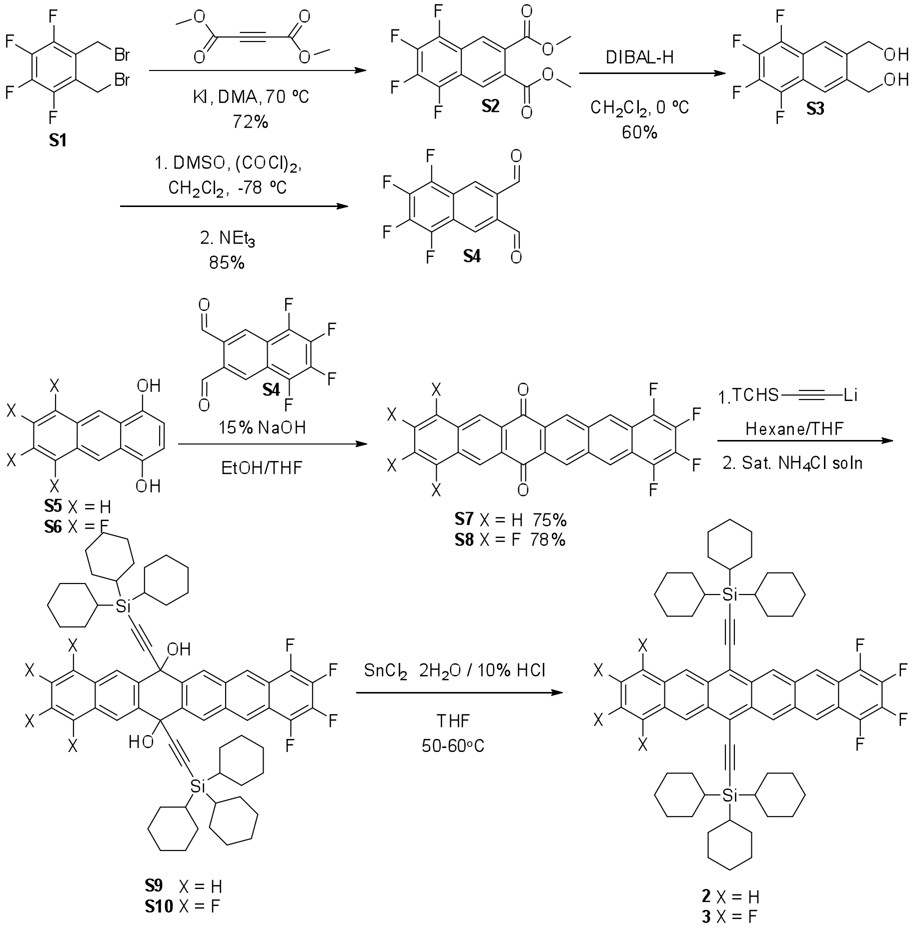
Supporting Information for:

Synthesis and Device Study of Stable Hexacene Derivatives

Balaji Purushothaman,[a,b] Mark J. Kendrick,[c] Daniel David,[d] Jeremy W. Ward,[d] Liyang Yu,[e] Natalie Stingelin,[e] Oana D. Jurchescu,[d] Oksana Ostroverkhova[c] and John E. Anthony*[a]

[a] Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055, USA.
[b] Current address: School of Chemistry, Bio21 Institute, The University of Melbourne, Parkville, VIC 3010, Australia
[c] Department of Physics, Oregon State University, Corvallis, OR 97331, USA.
[d] Department of Physics, Wake Forest University, Winston-Salem, NC 27109, USA.
[e] Department of Materials and Centre for Plastic Electronics, Imperial College London, London, SW7 2AZ, United Kingdom
anthony@uky.edu

