7370(4)	9009(2)	10736(2)	71(1)
C(12)	7322(4)	9150(2)	11371(2)	68(1)
C(13)	7327(4)	9972(2)	11702(2)	71(1)
C(14)	7287(5)	10117(3)	12326(2)	77(1)
C(15)	7274(5)	10943(3)	12676(2)	87(1)
C(16)	7267(6)	11071(3)	13285(3)	101(2)
C(17)	8246(5)	2993(3)	6703(2)	81(1)
C(18)	8153(4)	3079(2)	7311(2)	74(1)
C(19)	7999(4)	3854(2)	7665(2)	68(1)
C(20)	7874(4)	3949(2)	8282(2)	68(1)
C(21)	7744(4)	4732(2)	8619(2)	67(1)
C(22)	7654(4)	4853(2)	9253(2)	68(1)
C(23)	7517(4)	5623(2)	9564(2)	67(1)
C(24)	7371(4)	5904(2)	10208(2)	69(1)
C(25)	7265(4)	6752(2)	10262(2)	68(1)
C(26)	7241(4)	7490(2)	10739(2)	69(1)
C(27)	7210(4)	7608(2)	11350(2)	67(1)
C(28)	7266(4)	8441(2)	11708(2)	69(1)
C(29)	7220(4)	8585(3)	12333(2)	72(1)
C(30)	7248(5)	9418(3)	12665(2)	78(1)
C(31)	7278(6)	9597(3)	13313(2)	94(1)
C(32)	7290(7)	10394(3)	13619(2)	106(2)
C(33)	7673(5)	6063(3)	7327(2)	73(1)
C(34)	6357(6)	6072(3)	6952(2)	90(1)
C(35)	6243(6)	6752(3)	6650(3)	99(1)
C(36)	7403(6)	7410(3)	6714(2)	96(1)
C(37)	8719(6)	7418(3)	7094(2)	97(1)
C(38)	8827(5)	6741(3)	7395(2)	83(1)

C(39)	7415(5)	8417(2)	9273(2)	73(1)
C(40)	6517(5)	8104(3)	8676(2)	81(1)
C(41)	6508(6)	8573(3)	8227(2)	95(1)
C(42)	7406(6)	9400(3)	8339(2)	95(1)
C(43)	8323(6)	9706(3)	8932(2)	94(1)
C(44)	8330(5)	9228(3)	9396(2)	84(1)
C(45)	7422(4)	10710(2)	11352(2)	72(1)
C(46)	6182(5)	10833(3)	10979(3)	96(1)
C(47)	6298(6)	11512(4)	10670(3)	101(2)
C(48)	7593(6)	12051(3)	10710(2)	91(1)
C(49)	8810(6)	11914(3)	11067(2)	95(1)
C(50)	8724(5)	11250(3)	11385(2)	86(1)
C(51)	7834(4)	3199(2)	8608(2)	69(1)
C(52)	9064(5)	2912(3)	8801(2)	82(1)
C(53)	8987(5)	2219(3)	9097(2)	85(1)
C(54)	7702(5)	1799(3)	9193(2)	84(1)
C(55)	6467(5)	2078(3)	8997(2)	82(1)
C(56)	6552(4)	2770(3)	8700(2)	76(1)
C(57)	7329(4)	5368(2)	10677(2)	69(1)
C(58)	6282(4)	5351(3)	11039(2)	74(1)
C(59)	6218(5)	4857(3)	11481(2)	80(1)
C(60)	7193(5)	4347(2)	11598(2)	79(1)
C(61)	8235(5)	4371(3)	11258(2)	80(1)
C(62)	8309(4)	4865(2)	10802(2)	73(1)
C(63)	7077(4)	7849(3)	12672(2)	75(1)
C(64)	5831(5)	7580(3)	12874(2)	79(1)
C(65)	5675(5)	6898(3)	13178(2)	88(1)
C(66)	6764(5)	6473(3)	13272(2)	88(1)
C(67)	7990(5)	6730(3)	13076(2)	90(1)
C(68)	8161(5)	7409(3)	12777(2)	78(1)
C(69)	7348(8)	9913(4)	7834(3)	115(2)

C(70)	8695(8)	10130(5)	7664(4)	139(2)
C(71)	8583(8)	10550(5)	7067(4)	131(2)
C(72)	7943(11)	9947(5)	6464(4)	151(3)
C(73)	7749(10)	10373(5)	5907(4)	145(2)
C(74)	6437(9)	10790(5)	5833(3)	141(3)
C(75)	6346(9)	11289(5)	5314(3)	138(2)
C(76)	5120(8)	11725(6)	5239(4)	149(3)
C(77)	5110(10)	12179(8)	4688(4)	179(3)
C(78)	7128(6)	3816(3)	12091(2)	90(1)
C(79)	7968(5)	4289(3)	12743(2)	88(1)
C(80)	8022(6)	3754(3)	13239(2)	99(1)
C(81)	8772(8)	4267(5)	13896(3)	126(2)
C(82)	8857(9)	3762(5)	14408(3)	129(2)
C(83)	9958(9)	3229(6)	14393(3)	146(2)
C(84)	10029(8)	2657(6)	14883(3)	137(2)
C(85)	11006(10)	2103(6)	14846(4)	149(3)
C(86)	11019(10)	1512(6)	15291(4)	149(3)

Table S13. Bond lengths [A] and angles [deg] for **DAP2**.

C(1)-C(2)	1.362(6)
C(1)-C(17)	1.413(6)
C(1)-H(1A)	0.9500
C(2)-C(3)	1.406(6)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.418(5)
C(3)-C(19)	1.452(6)
C(4)-C(5)	1.374(6)
C(4)-C(33)	1.497(6)
C(5)-C(6)	1.440(5)

C(5)-C(21)	1.461(5)
C(6)-C(7)	1.331(5)
C(6)-H(6A)	0.9500
C(7)-C(23)	1.451(5)
C(7)-C(8)	1.473(5)
C(8)-C(9)	1.365(5)
C(8)-C(25)	1.411(6)
C(9)-C(10)	1.469(6)
C(9)-C(39)	1.476(6)
C(10)-C(11)	1.375(5)
C(10)-C(26)	1.449(6)
C(11)-C(12)	1.401(6)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.412(5)
C(12)-C(28)	1.463(6)
C(13)-C(14)	1.376(6)
C(13)-C(45)	1.524(6)
C(14)-C(15)	1.438(5)
C(14)-C(30)	1.452(6)
C(15)-C(16)	1.334(6)
C(15)-H(15A)	0.9500
C(16)-C(32)	1.418(7)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.356(6)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.422(5)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.384(6)
C(20)-C(21)	1.407(5)
C(20)-C(51)	1.507(5)
C(21)-C(22)	1.410(5)

C(22)-C(23)	1.369(5)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.472(5)
C(24)-C(25)	1.387(5)
C(24)-C(57)	1.457(6)
C(25)-C(26)	1.472(5)
C(26)-C(27)	1.343(5)
C(27)-C(28)	1.437(5)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.378(6)
C(29)-C(30)	1.422(6)
C(29)-C(63)	1.505(6)
C(30)-C(31)	1.414(6)
C(31)-C(32)	1.355(7)
C(31)-H(31A)	0.9500
C(32)-H(32A)	0.9500
C(33)-C(38)	1.364(6)
C(33)-C(34)	1.388(6)
C(34)-C(35)	1.391(7)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.350(7)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.385(7)
C(36)-H(36A)	0.9500
C(37)-C(38)	1.383(6)
C(37)-H(37A)	0.9500
C(38)-H(38A)	0.9500
C(39)-C(44)	1.378(6)
C(39)-C(40)	1.386(6)
C(40)-C(41)	1.344(6)
C(40)-H(40A)	0.9500

C(41)-C(42)	1.395(8)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.386(7)
C(42)-C(69)	1.495(7)
C(43)-C(44)	1.380(6)
C(43)-H(43A)	0.9500
C(44)-H(44A)	0.9500
C(45)-C(50)	1.363(6)
C(45)-C(46)	1.393(6)
C(46)-C(47)	1.383(7)
C(46)-H(46A)	0.9500
C(47)-C(48)	1.355(8)
C(47)-H(47A)	0.9500
C(48)-C(49)	1.369(7)
C(48)-H(48A)	0.9500
C(49)-C(50)	1.375(6)
C(49)-H(49A)	0.9500
C(50)-H(50A)	0.9500
C(51)-C(56)	1.367(6)
C(51)-C(52)	1.388(5)
C(52)-C(53)	1.384(6)
C(52)-H(52A)	0.9500
C(53)-C(54)	1.369(6)
C(53)-H(53A)	0.9500
C(54)-C(55)	1.386(6)
C(54)-H(54A)	0.9500
C(55)-C(56)	1.383(6)
C(55)-H(55A)	0.9500
C(56)-H(56A)	0.9500
C(57)-C(62)	1.393(5)
C(57)-C(58)	1.414(6)

C(58)-C(59)	1.363(6)
C(58)-H(58A)	0.9500
C(59)-C(60)	1.395(6)
C(59)-H(59A)	0.9500
C(60)-C(61)	1.376(6)
C(60)-C(78)	1.499(6)
C(61)-C(62)	1.389(6)
C(61)-H(61A)	0.9500
C(62)-H(62A)	0.9500
C(63)-C(64)	1.386(6)
C(63)-C(68)	1.393(5)
C(64)-C(65)	1.380(6)
C(64)-H(64A)	0.9500
C(65)-C(66)	1.380(6)
C(65)-H(65A)	0.9500
C(66)-C(67)	1.358(7)
C(66)-H(66A)	0.9500
C(67)-C(68)	1.370(6)
C(67)-H(67A)	0.9500
C(68)-H(68A)	0.9500
C(69)-C(70)	1.425(9)
C(69)-H(69A)	0.9900
C(69)-H(69B)	0.9900
C(70)-C(71)	1.576(9)
C(70)-H(70A)	0.9900
C(70)-H(70B)	0.9900
C(71)-C(72)	1.459(10)
C(71)-H(71A)	0.9900
C(71)-H(71B)	0.9900
C(72)-C(73)	1.507(10)
C(72)-H(72A)	0.9900

C(72)-H(72B)	0.9900
C(73)-C(74)	1.557(11)
C(73)-H(73A)	0.9900
C(73)-H(73B)	0.9900
C(74)-C(75)	1.507(10)
C(74)-H(74A)	0.9900
C(74)-H(74B)	0.9900
C(75)-C(76)	1.503(11)
C(75)-H(75A)	0.9900
C(75)-H(75B)	0.9900
C(76)-C(77)	1.522(10)
C(76)-H(76A)	0.9900
C(76)-H(76B)	0.9900
C(77)-H(77A)	0.9800
C(77)-H(77B)	0.9800
C(77)-H(77C)	0.9800
C(78)-C(79)	1.505(7)
C(78)-H(78A)	0.9900
C(78)-H(78B)	0.9900
C(79)-C(80)	1.504(7)
C(79)-H(79A)	0.9900
C(79)-H(79B)	0.9900
C(80)-C(81)	1.512(8)
C(80)-H(80A)	0.9900
C(80)-H(80B)	0.9900
C(81)-C(82)	1.501(8)
C(81)-H(81A)	0.9900
C(81)-H(81B)	0.9900
C(82)-C(83)	1.510(10)
C(82)-H(82A)	0.9900
C(82)-H(82B)	0.9900

C(83)-C(84)	1.538(9)
C(83)-H(83A)	0.9900
C(83)-H(83B)	0.9900
C(84)-C(85)	1.440(10)
C(84)-H(84A)	0.9900
C(84)-H(84B)	0.9900
C(85)-C(86)	1.480(10)
C(85)-H(85A)	0.9900
C(85)-H(85B)	0.9900
C(86)-H(86A)	0.9800
C(86)-H(86B)	0.9800
C(86)-H(86C)	0.9800
C(2)-C(1)-C(17)	118.2(4)
C(2)-C(1)-H(1A)	120.9
C(17)-C(1)-H(1A)	120.9
C(1)-C(2)-C(3)	122.9(4)
C(1)-C(2)-H(2A)	118.6
C(3)-C(2)-H(2A)	118.6
C(2)-C(3)-C(4)	122.8(4)
C(2)-C(3)-C(19)	119.1(3)
C(4)-C(3)-C(19)	118.1(4)
C(5)-C(4)-C(3)	120.8(3)
C(5)-C(4)-C(33)	120.4(3)
C(3)-C(4)-C(33)	118.8(4)
C(4)-C(5)-C(6)	121.6(3)
C(4)-C(5)-C(21)	121.5(3)
C(6)-C(5)-C(21)	117.0(4)
C(7)-C(6)-C(5)	121.3(3)
C(7)-C(6)-H(6A)	119.3
C(5)-C(6)-H(6A)	119.3
C(6)-C(7)-C(23)	122.0(3)