Contents of Supplementary Data



Scheme S1: Synthesis of partially fluorinated trialkylsilylethynyl hexacenes

General synthesis: All solvents were purchased from Pharmco Aaper except anhydrous tetrahydrofuran which was purchased from Aldrich. n-Butyllithium (n-BuLi, 2.5M in Hexanes) and diisobutylaluminum hydride (1.0M in hexanes) were purchased from Aldrich. 1,4-dihdroxyanthracene[1], 5,6,7,8-tetrafluoro-1,4-anthraquinone[2] and 1,2-bis(bromomethyl)-3,4,5,6-tetrafluorobenzene[3] were prepared using previously reported literature method. All other reagents were purchased from Alfa Aesar. Chromatography was performed on silica gel (60 Å, 40-63 µm) purchased from Silicycle Inc. Thin layer chromatography was performed using Silica Gel HL TLC plates (w/UV254) purchased from Sorbent Technologies. UV-Vis absorbance spectra were recorded using Shimadzu UV-Vis Spectrophotometer model UV-2501PC. NMR spectra were recorded on Varian Inova 400MHz instrument. ^{1}H NMR chemical shifts are reported in ppm units and are referenced to the residual solvent peak. ^{19}F NMR chemical shifts are reported in ppm units relative to perfluorobenzene δ=-164.9 ppm. Mass spectra were recorded in either EI mode on JOEL JMS-700T MStation or MALDI mode on Bruker Daltonics Autoflex MALDI-TOFMS. Electrochemical analysis was performed using BAS CV-50W voltammetric analyzer performed on 0.1M Bu_4NPF_6 solution in dichloromethane with ferrocene as internal standard.

Dimethyl-5,6,7,8-tetrafluoronaphthalene-2,3-dicarboxylate (S2)

To a 350 ml sealed tube equipped with a magnetic stir bar were added 15 g(44.65 mmol) of 1,2-bis(bromomethyl)-3,4,5,6-tetrafluorobenzene[3] (**4**), 12.69 g (89.3 mmol) of dimethyl acetylene dicarboxylate (DMAD). 140 ml of degassed DMA was added followed by 16.56 g of KI. The reaction mixture was heated to 70˚C and allowed to stir for 24h. 22.5 g of sodium bisulfite was dissolved in 1400 ml of water in a 2000 ml Erlenmeyer flask. The hot reaction mixture was poured into the stirring sodium bisulfite solution and allowed to stir for 30 min. The precipitate was filtered, washed with plenty of water and air dried to give the crude product. Purification by silica gel chromatography using 1:1 hexanes/DCM gave the pure product in 69% (9.7 g) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 2H), 3.96 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -150.37 – -150.48 (m), -156.57 – -156.65 (m). MS (EI 70eV) *m/z* = 316 (33%, M^+). HRMS (LDI) m/z (M+ Calc'd: 316.0359, Observed: 316.0361)

2,3-dimethanol-5,6,7,8-tetrafluoronaphthalene (S3)

11.56 g (36.56 mmol) of dimethyl-5,6,7,8-tetrafluoronaphthalene-2,3-dicarboxylate (**5**) was added to a flame dried, N_2 cooled 500 ml RB flask. 100 ml of DCM was added and the flask was cooled to 0˚C using ice water bath. 154 ml of 1M solution of DIBAL-H in hexanes was added drop wise and the reaction mixture was allowed to stir overnight. The reaction mixture was quenched by adding a saturated solution of NH_4Cl with cooling. The precipitated aluminum salts are filtered off and the filtrate is concentrated to give the diol dissolved in solution. The precipitates were heated at reflux in 500 ml ethyl acetate for an hour and the precipitates were filtered off, washed with ethyl acetate and the filtrate was saved. The process was repeated couple of times and the filtrate were combined together and solvent was removed to give white solid (5.54 g, 58%).^{1}H NMR (400 MHz, DMSO) δ 8.06 (s, 2H), 4.69 (s, 4H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -153.48 – -153.57 (m), -163.42 – -163.52 (m). MS (EI 70eV) *m/z* = 242 (40%, M^+-18). HRMS (LDI) m/z (M+ Calc'd: 260.0460, Observed: 260.0454)

5,6,7,8-tetrafluoronaphthalene-2,3-dicarbaldehyde (S4)

To a flame dried 500 ml round bottom flask equipped with a dropping funnel was added 60 ml of DCM followed by 4.7 ml (53.23 mmol) of oxalyl chloride under nitrogen. The resulting solution was cooled to -78˚C using a dry ice bath. 7.6 ml (106.46 mmol) of DMSO dissolved in 15 ml of DCM was added dropwise to the stirring solution of oxalyl chloride in DCM. The solution was stirred for 15 minutes and 5.54 g (21.3 mmol) of 2,3-dimethanol-5,6,7,8-tetrafluoronaphthalene (**6**) dissolved in 10 ml of DMSO was added dropwise with stirrring. After addition is complete the reaction mixture was allowed to stir for 2h. 53 ml (378 mmol) of triethylamine was slowly added to the reaction mixture at -78˚C and was allowed to slowly warm up to room temperature overnight. The next day reaction mixture was poured into ice cold water, extracted into DCM (3x250 ml) and finally was washed with water (4x300 ml). The solvent was removed under reduced pressure to give crude dialdehyde which was further purified by silica gel chromatography using straight DCM to give pure dialdehyde as a light golden yellow solid (4.64 g, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.63 (s, 1H), 8.69 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -148.21 – -148.29 (m), -153.76 – -153.84 (m). MS (EI 70eV) *m/z* = 256 (37%, M^+). Elem. Anal.: Calcd for $C_{12}H_4F_4O_2$: C, 56.27; H, 1.57. Found: C, 56.23; H, 1.54.

5,6,7,8-tetrafluoro-1,4-dihydroxyanthracene (S6)

To a nitrogen purged solution of 1:1 dioxane (15 ml) and water (15 ml) was added 1g (3.57 mmol) of 5,6,7,8-tetrafluoro-1,4-anthraquinone[2]. 2.61g (14.99 mmol) of sodium dithionite ($Na_2S_2O_4$) was added and the reaction mixture was stirred overnight under nitrogen atmosphere. The reaction mixture was poured into nitrogen purged water and the precipitated solids were washed with nitrogen purged water and dried under vaccum to give 800 mg (80%) of greenish yellow solid that oxidized rapidly in air – the material was used immediately after preparation.

1,2,3,4-tetrafluorohexacene-7, 14-dione (S7)
To a 250 ml round bottom flask equipped with a stir bar were added 250 mg (0.98mmol) of 5,6,7,8-tetrafluoronaphthalene-2,3-dicarbaldehyde and 226 mg (1.07 mmol) of 1,4-dihydroxyanthracene[1]. The mixture was then dissolved in minimal amount of 1:1 ethanol/THF. Drops of 15% aqueous NaOH solution was added to the stirring mixture until there was any observable precipitate formation and the thick slurry was allowed to stir for 30 minutes. 50 ml of methanol was added to the reaction mixture and the precipitates were filtered through a Büchner funnel, washed with methanol followed by THF and finally with ether to give an impressively insoluble yellow solid. Yield – 315 mg, 75%. MS (EI, 70 eV) $m/z = 430$ (100%, M^+)

1,2,3,4,9,10,11,12-octafluorohexacene-6,15-dione (S8)
To a 250 ml round bottom flask equipped with a stir bar were added 227 mg (0.88 mmol) of 5,6,7,8-tetrafluoronaphthalene-2,3-dicarbaldehyde and 250 mg (0.88 mmol) of 5,6,7,8-tetrafluoro-1,4-dihydroxyanthracene. The mixture was then dissolved in minimal amount of 1:1 ethanol/THF. Drops of 15% aqueous NaOH solution was added to the stirring mixture until there was any observable precipitate formation and the thick slurry was allowed to stir for 30 minutes. 50 ml of methanol was added to the reaction mixture and the precipitates were filtered through a Büchner funnel, washed with methanol followed by THF and finally with ether to give an insoluble light brown solid. Yield – 350 mg, 78%. MS (EI, 70 eV) $m/z = 502$ (100%, M^+)