C(6)-C(7)-C(8)	133.6(3)
C(23)-C(7)-C(8)	104.4(3)
C(9)-C(8)-C(25)	112.0(3)
C(9)-C(8)-C(7)	139.0(4)
C(25)-C(8)-C(7)	108.6(3)
C(8)-C(9)-C(10)	106.1(4)
C(8)-C(9)-C(39)	127.9(4)
C(10)-C(9)-C(39)	126.1(3)
C(11)-C(10)-C(26)	119.3(4)
C(11)-C(10)-C(9)	131.0(4)
C(26)-C(10)-C(9)	109.7(3)
C(10)-C(11)-C(12)	120.8(4)
C(10)-C(11)-H(11A)	119.6
C(12)-C(11)-H(11A)	119.6
C(11)-C(12)-C(13)	121.3(4)
C(11)-C(12)-C(28)	120.3(3)
C(13)-C(12)-C(28)	118.3(4)
C(14)-C(13)-C(12)	121.7(4)
C(14)-C(13)-C(45)	120.4(3)
C(12)-C(13)-C(45)	117.9(3)
C(13)-C(14)-C(15)	123.1(4)
C(13)-C(14)-C(30)	120.2(3)
C(15)-C(14)-C(30)	116.7(4)
C(16)-C(15)-C(14)	121.9(4)
C(16)-C(15)-H(15A)	119.0
C(14)-C(15)-H(15A)	119.0
C(15)-C(16)-C(32)	121.1(4)
C(15)-C(16)-H(16A)	119.5
C(32)-C(16)-H(16A)	119.5
C(18)-C(17)-C(1)	121.2(3)
C(18)-C(17)-H(17A)	119.4

C(1)-C(17)-H(17A)	119.4
C(17)-C(18)-C(19)	122.6(4)
C(17)-C(18)-H(18A)	118.7
C(19)-C(18)-H(18A)	118.7
C(20)-C(19)-C(18)	123.5(3)
C(20)-C(19)-C(3)	120.5(3)
C(18)-C(19)-C(3)	116.0(4)
C(19)-C(20)-C(21)	121.7(3)
C(19)-C(20)-C(51)	120.3(3)
C(21)-C(20)-C(51)	118.0(3)
C(20)-C(21)-C(22)	122.9(3)
C(20)-C(21)-C(5)	117.3(3)
C(22)-C(21)-C(5)	119.8(3)
C(23)-C(22)-C(21)	121.1(3)
C(23)-C(22)-H(22A)	119.4
C(21)-C(22)-H(22A)	119.4
C(22)-C(23)-C(7)	118.8(3)
C(22)-C(23)-C(24)	131.7(3)
C(7)-C(23)-C(24)	109.5(3)
C(25)-C(24)-C(57)	128.7(4)
C(25)-C(24)-C(23)	106.1(3)
C(57)-C(24)-C(23)	125.2(3)
C(24)-C(25)-C(8)	111.3(3)
C(24)-C(25)-C(26)	140.2(4)
C(8)-C(25)-C(26)	108.2(3)
C(27)-C(26)-C(10)	121.2(3)
C(27)-C(26)-C(25)	134.7(4)
C(10)-C(26)-C(25)	104.0(3)
C(26)-C(27)-C(28)	121.6(3)
C(26)-C(27)-H(27A)	119.2
C(28)-C(27)-H(27A)	119.2

C(29)-C(28)-C(27)	123.2(3)
C(29)-C(28)-C(12)	120.0(3)
C(27)-C(28)-C(12)	116.7(3)
C(28)-C(29)-C(30)	121.2(4)
C(28)-C(29)-C(63)	120.3(3)
C(30)-C(29)-C(63)	118.4(4)
C(31)-C(30)-C(29)	122.6(4)
C(31)-C(30)-C(14)	118.8(4)
C(29)-C(30)-C(14)	118.5(4)
C(32)-C(31)-C(30)	121.6(5)
C(32)-C(31)-H(31A)	119.2
C(30)-C(31)-H(31A)	119.2
C(31)-C(32)-C(16)	119.8(4)
C(31)-C(32)-H(32A)	120.1
C(16)-C(32)-H(32A)	120.1
C(38)-C(33)-C(34)	118.3(4)
C(38)-C(33)-C(4)	121.7(4)
C(34)-C(33)-C(4)	120.0(4)
C(33)-C(34)-C(35)	120.0(5)
C(33)-C(34)-H(34A)	120.0
C(35)-C(34)-H(34A)	120.0
C(36)-C(35)-C(34)	120.9(5)
C(36)-C(35)-H(35A)	119.6
C(34)-C(35)-H(35A)	119.6
C(35)-C(36)-C(37)	119.8(4)
C(35)-C(36)-H(36A)	120.1
C(37)-C(36)-H(36A)	120.1
C(38)-C(37)-C(36)	119.2(5)
C(38)-C(37)-H(37A)	120.4
C(36)-C(37)-H(37A)	120.4
C(33)-C(38)-C(37)	121.8(4)

C(33)-C(38)-H(38A)	119.1
C(37)-C(38)-H(38A)	119.1
C(44)-C(39)-C(40)	118.0(4)
C(44)-C(39)-C(9)	121.8(4)
C(40)-C(39)-C(9)	120.2(4)
C(41)-C(40)-C(39)	121.8(5)
C(41)-C(40)-H(40A)	119.1
C(39)-C(40)-H(40A)	119.1
C(40)-C(41)-C(42)	121.6(5)
C(40)-C(41)-H(41A)	119.2
C(42)-C(41)-H(41A)	119.2
C(43)-C(42)-C(41)	116.4(4)
C(43)-C(42)-C(69)	123.2(5)
C(41)-C(42)-C(69)	120.4(5)
C(44)-C(43)-C(42)	122.1(5)
C(44)-C(43)-H(43A)	118.9
C(42)-C(43)-H(43A)	118.9
C(39)-C(44)-C(43)	120.0(5)
C(39)-C(44)-H(44A)	120.0
C(43)-C(44)-H(44A)	120.0
C(50)-C(45)-C(46)	118.8(4)
C(50)-C(45)-C(13)	120.7(4)
C(46)-C(45)-C(13)	120.4(4)
C(47)-C(46)-C(45)	119.2(5)
C(47)-C(46)-H(46A)	120.4
C(45)-C(46)-H(46A)	120.4
C(48)-C(47)-C(46)	121.6(5)
C(48)-C(47)-H(47A)	119.2
C(46)-C(47)-H(47A)	119.2
C(47)-C(48)-C(49)	118.8(5)
C(47)-C(48)-H(48A)	120.6

C(49)-C(48)-H(48A)	120.6
C(48)-C(49)-C(50)	120.9(5)
C(48)-C(49)-H(49A)	119.6
C(50)-C(49)-H(49A)	119.6
C(45)-C(50)-C(49)	120.7(4)
C(45)-C(50)-H(50A)	119.6
C(49)-C(50)-H(50A)	119.6
C(56)-C(51)-C(52)	118.8(4)
C(56)-C(51)-C(20)	119.7(3)
C(52)-C(51)-C(20)	121.6(4)
C(53)-C(52)-C(51)	120.0(4)
C(53)-C(52)-H(52A)	120.0
C(51)-C(52)-H(52A)	120.0
C(54)-C(53)-C(52)	120.8(4)
C(54)-C(53)-H(53A)	119.6
C(52)-C(53)-H(53A)	119.6
C(53)-C(54)-C(55)	119.5(4)
C(53)-C(54)-H(54A)	120.3
C(55)-C(54)-H(54A)	120.3
C(56)-C(55)-C(54)	119.4(4)
C(56)-C(55)-H(55A)	120.3
C(54)-C(55)-H(55A)	120.3
C(51)-C(56)-C(55)	121.6(4)
C(51)-C(56)-H(56A)	119.2
C(55)-C(56)-H(56A)	119.2
C(62)-C(57)-C(58)	116.6(4)
C(62)-C(57)-C(24)	122.8(3)
C(58)-C(57)-C(24)	120.5(3)
C(59)-C(58)-C(57)	121.8(4)
C(59)-C(58)-H(58A)	119.1
C(57)-C(58)-H(58A)	119.1

C(58)-C(59)-C(60)	121.2(4)
C(58)-C(59)-H(59A)	119.4
C(60)-C(59)-H(59A)	119.4
C(61)-C(60)-C(59)	117.6(4)
C(61)-C(60)-C(78)	121.5(4)
C(59)-C(60)-C(78)	120.9(4)
C(60)-C(61)-C(62)	122.0(4)
C(60)-C(61)-H(61A)	119.0
C(62)-C(61)-H(61A)	119.0
C(61)-C(62)-C(57)	120.8(4)
C(61)-C(62)-H(62A)	119.6
C(57)-C(62)-H(62A)	119.6
C(64)-C(63)-C(68)	118.4(4)
C(64)-C(63)-C(29)	120.1(3)
C(68)-C(63)-C(29)	121.5(4)
C(65)-C(64)-C(63)	120.8(4)
C(65)-C(64)-H(64A)	119.6
C(63)-C(64)-H(64A)	119.6
C(66)-C(65)-C(64)	119.4(4)
C(66)-C(65)-H(65A)	120.3
C(64)-C(65)-H(65A)	120.3
C(67)-C(66)-C(65)	120.4(4)
C(67)-C(66)-H(66A)	119.8
C(65)-C(66)-H(66A)	119.8
C(66)-C(67)-C(68)	120.7(4)
C(66)-C(67)-H(67A)	119.7
C(68)-C(67)-H(67A)	119.7
C(67)-C(68)-C(63)	120.3(4)
C(67)-C(68)-H(68A)	119.8
C(63)-C(68)-H(68A)	119.8
C(70)-C(69)-C(42)	112.6(5)

C(70)-C(69)-H(69A)	109.1
C(42)-C(69)-H(69A)	109.1
C(70)-C(69)-H(69B)	109.1
C(42)-C(69)-H(69B)	109.1
H(69A)-C(69)-H(69B)	107.8
C(69)-C(70)-C(71)	112.7(5)
C(69)-C(70)-H(70A)	109.0
C(71)-C(70)-H(70A)	109.0
C(69)-C(70)-H(70B)	109.0
C(71)-C(70)-H(70B)	109.0
H(70A)-C(70)-H(70B)	107.8
C(72)-C(71)-C(70)	115.3(7)
C(72)-C(71)-H(71A)	108.4
C(70)-C(71)-H(71A)	108.4
C(72)-C(71)-H(71B)	108.4
C(70)-C(71)-H(71B)	108.4
H(71A)-C(71)-H(71B)	107.5
C(71)-C(72)-C(73)	114.1(7)
C(71)-C(72)-H(72A)	108.7
C(73)-C(72)-H(72A)	108.7
C(71)-C(72)-H(72B)	108.7
C(73)-C(72)-H(72B)	108.7
H(72A)-C(72)-H(72B)	107.6
C(72)-C(73)-C(74)	114.0(6)
C(72)-C(73)-H(73A)	108.7
C(74)-C(73)-H(73A)	108.7
C(72)-C(73)-H(73B)	108.7
C(74)-C(73)-H(73B)	108.7
H(73A)-C(73)-H(73B)	107.6
C(75)-C(74)-C(73)	113.3(6)
C(75)-C(74)-H(74A)	108.9

C(73)-C(74)-H(74A)	108.9
C(75)-C(74)-H(74B)	108.9
C(73)-C(74)-H(74B)	108.9
H(74A)-C(74)-H(74B)	107.7
C(76)-C(75)-C(74)	115.1(6)
C(76)-C(75)-H(75A)	108.5
C(74)-C(75)-H(75A)	108.5
C(76)-C(75)-H(75B)	108.5
C(74)-C(75)-H(75B)	108.5
H(75A)-C(75)-H(75B)	107.5
C(75)-C(76)-C(77)	110.2(7)
C(75)-C(76)-H(76A)	109.6
C(77)-C(76)-H(76A)	109.6
C(75)-C(76)-H(76B)	109.6
C(77)-C(76)-H(76B)	109.6
H(76A)-C(76)-H(76B)	108.1
C(76)-C(77)-H(77A)	109.5
C(76)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	109.5
C(76)-C(77)-H(77C)	109.5
H(77A)-C(77)-H(77C)	109.5
H(77B)-C(77)-H(77C)	109.5
C(60)-C(78)-C(79)	114.4(4)
C(60)-C(78)-H(78A)	108.7
C(79)-C(78)-H(78A)	108.7
C(60)-C(78)-H(78B)	108.7
C(79)-C(78)-H(78B)	108.7
H(78A)-C(78)-H(78B)	107.6
C(78)-C(79)-C(80)	115.7(4)
C(78)-C(79)-H(79A)	108.4
C(80)-C(79)-H(79A)	108.4