7,14-bis(tricyclohexylsilylethynyl)-1,2,3,4-tetrafluorohexacene (2)
To a flame dried 100 ml flask cooled under nitrogen was added 4.65 mmol of acetylene, followed by 5 ml of hexanes. The reaction mixture was then placed in an ice bath. 1.7 ml of n-BuLi (4.18 mmol, 2.5 M solution in hexanes) was added dropwise and the reaction mixture stirred at 0 °C for an hour. 13 ml of hexanes was added followed by 2 ml of anhydrous THF. 500 mg (1.16 mmol) of powdered 1,2,3,4-tetrafluorohexacene-7,14-dione was then added to the reaction mixture. After 3h another 2 ml of anhydrous THF was added and allowed to stir overnight. The reaction mixture was quenched with saturated NH_4Cl solution and extracted into ether. The combined ether layers were washed with water and dried over anhydrous $MgSO_4$. The excess acetylene was recovered from the crude product by elution through a pad of silica gel initially with hexanes. The crude diol was obtained as a mixture of *syn* and *anti* isomers by slowly increasing the ratio of hexanes:DCM to 7:3. To a 50 ml round bottom flask equipped with a magnetic stir bar were added 250 mg of crude diol, 20 ml of THF. Nitrogen gas was bubbled through the solution for 30 min. 2 ml of 10% aqueous HCl was added

followed by 3 g of $SnCl_2 \cdot 2H_2O$ and the reaction mixture was placed in an oil bath maintained at 50˚C. The reaction was followed by TLC by monitoring the disappearance of diol. Fluorinated hexacene precipitates as crystalline solid during the course of the reaction. The precipitated solids were filtered and washed with 50 ml of 1:1 THF/acetone mixture followed by plenty of methanol. Finally the solids were washed with acetone followed by 15 ml of hexanes to give crystalline green powder. Yield - 183 mg (76%). The hexacene was further purified by recrystallization in hexanes/DCM. ^1H NMR (400 MHz, $CDCl_3$) δ 9.65 (s, 2H), 9.25 (s, 2H), 8.79 (s, 2H), 7.94 (dd, *J* = 6.6, 3.2 Hz, 2H), 7.42 (dd, *J* = 6.7, 3.0 Hz, 2H), 2.13 (d, *J* = 12.9 Hz, 12H), 1.96 – 1.79 (m, 18H), 1.72 – 1.58 (m, 12H), 1.48 – 1.31 (m, 18H), 1.25 (tt, *J* = 12.8, 2.8 Hz, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -153.93 – -154.06 (m), -162.04 – -162.13 (m). MS (LDI) *m/z* = 1000.54 (100%, M^+). Elem. Anal.: Calcd for $C_{66}H_{76}F_4Si_2$: C, 79.15; H, 7.65. Found: C, 79.11; H, 7.69.

Note: The conversion of the intermediate diol to final hexacene was done in the dark. Solvents were degassed with nitrogen prior to use for recrystallization.

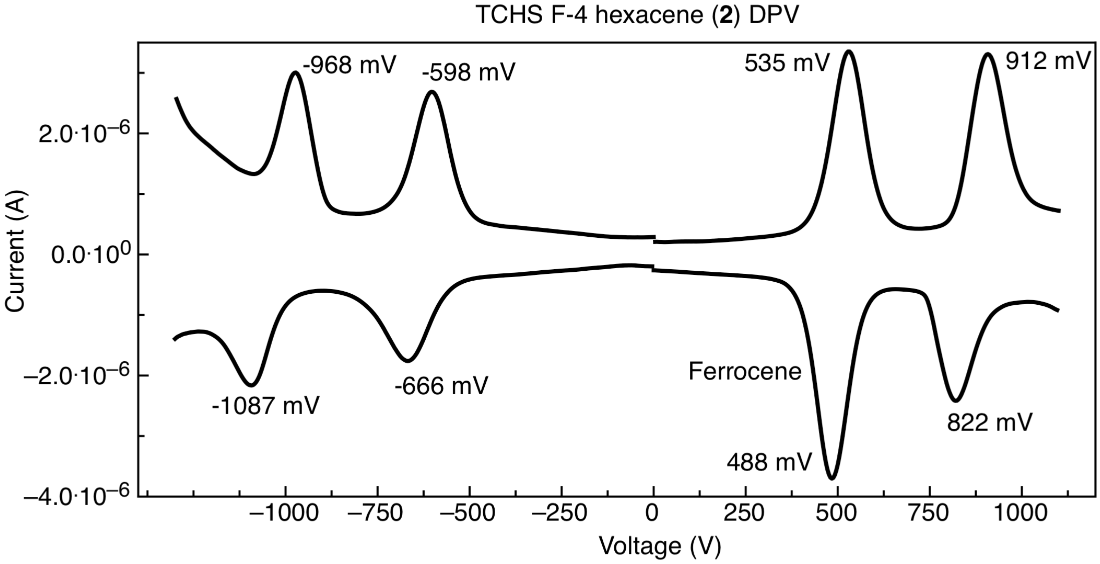
6,15-bis(tricyclohexylsilylethynyl)-1,2,3,4,9,10,11,12-octafluorohexacene (3)

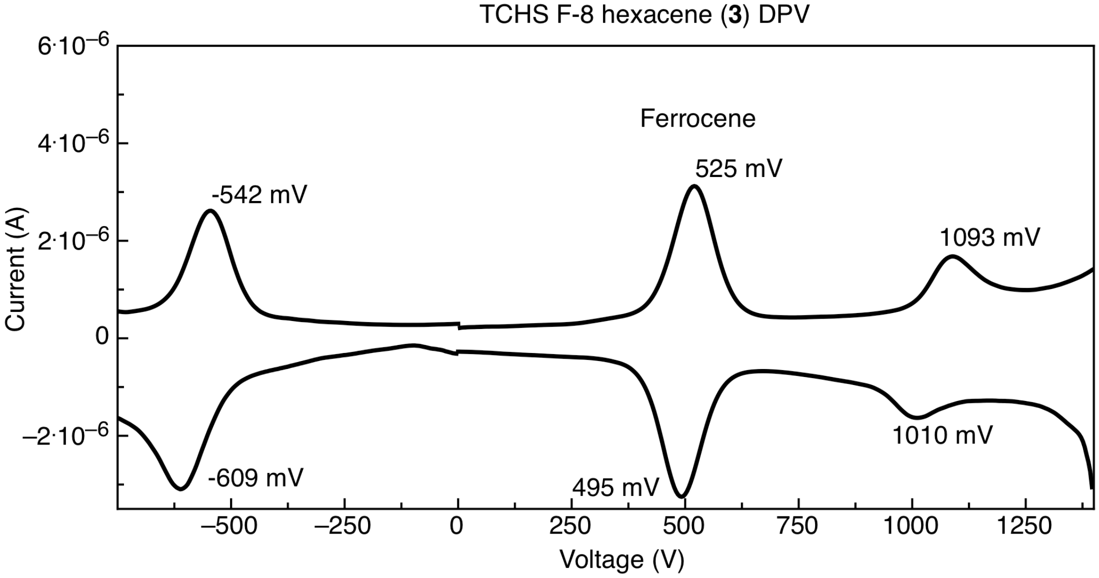
To a flame dried 100 ml flask cooled under nitrogen was added 7.96 mmol of acetylene, followed by 5 ml of hexanes. The reaction mixture was then placed in an ice bath. 2.9 ml of n-BuLi (7.25 mmol, 2.5 M solution in hexanes) was added dropwise and the reaction mixture stirred at 0 °C for an hour. 13 ml of hexanes was added followed by 2 ml of anhydrous THF. 1 g (1.99 mmol) of pulverized 1,2,3,4,9,10,11,12-octafluorohexacene-6,15-dione was then added to the reaction mixture. After 3 h another 2 ml of anhydrous THF was added and allowed to stir overnight. The reaction mixture was quenched with saturated NH_4Cl solution and extracted into ether. The combined ether layers were washed with water and dried over anhydrous $MgSO_4$. The excess acetylene was recovered from the crude product by elution through a pad of silica gel initially with hexanes. The crude diol was obtained as a mixture of *syn* and *anti* isomers by slowly increasing the ratio of hexanes:DCM to 7:3. To a 50 ml round bottom flask equipped with a magnetic stir bar were added 250 mg of crude diol, 20 ml of THF. Nitrogen gas was bubbled through the solution for 30 min. 2 ml of 10% aqueous HCl was added followed by 3 g of $SnCl_2 \cdot 2H_2O$ and the reaction mixture was placed in an oil bath maintained at 60˚C. The reaction was followed by TLC by monitoring the disappearance of diol. Fluorinated hexacene precipitates as crystalline solid during the course of the reaction. The precipitated solids were filtered and washed with 50 ml of 1:1 THF/acetone mixture followed by plenty of methanol. Finally the solids were washed with acetone followed by 15 ml of hexanes to give crystalline green powder. Yield - 169 mg (70%). The hexacene was further purified by recrystallization in hexanes/toluene. ^1H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 2H), 9.48 (s, 2H), 2.10 (d, *J* = 12.6 Hz, 12H), 1.93 – 1.8 (m, 18H), 1.7 – 1.56 (m, 12H), 1.46 – 1.31 (m, 18H), 1.24 (tt, *J* = 12.8, 2.9 Hz, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -153.25 – -153.35 (m), -153.66 – -153.77 (m), -160.45 – -160.55 (m), -161.18 – -161.32 (m). MS (LDI) *m/z* = 1072.5 (100%, M^+). Elem. Anal.: Calcd for $C_{66}H_{72}F_8Si_2 \cdot 0.25C_7H_8$: C, 74.21; H, 6.80. Found: C, 74.25; H, 6.76.