C(78)-C(79)-H(79B)	108.4
C(80)-C(79)-H(79B)	108.4
H(79A)-C(79)-H(79B)	107.4
C(79)-C(80)-C(81)	114.0(5)
C(79)-C(80)-H(80A)	108.8
C(81)-C(80)-H(80A)	108.8
C(79)-C(80)-H(80B)	108.8
C(81)-C(80)-H(80B)	108.8
H(80A)-C(80)-H(80B)	107.6
C(82)-C(81)-C(80)	116.0(6)
C(82)-C(81)-H(81A)	108.3
C(80)-C(81)-H(81A)	108.3
C(82)-C(81)-H(81B)	108.3
C(80)-C(81)-H(81B)	108.3
H(81A)-C(81)-H(81B)	107.4
C(81)-C(82)-C(83)	112.5(6)
C(81)-C(82)-H(82A)	109.1
C(83)-C(82)-H(82A)	109.1
C(81)-C(82)-H(82B)	109.1
C(83)-C(82)-H(82B)	109.1
H(82A)-C(82)-H(82B)	107.8
C(82)-C(83)-C(84)	114.8(6)
C(82)-C(83)-H(83A)	108.6
C(84)-C(83)-H(83A)	108.6
C(82)-C(83)-H(83B)	108.6
C(84)-C(83)-H(83B)	108.6
H(83A)-C(83)-H(83B)	107.5
C(85)-C(84)-C(83)	115.2(6)
C(85)-C(84)-H(84A)	108.5
C(83)-C(84)-H(84A)	108.5
C(85)-C(84)-H(84B)	108.5

C(83)-C(84)-H(84B)	108.5
H(84A)-C(84)-H(84B)	107.5
C(84)-C(85)-C(86)	115.6(6)
C(84)-C(85)-H(85A)	108.4
C(86)-C(85)-H(85A)	108.4
C(84)-C(85)-H(85B)	108.4
C(86)-C(85)-H(85B)	108.4
H(85A)-C(85)-H(85B)	107.4
C(85)-C(86)-H(86A)	109.5
C(85)-C(86)-H(86B)	109.5
H(86A)-C(86)-H(86B)	109.5
C(85)-C(86)-H(86C)	109.5
H(86A)-C(86)-H(86C)	109.5
H(86B)-C(86)-H(86C)	109.5

Table S14. Anisotropic displacement parameters (A^2 x 10^3) for**DAP2**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	85(3)	74(3)	93(3)	2(2)	25(2)	31(2)
C(2)	78(3)	60(2)	95(3)	6(2)	23(2)	27(2)
C(3)	65(2)	54(2)	104(3)	2(2)	21(2)	26(2)
C(4)	71(2)	53(2)	93(3)	8(2)	22(2)	26(2)
C(5)	69(2)	49(2)	94(3)	8(2)	18(2)	29(2)
C(6)	68(2)	48(2)	99(3)	7(2)	17(2)	24(2)
C(7)	71(2)	49(2)	85(3)	4(2)	15(2)	28(2)
C(8)	66(2)	57(2)	79(2)	5(2)	15(2)	31(2)
C(9)	64(2)	53(2)	92(3)	2(2)	16(2)	29(2)

C(10)	63(2)	51(2)	97(3)	6(2)	21(2)	30(2)
C(11)	66(2)	54(2)	98(3)	10(2)	20(2)	28(2)
C(12)	66(2)	48(2)	91(3)	1(2)	19(2)	27(2)
C(13)	65(2)	51(2)	95(3)	1(2)	15(2)	23(2)
C(14)	80(3)	56(2)	97(3)	6(2)	24(2)	27(2)
C(15)	101(3)	54(2)	109(4)	-2(2)	31(2)	32(2)
C(16)	134(4)	60(3)	111(4)	-9(2)	47(3)	34(3)
C(17)	84(3)	59(2)	103(3)	1(2)	29(2)	29(2)
C(18)	76(2)	51(2)	97(3)	4(2)	20(2)	28(2)
C(19)	63(2)	47(2)	95(3)	6(2)	20(2)	21(2)
C(20)	61(2)	47(2)	96(3)	6(2)	18(2)	25(2)
C(21)	60(2)	49(2)	92(3)	6(2)	19(2)	24(2)
C(22)	65(2)	47(2)	94(3)	9(2)	18(2)	23(2)
C(23)	63(2)	48(2)	92(3)	7(2)	17(2)	25(2)
C(24)	60(2)	53(2)	93(3)	5(2)	16(2)	22(2)
C(25)	59(2)	56(2)	92(3)	2(2)	17(2)	33(2)
C(26)	62(2)	55(2)	90(3)	3(2)	17(2)	28(2)
C(27)	61(2)	47(2)	97(3)	8(2)	20(2)	24(2)
C(28)	64(2)	54(2)	92(3)	4(2)	22(2)	27(2)
C(29)	62(2)	60(2)	96(3)	9(2)	21(2)	25(2)
C(30)	82(3)	63(2)	93(3)	3(2)	29(2)	28(2)
C(31)	111(4)	75(3)	104(4)	11(2)	35(3)	35(3)
C(32)	148(5)	74(3)	96(3)	-4(2)	39(3)	35(3)
C(33)	81(3)	59(2)	83(3)	5(2)	21(2)	29(2)
C(34)	95(3)	75(3)	101(3)	12(2)	21(2)	28(2)
C(35)	95(3)	87(3)	117(4)	28(3)	13(3)	33(3)
C(36)	119(4)	77(3)	104(3)	25(2)	28(3)	49(3)
C(37)	112(4)	69(3)	113(4)	13(2)	31(3)	26(2)
C(38)	84(3)	69(3)	105(3)	19(2)	25(2)	32(2)
C(39)	83(3)	50(2)	89(3)	2(2)	22(2)	31(2)
C(40)	94(3)	63(2)	90(3)	5(2)	16(2)	41(2)

C(41)	112(4)	84(3)	92(3)	7(2)	10(2)	51(3)
C(42)	122(4)	73(3)	105(4)	18(2)	27(3)	55(3)
C(43)	132(4)	60(3)	95(3)	11(2)	25(3)	43(3)
C(44)	86(3)	64(3)	104(3)	10(2)	20(2)	31(2)
C(45)	80(3)	51(2)	91(3)	0(2)	24(2)	35(2)
C(46)	81(3)	81(3)	136(4)	22(3)	27(3)	41(2)
C(47)	96(4)	88(3)	133(4)	25(3)	25(3)	54(3)
C(48)	115(4)	66(3)	99(3)	14(2)	29(3)	38(3)
C(49)	101(3)	65(3)	117(4)	15(2)	26(3)	17(2)
C(50)	79(3)	65(3)	110(3)	9(2)	14(2)	25(2)
C(51)	71(2)	42(2)	94(3)	-1(2)	22(2)	22(2)
C(52)	71(2)	54(2)	123(3)	11(2)	24(2)	27(2)
C(53)	72(3)	57(2)	127(4)	14(2)	17(2)	32(2)
C(54)	83(3)	57(2)	117(3)	18(2)	23(2)	32(2)
C(55)	72(2)	65(3)	115(3)	19(2)	27(2)	26(2)
C(56)	68(2)	62(2)	103(3)	14(2)	20(2)	29(2)
C(57)	71(2)	50(2)	82(2)	-2(2)	17(2)	22(2)
C(58)	71(2)	62(2)	92(3)	6(2)	18(2)	30(2)
C(59)	71(2)	67(2)	103(3)	11(2)	24(2)	19(2)
C(60)	85(3)	55(2)	93(3)	9(2)	19(2)	15(2)
C(61)	81(3)	60(2)	105(3)	14(2)	19(2)	34(2)
C(62)	73(2)	58(2)	92(3)	6(2)	22(2)	27(2)
C(63)	75(2)	63(2)	87(3)	3(2)	22(2)	24(2)
C(64)	72(2)	77(3)	87(3)	8(2)	20(2)	25(2)
C(65)	82(3)	83(3)	97(3)	12(2)	25(2)	19(2)
C(66)	87(3)	73(3)	106(3)	18(2)	26(2)	23(2)
C(67)	82(3)	72(3)	116(3)	14(2)	20(2)	29(2)
C(68)	75(2)	64(2)	101(3)	13(2)	25(2)	28(2)
C(69)	145(5)	100(4)	117(4)	25(3)	40(3)	52(4)
C(70)	112(5)	119(5)	198(7)	57(5)	28(4)	47(4)
C(71)	125(5)	116(5)	165(6)	55(5)	39(4)	31(4)

C(72)	216(8)	107(5)	140(6)	12(4)	64(5)	48(5)
C(73)	177(7)	132(6)	137(6)	19(4)	61(5)	47(5)
C(74)	166(7)	114(5)	121(5)	3(4)	50(4)	-14(5)
C(75)	158(6)	144(6)	91(4)	-6(4)	32(4)	10(5)
C(76)	102(5)	174(7)	151(6)	14(5)	18(4)	18(5)
C(77)	140(6)	231(11)	153(7)	50(7)	9(5)	35(6)
C(78)	96(3)	63(3)	114(4)	16(2)	26(3)	26(2)
C(79)	98(3)	75(3)	95(3)	16(2)	24(2)	29(2)
C(80)	102(3)	88(3)	116(4)	24(3)	31(3)	37(3)
C(81)	157(6)	125(5)	95(4)	35(3)	33(3)	21(4)
C(82)	151(6)	127(5)	113(4)	24(4)	39(4)	39(4)
C(83)	151(6)	168(7)	125(5)	40(5)	51(4)	30(5)
C(84)	130(5)	177(7)	124(5)	52(5)	46(4)	56(5)
C(85)	155(6)	177(7)	133(5)	40(5)	47(4)	64(6)
C(86)	168(7)	161(7)	145(6)	36(5)	53(5)	85(6)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **DAP2**.

	x	y	z	U(eq)
H(1A)	8277	3619	5961	100
H(2A)	7959	4887	6487	93
H(6A)	7535	6709	8431	86
H(11A)	7433	9477	10526	85
H(15A)	7272	11411	12467	105
H(16A)	7246	11624	13498	121
H(17A)	8347	2461	6487	97
H(18A)	8192	2602	7509	89

H(22A)	7688	4392	9469	82
H(27A)	7151	7129	11549	81
H(31A)	7290	9147	13541	113
H(32A)	7314	10500	14055	127
H(34A)	5532	5612	6902	109
H(35A)	5338	6754	6394	119
H(36A)	7317	7867	6499	115
H(37A)	9538	7882	7147	117
H(38A)	9730	6748	7657	100
H(40A)	5892	7542	8581	97
H(41A)	5874	8335	7824	114
H(43A)	8968	10261	9023	112
H(44A)	8965	9459	9799	101
H(46A)	5266	10455	10938	115
H(47A)	5449	11603	10423	121
H(48A)	7655	12515	10495	109
H(49A)	9726	12283	11095	114
H(50A)	9580	11165	11631	103
H(52A)	9959	3192	8731	98
H(53A)	9837	2032	9235	102
H(54A)	7656	1320	9393	101
H(55A)	5571	1798	9066	98
H(56A)	5700	2951	8557	91
H(58A)	5605	5693	10972	89
H(59A)	5495	4860	11713	96
H(61A)	8925	4040	11337	96
H(62A)	9037	4860	10573	88
H(64A)	5076	7867	12803	94
H(65A)	4825	6723	13322	105
H(66A)	6656	5997	13475	106
H(67A)	8737	6436	13146	108

H(68A)	9023	7581	12641	94
H(69A)	6596	9576	7458	138
H(69B)	7069	10450	7982	138
H(70A)	9046	9601	7577	166
H(70B)	9413	10538	8022	166
H(71A)	8002	10981	7112	158
H(71B)	9566	10862	7060	158
H(72A)	6989	9603	6480	182
H(72B)	8565	9543	6402	182
H(73A)	7624	9937	5520	174
H(73B)	8639	10825	5949	174
H(74A)	5536	10330	5746	169
H(74B)	6508	11183	6235	169
H(75A)	7265	11733	5395	166
H(75B)	6250	10889	4912	166
H(76A)	5228	12152	5629	178
H(76B)	4192	11291	5164	178
H(77A)	4291	12448	4635	268
H(77B)	5019	11758	4303	268
H(77C)	6014	12625	4770	268
H(78A)	7502	3305	11970	108
H(78B)	6104	3605	12100	108
H(79A)	7540	4772	12875	106
H(79B)	8971	4542	12724	106
H(80A)	8529	3302	13129	119
H(80B)	7022	3462	13237	119
H(81A)	9767	4563	13893	151
H(81B)	8261	4720	14002	151
H(82A)	7895	3375	14363	155
H(82B)	9112	4166	14821	155
H(83A)	10923	3624	14461	175

H(83B)	9734	2856	13969	175
H(84A)	10321	3034	15308	164
H(84B)	9047	2292	14835	164
H(85A)	11997	2470	14920	179
H(85B)	10752	1753	14413	179
H(86A)	11770	1200	15253	223
H(86B)	10075	1099	15192	223
H(86C)	11220	1847	15721	223

Table S16. Torsion angles [deg] for **DAP2**.