Note: The conversion of the intermediate diol to final hexacene was done in the dark. Solvents were degassed with nitrogen prior to use for recrystallization.

Experimental details for Differential Pulse Voltammetry (DPV):

Electrochemical analysis were performed on hexacenes **2&3** using BAS CV-50W voltammetric analyzer in a three electrode cell configuration consisting of silver wire as a pseudo reference electrode, platinum button as the working electrode and platinum wire as counter electrode. All experiments were done in 0.1M solution of tetrabutylammonium hexafluorophosphate in dichloromethane. Oxidation and reduction potential were calibrated with respect to ferrocene/ferrocenium redox couple. In order to obtain reduction potential, the solution was purged with nitrogen for 10 minutes and the analysis were performed under nitrogen. A scan rate of 20 mV/s was used for DPV measurements. Oxidation and reduction potentials were then converted to vacuum energy levels according to reported literature methods[4,5]. DPV data, including raw peak values, are shown below.





Optical and electronic characterization methods

For optical absorption and photoluminescent (PL) emission measurements in solution, compounds **1-3** were dissolved at 10^{-4} M concentrations in de-oxygenated toluene. Absorption of light from a halogen lamp (LS-1, Ocean Optics) in samples was measured using an Ocean Optics USB2000 spectrometer. For PL measurements, the custom made experimental set up was used.[6] The samples were excited with a 633 nm HeNe laser, and the PL emission was measured using a calibrated Ocean Optics USB2000 spectrometer.

For dark and photocurrent measurements, solutions were prepared at concentrations ranging between 10^{-2} M and 10^{-3} M. Films were drop-cast onto glass substrates with photolithographically deposited Cr/Au interdigitated electrode pairs (either 5 nm/50 nm or 1 nm/50 nm thick). Each interdigitated electrode pair consisted of 10 pairs of 0.85 mm long and 25 μm wide fingers, with a 25 μm gap between the fingers of opposing electrodes. Samples were mounted in a custom built fixture and photoexcited from the substrate side with ~190 mW/cm^2 of 765 nm cw laser light from a Ti:Sapphire source (Kapteyn-Murnane Labs). For both dark and photocurrent measurements, voltage was applied to the sample and current measured using a Keithley 237 source/measure unit.

Photodegradation testing

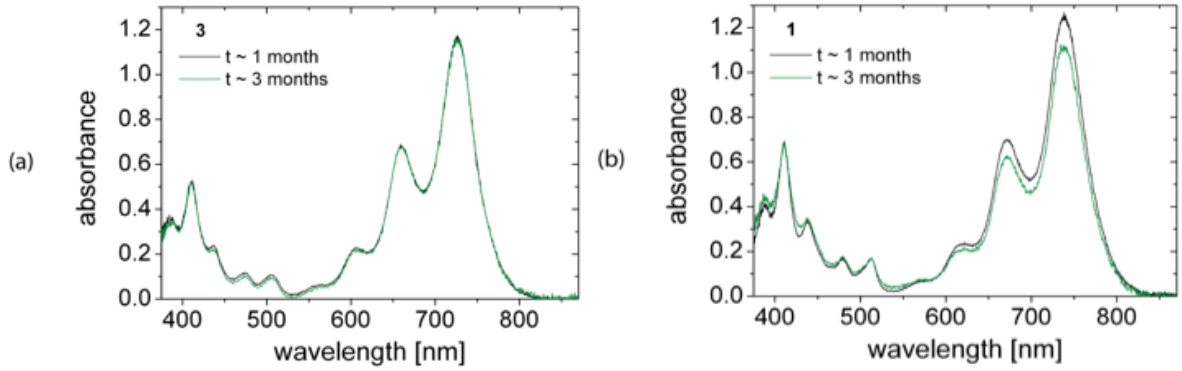


Figure S1: Optical absorption spectra of (a) **3** and (b) **1** in toluene. Spectra were measured in freshly made solutions of powders stored for ~1 month and ~3 months after synthesis. Compounds were stored in the dark at room temperature in air between measurements. The addition of fluorine to the acene backbone increased the stability, such that the stability of **3** > **2** > **1.** In particular, no powder degradation was observed in compound **3**.

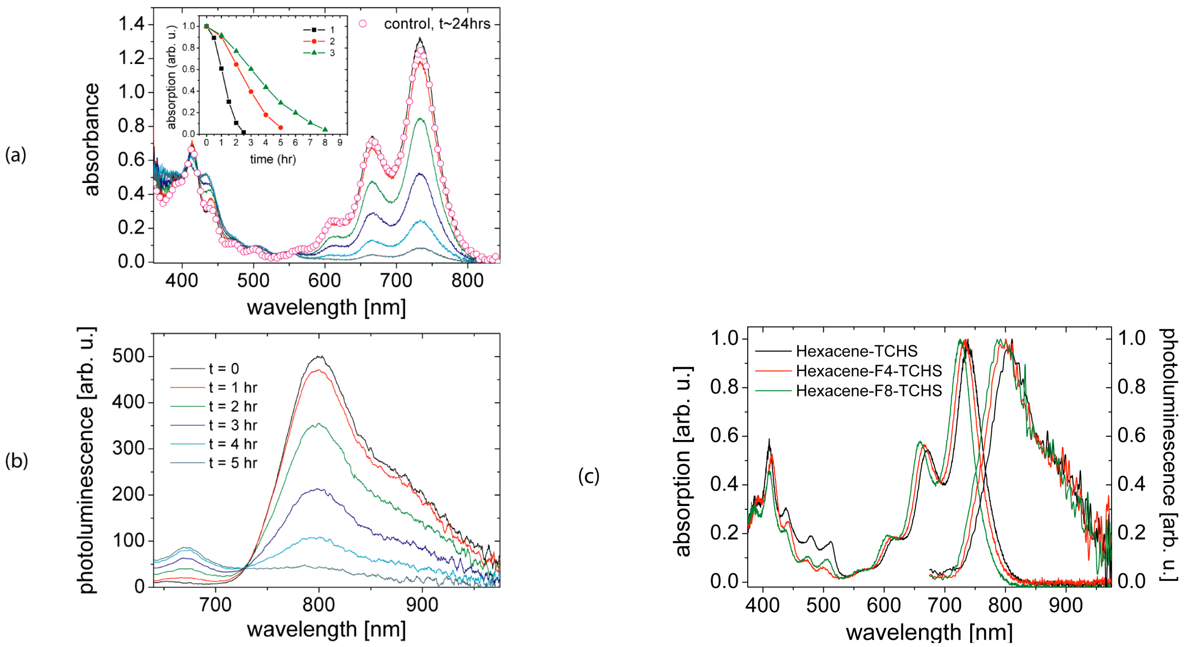


Figure S2: (a) Absorption and (b) PL spectra of **2** in toluene. Measurements were taken at one hour intervals with the solution exposed to fume hood lighting, in air, between measurements to monitor photostability. As a control, absorption measurements were taken on a similar solution that was stored in air in the dark. The control solution showed almost no change in absorption after t ~ 24 hrs. Inset of (a): Integrated absorption spectra (640nm < λ < 824nm) as a function of light exposure time for **1-3** (lines connecting data points added for clarity). The addition of fluorine to the acene backbone increased the photostability in solution, with compound **3** being the most stable. (c) Absorption and emission spectra of pristine **1** – **3** in toluene.