C(17)-C(1)-C(2)-C(3)	2.2(7)
C(1)-C(2)-C(3)-C(4)	179.8(4)
C(1)-C(2)-C(3)-C(19)	-2.5(6)
C(2)-C(3)-C(4)-C(5)	179.9(4)
C(19)-C(3)-C(4)-C(5)	2.1(6)
C(2)-C(3)-C(4)-C(33)	0.2(6)
C(19)-C(3)-C(4)-C(33)	-177.5(3)
C(3)-C(4)-C(5)-C(6)	178.8(3)
C(33)-C(4)-C(5)-C(6)	-1.5(6)
C(3)-C(4)-C(5)-C(21)	-2.8(6)
C(33)-C(4)-C(5)-C(21)	176.8(4)
C(4)-C(5)-C(6)-C(7)	178.9(4)
C(21)-C(5)-C(6)-C(7)	0.5(6)
C(5)-C(6)-C(7)-C(23)	-0.1(6)
C(5)-C(6)-C(7)-C(8)	179.9(4)
C(6)-C(7)-C(8)-C(9)	-8.4(8)
C(23)-C(7)-C(8)-C(9)	171.6(5)
C(6)-C(7)-C(8)-C(25)	179.2(4)

C(23)-C(7)-C(8)-C(25)	-0.8(4)
C(25)-C(8)-C(9)-C(10)	0.3(4)
C(7)-C(8)-C(9)-C(10)	-171.9(4)
C(25)-C(8)-C(9)-C(39)	-179.4(4)
C(7)-C(8)-C(9)-C(39)	8.3(8)
C(8)-C(9)-C(10)-C(11)	178.5(4)
C(39)-C(9)-C(10)-C(11)	-1.7(7)
C(8)-C(9)-C(10)-C(26)	-1.2(4)
C(39)-C(9)-C(10)-C(26)	178.6(3)
C(26)-C(10)-C(11)-C(12)	-0.4(5)
C(9)-C(10)-C(11)-C(12)	179.9(4)
C(10)-C(11)-C(12)-C(13)	-178.3(3)
C(10)-C(11)-C(12)-C(28)	1.7(6)
C(11)-C(12)-C(13)-C(14)	-179.7(3)
C(28)-C(12)-C(13)-C(14)	0.3(6)
C(11)-C(12)-C(13)-C(45)	-1.5(5)
C(28)-C(12)-C(13)-C(45)	178.5(3)
C(12)-C(13)-C(14)-C(15)	-179.3(4)
C(45)-C(13)-C(14)-C(15)	2.5(6)
C(12)-C(13)-C(14)-C(30)	0.4(6)
C(45)-C(13)-C(14)-C(30)	-177.8(4)
C(13)-C(14)-C(15)-C(16)	-178.5(4)
C(30)-C(14)-C(15)-C(16)	1.7(7)
C(14)-C(15)-C(16)-C(32)	0.8(8)
C(2)-C(1)-C(17)-C(18)	-1.0(7)
C(1)-C(17)-C(18)-C(19)	0.1(6)
C(17)-C(18)-C(19)-C(20)	178.7(4)
C(17)-C(18)-C(19)-C(3)	-0.3(6)
C(2)-C(3)-C(19)-C(20)	-177.6(4)
C(4)-C(3)-C(19)-C(20)	0.2(5)
C(2)-C(3)-C(19)-C(18)	1.4(5)

C(4)-C(3)-C(19)-C(18)	179.2(4)
C(18)-C(19)-C(20)-C(21)	179.1(3)
C(3)-C(19)-C(20)-C(21)	-1.9(6)
C(18)-C(19)-C(20)-C(51)	-2.6(6)
C(3)-C(19)-C(20)-C(51)	176.4(3)
C(19)-C(20)-C(21)-C(22)	-178.3(3)
C(51)-C(20)-C(21)-C(22)	3.4(5)
C(19)-C(20)-C(21)-C(5)	1.3(5)
C(51)-C(20)-C(21)-C(5)	-177.0(3)
C(4)-C(5)-C(21)-C(20)	1.0(5)
C(6)-C(5)-C(21)-C(20)	179.5(3)
C(4)-C(5)-C(21)-C(22)	-179.3(3)
C(6)-C(5)-C(21)-C(22)	-0.9(5)
C(20)-C(21)-C(22)-C(23)	-179.5(3)
C(5)-C(21)-C(22)-C(23)	0.9(5)
C(21)-C(22)-C(23)-C(7)	-0.4(5)
C(21)-C(22)-C(23)-C(24)	178.4(4)
C(6)-C(7)-C(23)-C(22)	0.0(6)
C(8)-C(7)-C(23)-C(22)	-179.9(3)
C(6)-C(7)-C(23)-C(24)	-179.1(3)
C(8)-C(7)-C(23)-C(24)	1.0(4)
C(22)-C(23)-C(24)-C(25)	-179.7(4)
C(7)-C(23)-C(24)-C(25)	-0.8(4)
C(22)-C(23)-C(24)-C(57)	-0.6(6)
C(7)-C(23)-C(24)-C(57)	178.4(3)
C(57)-C(24)-C(25)-C(8)	-178.9(4)
C(23)-C(24)-C(25)-C(8)	0.2(4)
C(57)-C(24)-C(25)-C(26)	8.8(8)
C(23)-C(24)-C(25)-C(26)	-172.1(4)
C(9)-C(8)-C(25)-C(24)	-174.2(3)
C(7)-C(8)-C(25)-C(24)	0.4(4)

C(9)-C(8)-C(25)-C(26)	0.6(4)
C(7)-C(8)-C(25)-C(26)	175.3(3)
C(11)-C(10)-C(26)-C(27)	-0.4(5)
C(9)-C(10)-C(26)-C(27)	179.3(3)
C(11)-C(10)-C(26)-C(25)	-178.2(3)
C(9)-C(10)-C(26)-C(25)	1.5(4)
C(24)-C(25)-C(26)-C(27)	-6.2(8)
C(8)-C(25)-C(26)-C(27)	-178.7(4)
C(24)-C(25)-C(26)-C(10)	171.2(5)
C(8)-C(25)-C(26)-C(10)	-1.3(4)
C(10)-C(26)-C(27)-C(28)	-0.2(5)
C(25)-C(26)-C(27)-C(28)	176.9(4)
C(26)-C(27)-C(28)-C(29)	179.3(3)
C(26)-C(27)-C(28)-C(12)	1.4(5)
C(11)-C(12)-C(28)-C(29)	179.9(3)
C(13)-C(12)-C(28)-C(29)	-0.1(5)
C(11)-C(12)-C(28)-C(27)	-2.2(5)
C(13)-C(12)-C(28)-C(27)	177.8(3)
C(27)-C(28)-C(29)-C(30)	-178.7(3)
C(12)-C(28)-C(29)-C(30)	-0.9(6)
C(27)-C(28)-C(29)-C(63)	-1.2(6)
C(12)-C(28)-C(29)-C(63)	176.5(3)
C(28)-C(29)-C(30)-C(31)	-176.7(4)
C(63)-C(29)-C(30)-C(31)	5.8(6)
C(28)-C(29)-C(30)-C(14)	1.6(6)
C(63)-C(29)-C(30)-C(14)	-175.9(4)
C(13)-C(14)-C(30)-C(31)	177.0(4)
C(15)-C(14)-C(30)-C(31)	-3.3(6)
C(13)-C(14)-C(30)-C(29)	-1.4(6)
C(15)-C(14)-C(30)-C(29)	178.4(4)
C(29)-C(30)-C(31)-C(32)	-179.4(5)

C(14)-C(30)-C(31)-C(32)	2.4(7)
C(30)-C(31)-C(32)-C(16)	0.3(9)
C(15)-C(16)-C(32)-C(31)	-1.9(9)
C(5)-C(4)-C(33)-C(38)	80.2(5)
C(3)-C(4)-C(33)-C(38)	-100.2(5)
C(5)-C(4)-C(33)-C(34)	-97.0(5)
C(3)-C(4)-C(33)-C(34)	82.6(5)
C(38)-C(33)-C(34)-C(35)	1.0(6)
C(4)-C(33)-C(34)-C(35)	178.3(4)
C(33)-C(34)-C(35)-C(36)	0.1(8)
C(34)-C(35)-C(36)-C(37)	-1.1(8)
C(35)-C(36)-C(37)-C(38)	0.9(7)
C(34)-C(33)-C(38)-C(37)	-1.2(6)
C(4)-C(33)-C(38)-C(37)	-178.4(4)
C(36)-C(37)-C(38)-C(33)	0.2(7)
C(8)-C(9)-C(39)-C(44)	-135.6(4)
C(10)-C(9)-C(39)-C(44)	44.7(5)
C(8)-C(9)-C(39)-C(40)	45.3(6)
C(10)-C(9)-C(39)-C(40)	-134.4(4)
C(44)-C(39)-C(40)-C(41)	-1.0(6)
C(9)-C(39)-C(40)-C(41)	178.1(4)
C(39)-C(40)-C(41)-C(42)	0.2(7)
C(40)-C(41)-C(42)-C(43)	1.1(7)
C(40)-C(41)-C(42)-C(69)	-178.8(4)
C(41)-C(42)-C(43)-C(44)	-1.5(7)
C(69)-C(42)-C(43)-C(44)	178.3(4)
C(40)-C(39)-C(44)-C(43)	0.6(6)
C(9)-C(39)-C(44)-C(43)	-178.5(4)
C(42)-C(43)-C(44)-C(39)	0.7(7)
C(14)-C(13)-C(45)-C(50)	83.9(5)
C(12)-C(13)-C(45)-C(50)	-94.3(5)

C(14)-C(13)-C(45)-C(46)	-97.6(5)
C(12)-C(13)-C(45)-C(46)	84.1(5)
C(50)-C(45)-C(46)-C(47)	-2.0(6)
C(13)-C(45)-C(46)-C(47)	179.6(4)
C(45)-C(46)-C(47)-C(48)	1.3(7)
C(46)-C(47)-C(48)-C(49)	0.1(7)
C(47)-C(48)-C(49)-C(50)	-0.8(7)
C(46)-C(45)-C(50)-C(49)	1.3(6)
C(13)-C(45)-C(50)-C(49)	179.7(4)
C(48)-C(49)-C(50)-C(45)	0.1(7)
C(19)-C(20)-C(51)-C(56)	-104.8(4)
C(21)-C(20)-C(51)-C(56)	73.6(5)
C(19)-C(20)-C(51)-C(52)	73.3(5)
C(21)-C(20)-C(51)-C(52)	-108.3(4)
C(56)-C(51)-C(52)-C(53)	-1.7(6)
C(20)-C(51)-C(52)-C(53)	-179.8(4)
C(51)-C(52)-C(53)-C(54)	1.1(7)
C(52)-C(53)-C(54)-C(55)	-0.7(7)
C(53)-C(54)-C(55)-C(56)	0.9(7)
C(52)-C(51)-C(56)-C(55)	2.0(6)
C(20)-C(51)-C(56)-C(55)	-179.9(4)
C(54)-C(55)-C(56)-C(51)	-1.6(6)
C(25)-C(24)-C(57)-C(62)	-134.0(4)
C(23)-C(24)-C(57)-C(62)	47.1(6)
C(25)-C(24)-C(57)-C(58)	44.8(6)
C(23)-C(24)-C(57)-C(58)	-134.2(4)
C(62)-C(57)-C(58)-C(59)	-1.1(6)
C(24)-C(57)-C(58)-C(59)	-179.9(4)
C(57)-C(58)-C(59)-C(60)	0.3(7)
C(58)-C(59)-C(60)-C(61)	0.9(6)
C(58)-C(59)-C(60)-C(78)	179.1(4)

C(59)-C(60)-C(61)-C(62)	-1.5(6)
C(78)-C(60)-C(61)-C(62)	-179.7(4)
C(60)-C(61)-C(62)-C(57)	0.8(7)
C(58)-C(57)-C(62)-C(61)	0.5(6)
C(24)-C(57)-C(62)-C(61)	179.3(4)
C(28)-C(29)-C(63)-C(64)	-113.0(4)
C(30)-C(29)-C(63)-C(64)	64.5(5)
C(28)-C(29)-C(63)-C(68)	65.3(5)
C(30)-C(29)-C(63)-C(68)	-117.2(4)
C(68)-C(63)-C(64)-C(65)	0.7(6)
C(29)-C(63)-C(64)-C(65)	179.1(4)
C(63)-C(64)-C(65)-C(66)	-1.1(7)
C(64)-C(65)-C(66)-C(67)	1.0(7)
C(65)-C(66)-C(67)-C(68)	-0.6(7)
C(66)-C(67)-C(68)-C(63)	0.2(7)
C(64)-C(63)-C(68)-C(67)	-0.3(6)
C(29)-C(63)-C(68)-C(67)	-178.6(4)
C(43)-C(42)-C(69)-C(70)	60.7(7)
C(41)-C(42)-C(69)-C(70)	-119.4(6)
C(42)-C(69)-C(70)-C(71)	171.6(6)
C(69)-C(70)-C(71)-C(72)	-77.5(9)
C(70)-C(71)-C(72)-C(73)	175.7(6)
C(71)-C(72)-C(73)-C(74)	-76.9(10)
C(72)-C(73)-C(74)-C(75)	174.2(6)
C(73)-C(74)-C(75)-C(76)	-178.2(6)
C(74)-C(75)-C(76)-C(77)	-178.0(7)
C(61)-C(60)-C(78)-C(79)	91.1(5)
C(59)-C(60)-C(78)-C(79)	-87.0(5)
C(60)-C(78)-C(79)-C(80)	-175.3(4)
C(78)-C(79)-C(80)-C(81)	-175.3(5)
C(79)-C(80)-C(81)-C(82)	-179.8(5)

C(80)-C(81)-C(82)-C(83)	74.2(8)
C(81)-C(82)-C(83)-C(84)	-176.6(6)
C(82)-C(83)-C(84)-C(85)	176.0(8)
C(83)-C(84)-C(85)-C(86)	-176.5(8)

7. NMR spectra of all new compounds

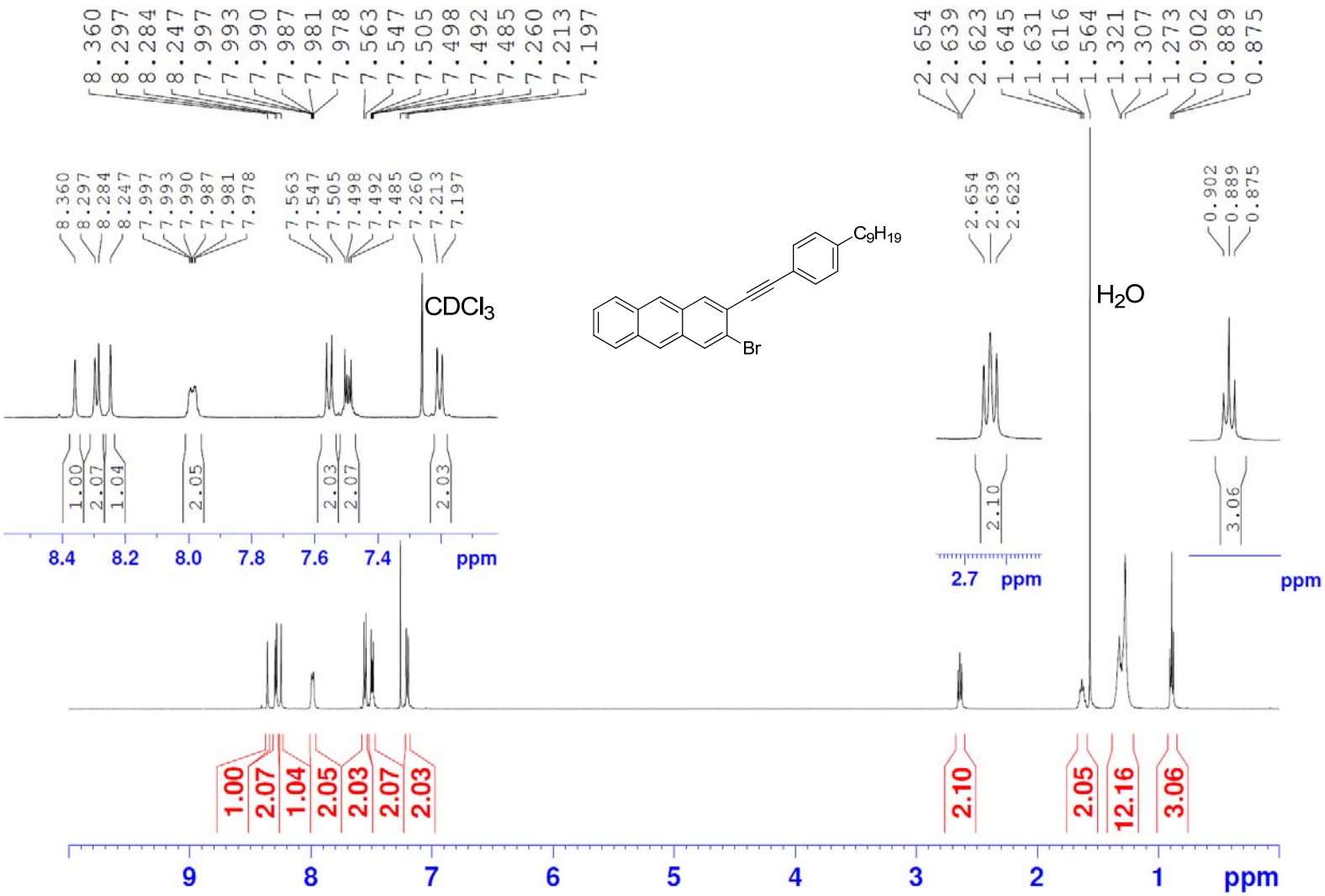


Fig. S10 ^{1}H NMR (500 MHz) spectrum of compound **2** in $CDCl_3$

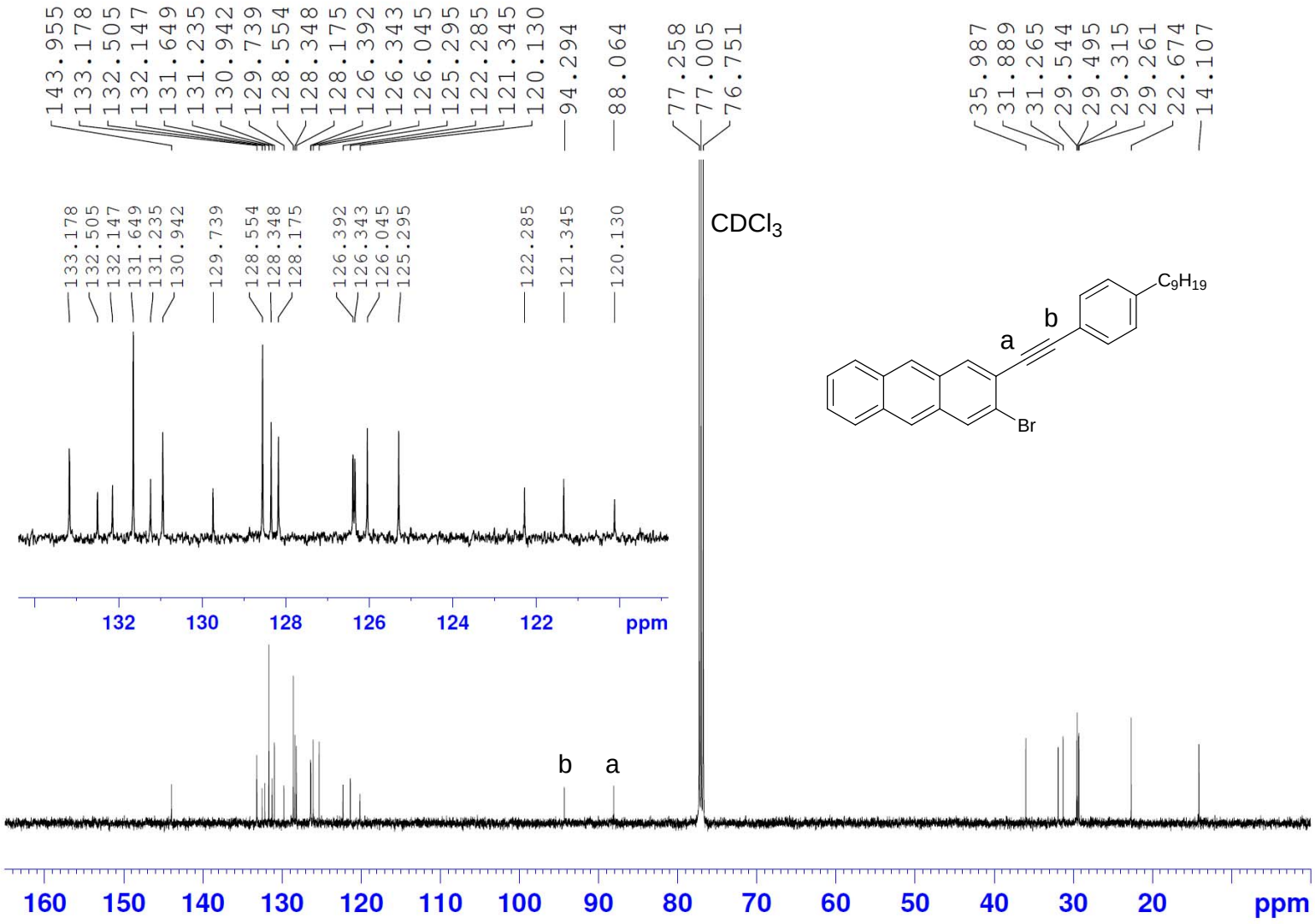


Fig. S11 ^{13}C NMR (125 MHz) spectrum of compound **2** in $CDCl_3$

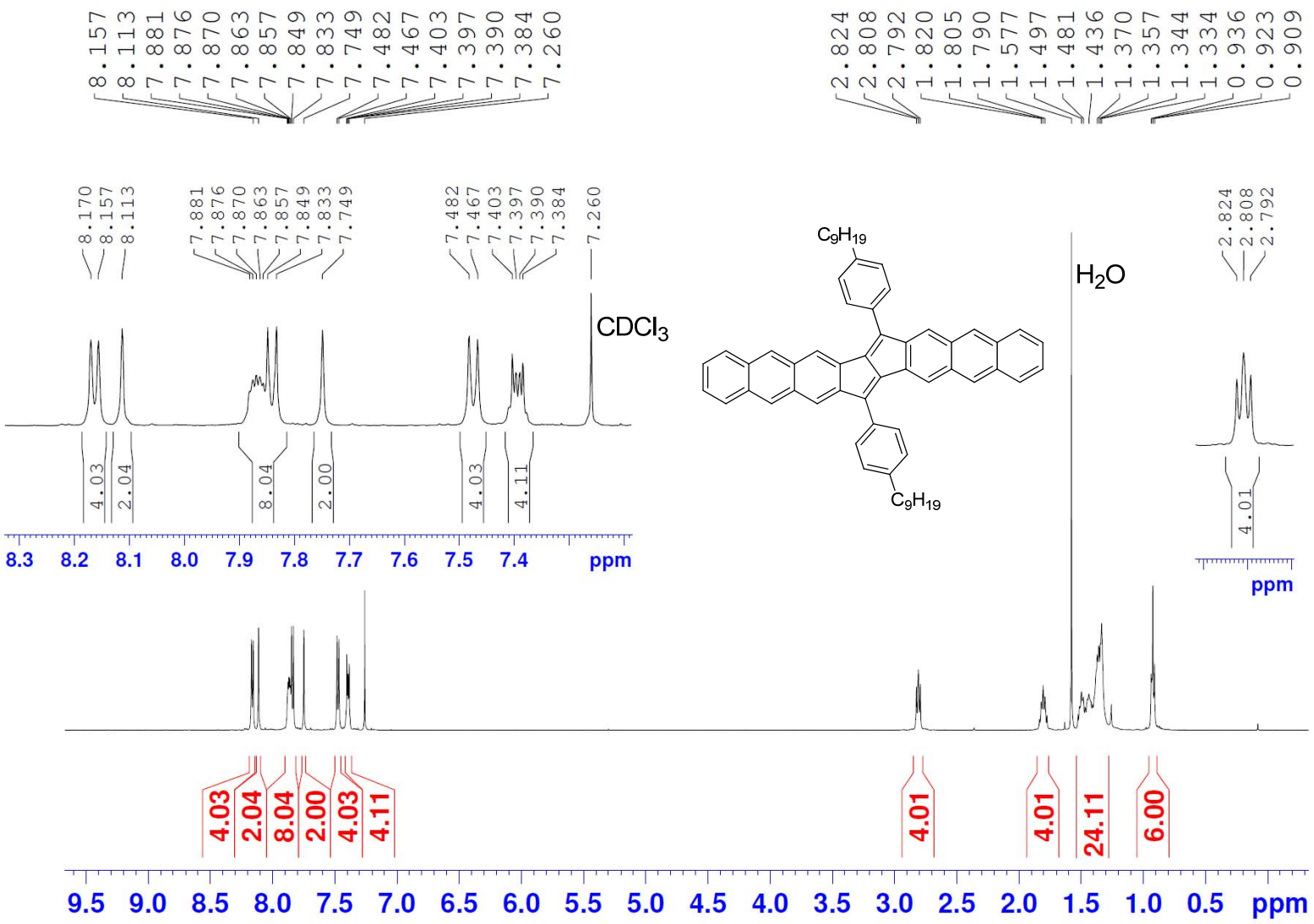


Fig. S12 ^{1}H NMR (500 MHz) spectrum of compound **DAP1** in $CDCl_3$

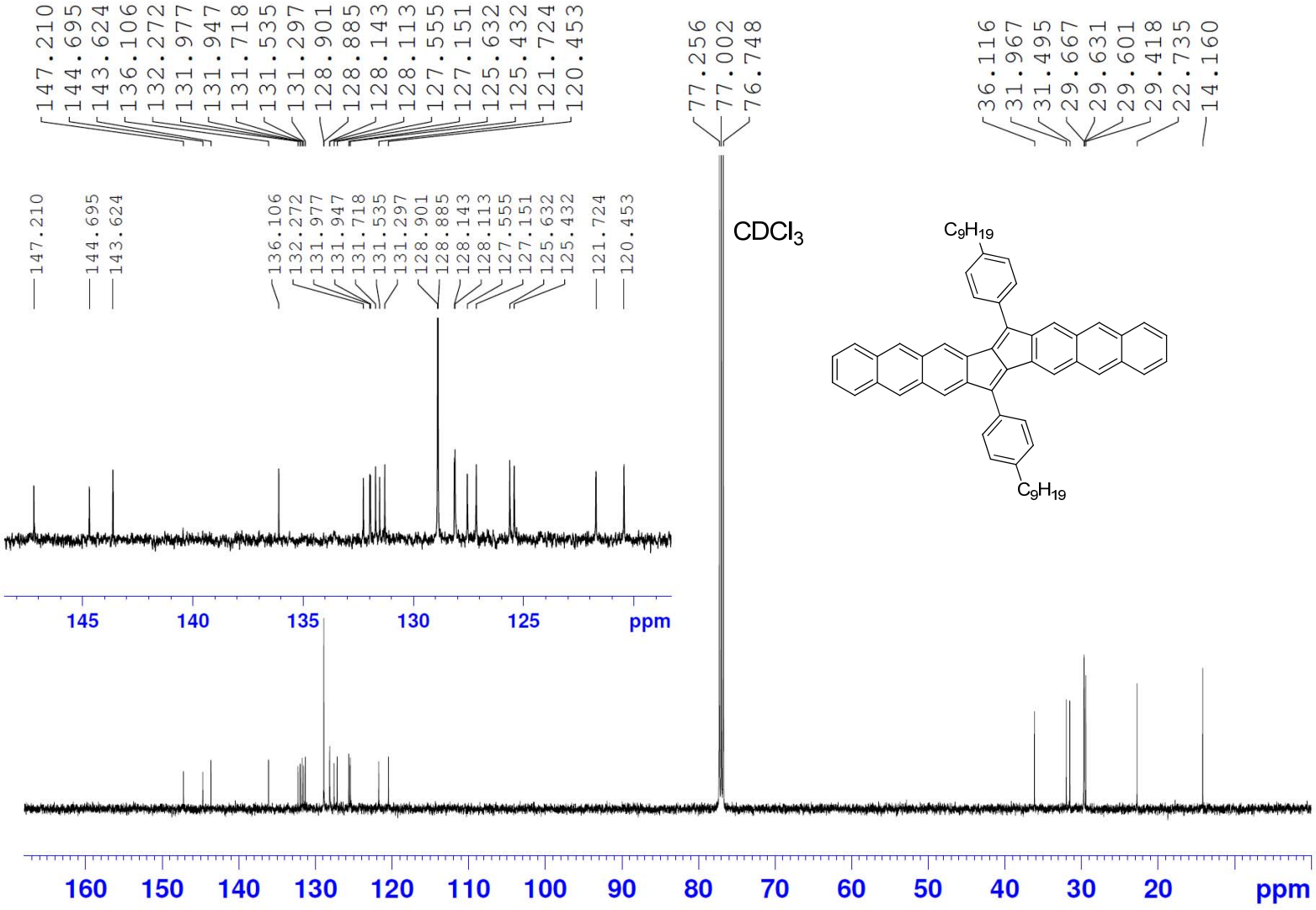


Fig. S13 ^{13}C NMR (125 MHz) spectrum of compound **DAP1** in $CDCl_3$

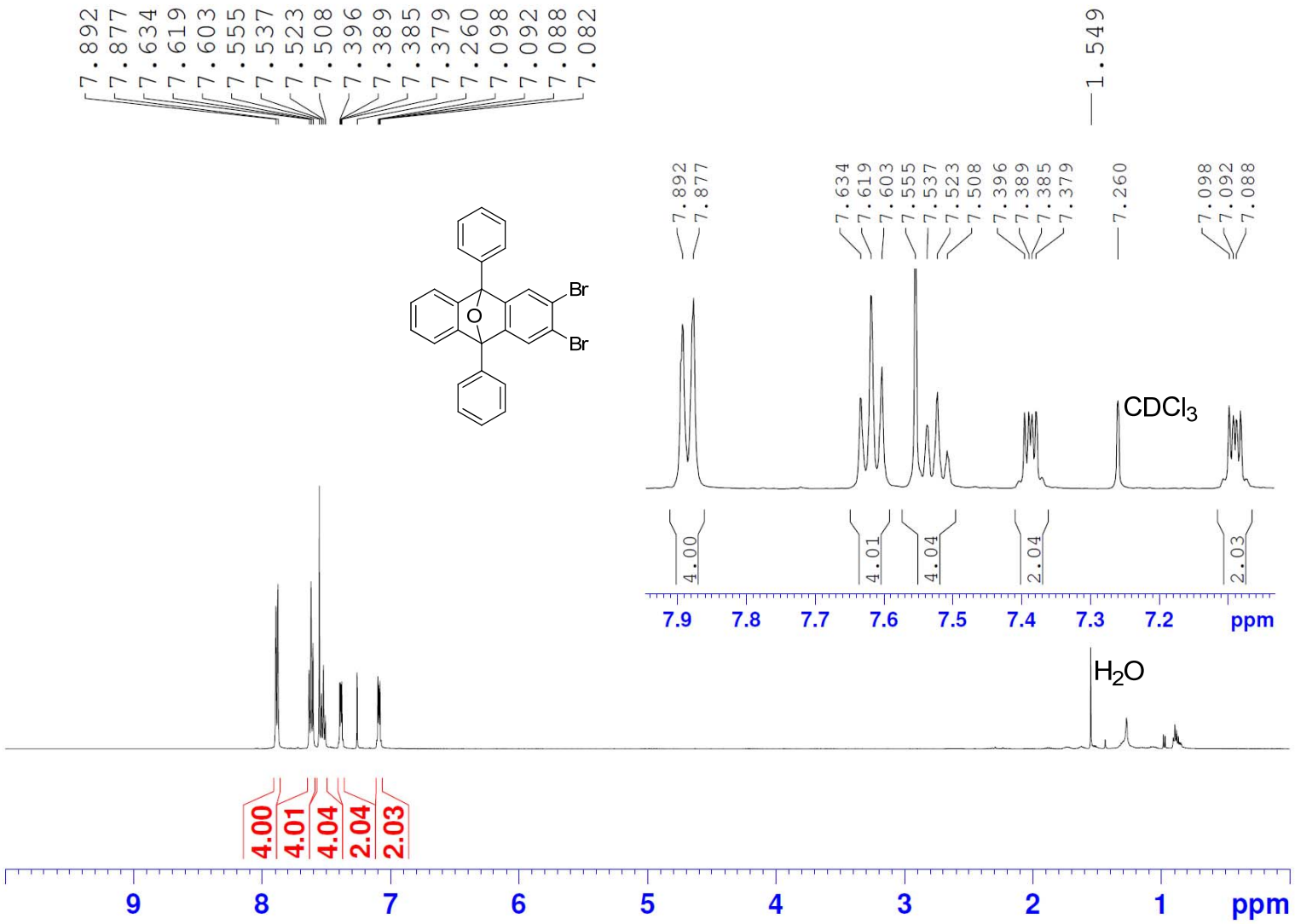


Fig. S14 ^{1}H NMR (500 MHz) spectrum of compound **4** in $CDCl_3$

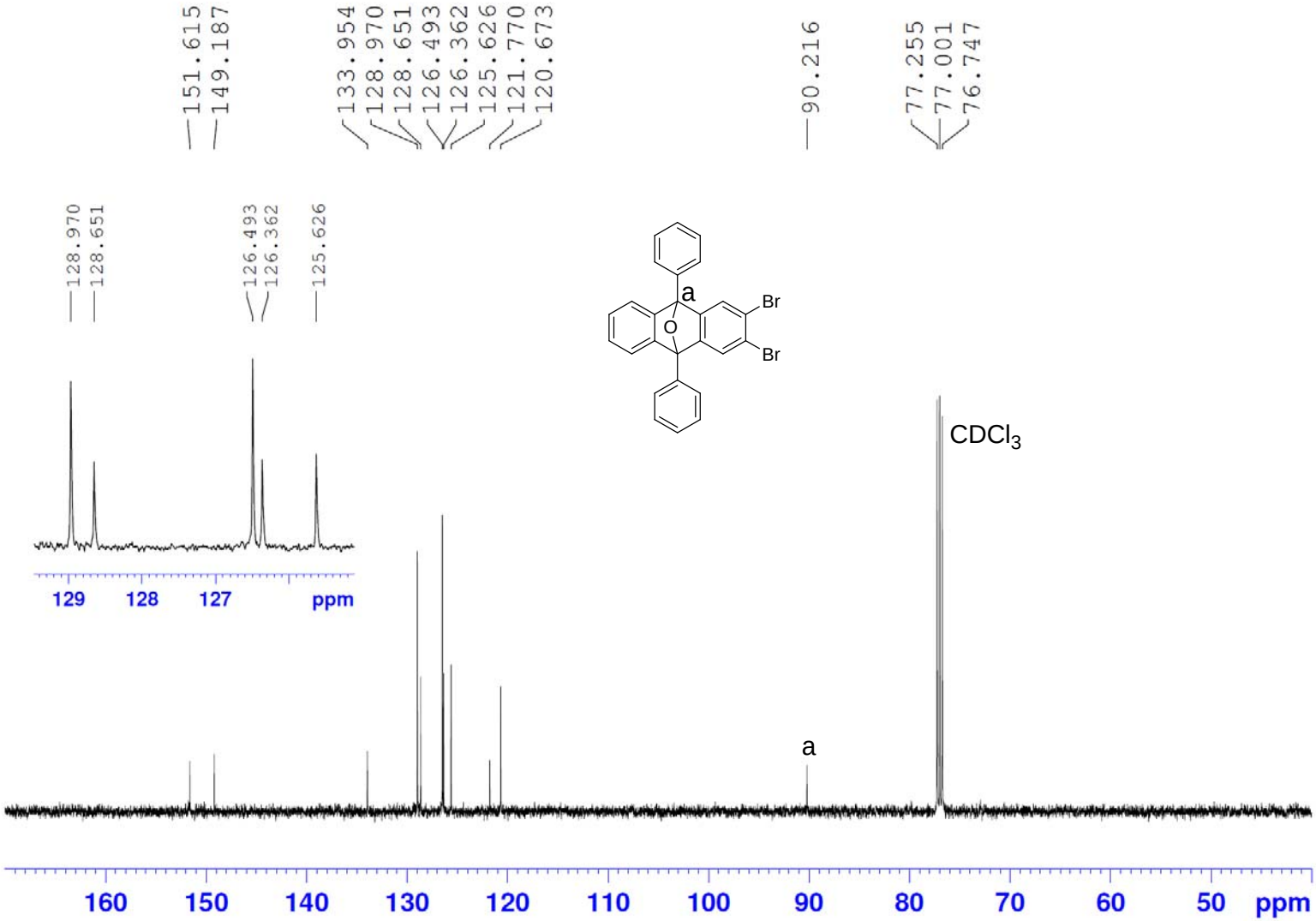


Fig. S15 ^{13}C NMR (125 MHz) spectrum of compound **4** in $CDCl_3$

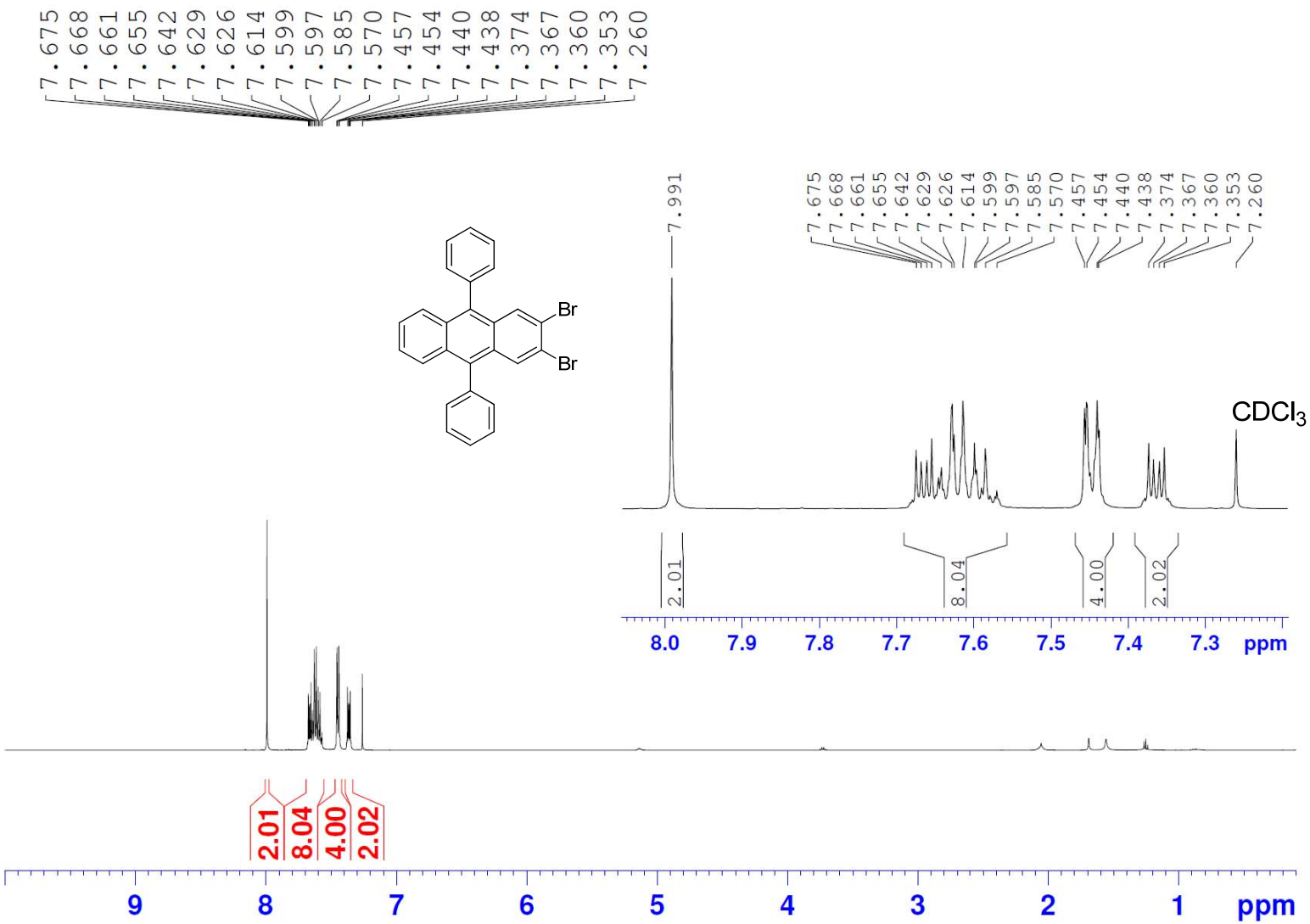


Fig. S16 ^{1}H NMR (500 MHz) spectrum of compound **5** in $CDCl_3$

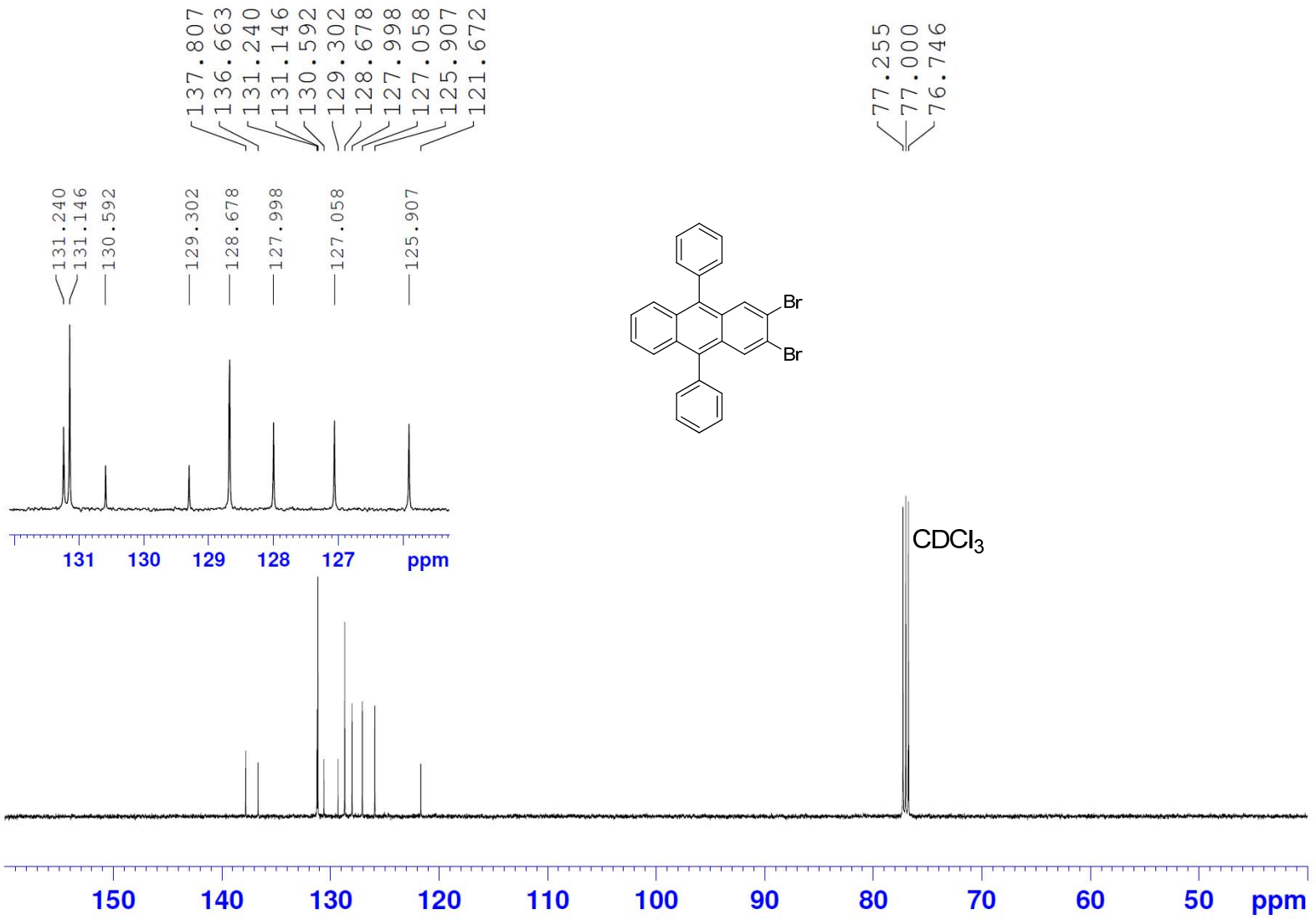


Fig. S17 ^{13}C NMR (125 MHz) spectrum of compound **5** in $CDCl_3$

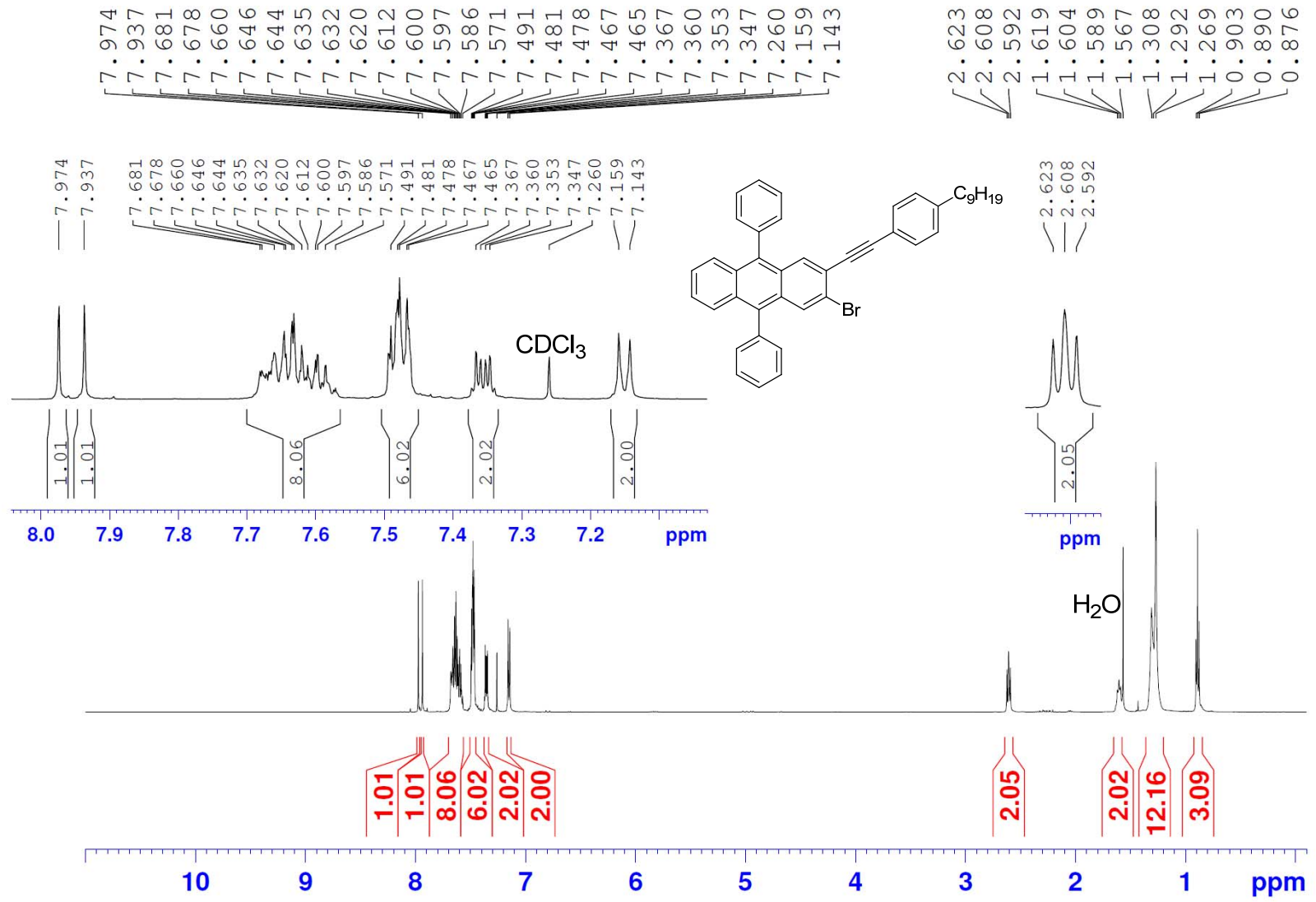


Fig. S18 ^{1}H NMR (500 MHz) spectrum of compound **6** in $CDCl_3$

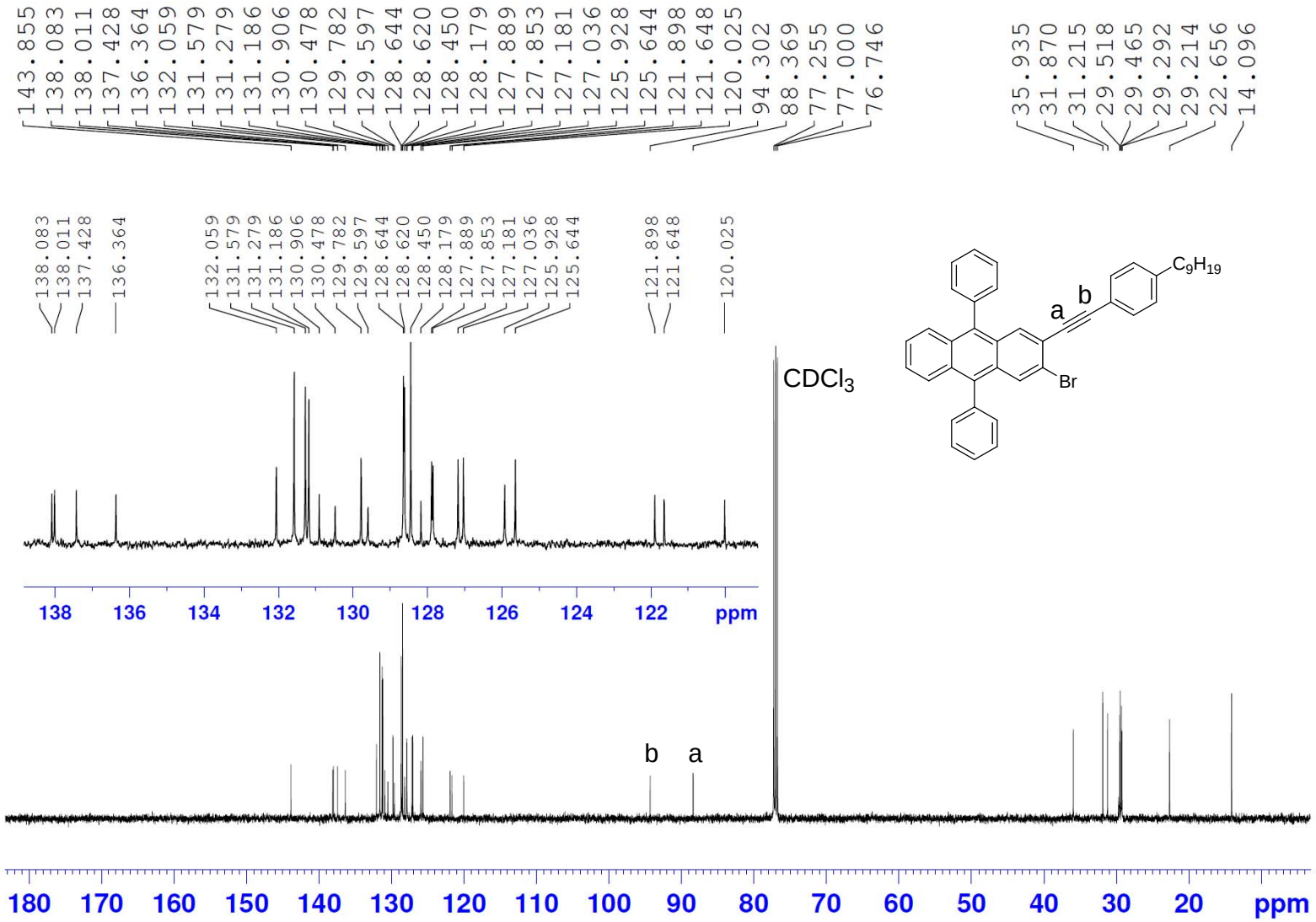


Fig. S19 ^{13}C NMR (125 MHz) spectrum of compound **6** in $CDCl_3$

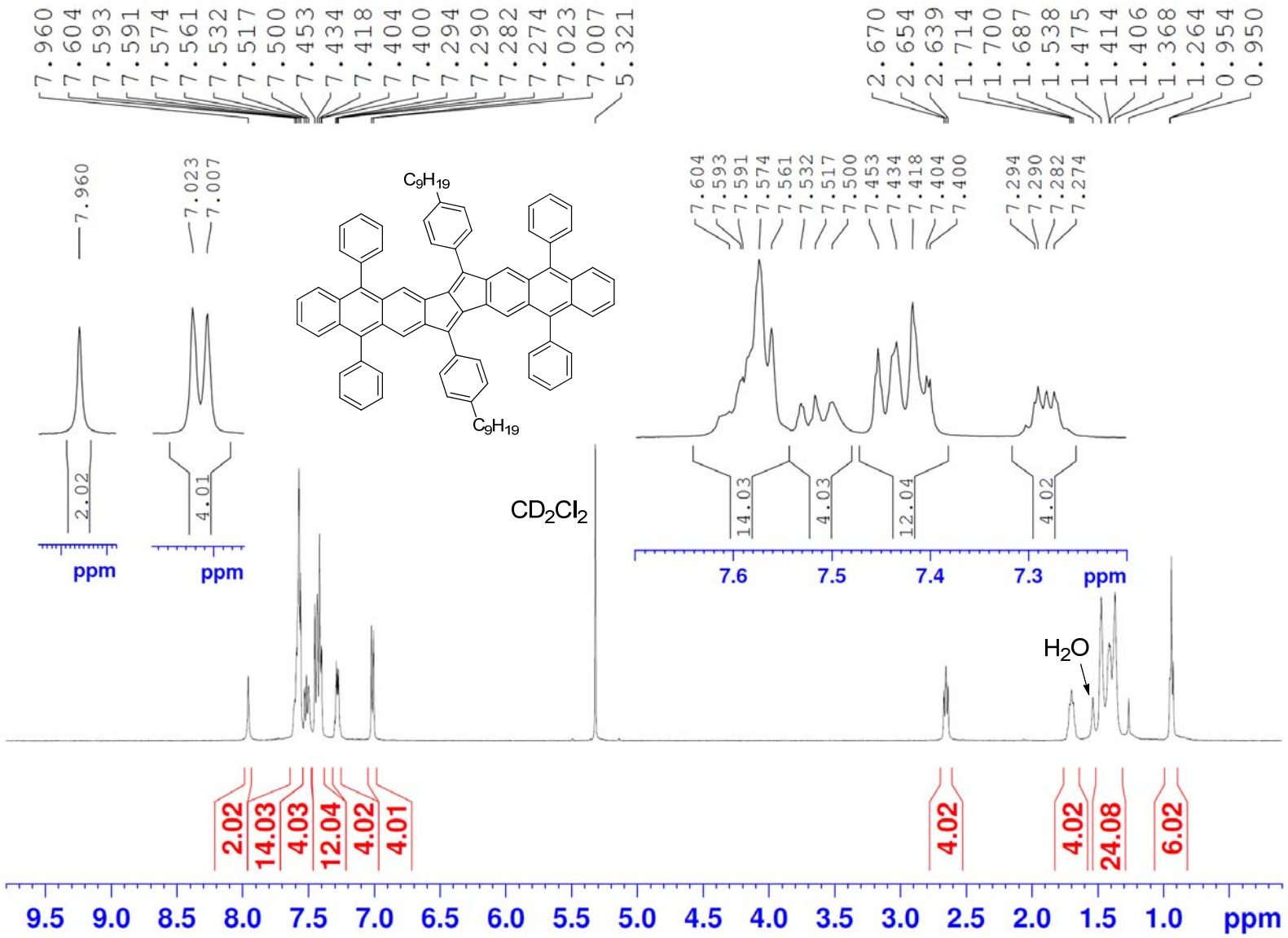


Fig. S20 ^{1}H NMR (500 MHz) spectrum of compound **DAP2** in CD_2Cl_2

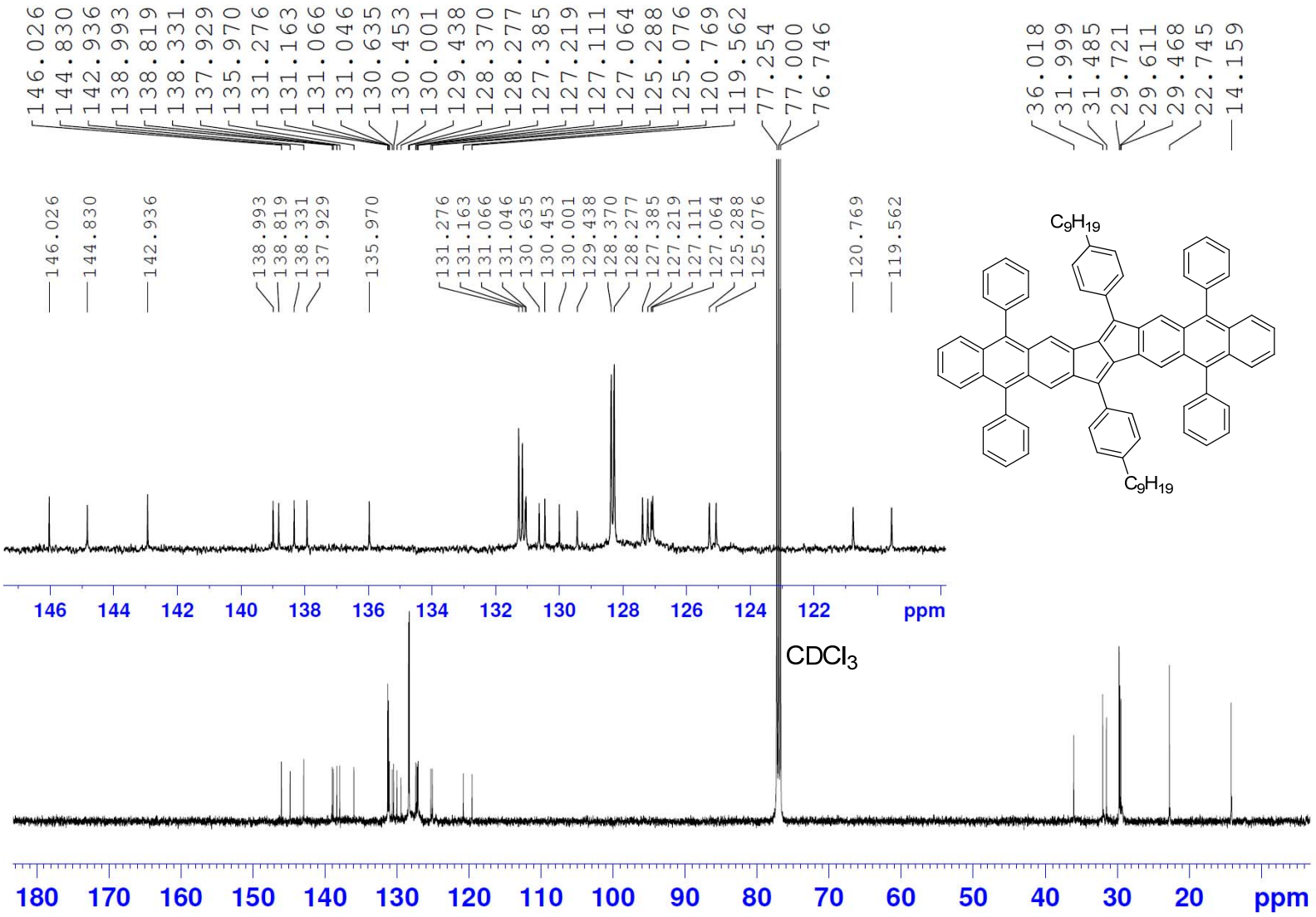


Fig. S21 ^{13}C NMR (125 MHz) spectrum of compound **DAP2** in $CDCl_3$