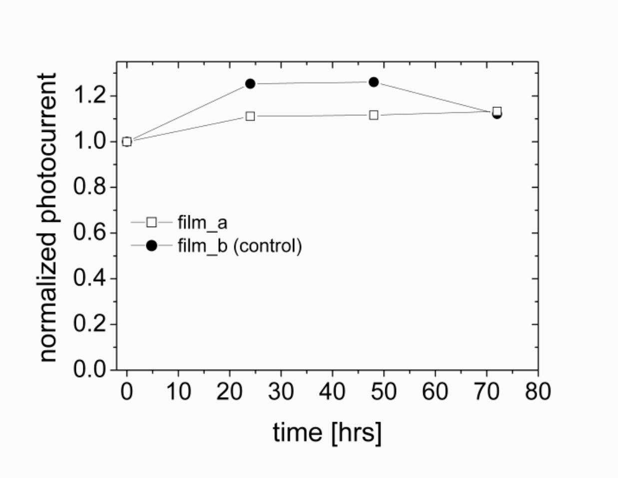


Figure S3: Photocurrent measured in thin films of **2** under 765 nm photoexcitation at 150 V, normalized at its value at t = 0 (freshly prepared film). Measurements were taken at ~24 hr intervals after film preparation to monitor film photostability. Between measurements, both films were stored in air. Film_a was stored under fume hood lights and film_b was stored in the dark, as a control. Films were considerably more robust with respect to degradation as compared to solutions. In particular, no photocurrent degradation was observed even after 72 hrs of illumination in thin films of compound **2**.

SCLC effective mobilities

In the case of the planar electrode geometry used in our experiments, the current flows along a thin layer of unknown thickness, and the current density (*j*) is expressed in units of A/m (as opposed to A/m^2 for the "sandwich" electrode geometry) (Fig.2(b)). Although there is no analytical solution for the *j*-*V* relationship in a film of finite thickness, such as our films, Eqs.(1) and (2) provide solutions for the limiting cases of an infinitely thin film and infinite half space, respectively.[7]

$$\text{Thin-film:} \qquad j = \frac{2\mu\varepsilon\varepsilon_o}{\pi}\frac{V^2}{L^2} \qquad (1)$$

$$\text{Half space:} \qquad j = 0.28\mu\varepsilon\varepsilon_o\frac{V^2}{L^2} \qquad (2)$$

Here *L* is the gap between the electrodes, ε is the relative dielectric constant of the film, ε_o is the dielectric permittivity of vacuum, and *V* is the voltage applied to the sample. In our calculations we assumed a value of ε =3.5 for all films. The values for the effective charge carrier mobilities (μ) calculated in films of compounds **1-3** in the thin-film and half-space approximations are presented in Table S1. These define lower and higher bounds, respectively, of the "true" effective mobility values.

	μ, thin-film [cm^2/(V s)]	μ, half-space [cm^2/(V s)]
1	$1.7\text{x}10^{-4}$	$3.8\text{x}10^{-4}$
2	$8.4\text{x}10^{-3}$	$1.9\text{x}10^{-2}$
3	$6.9\text{x}10^{-4}$	$1.6\text{x}10^{-3}$

Table S1: Thin-film and half-space effective charge carrier mobility for **1-3**.

Field-Effect Transistor Measurements – compound 2

Heavily doped Si was used as the gate electrode and 300 nm of thermally grown SiO_2 at its surface served as gate dielectric. Ti/Au source and drain contacts were deposited by e-beam evaporation. The contacts were chemically modified by using pentafluorobenzene thiol (PFBT), a self-assembly monolayer which was reported to improve the performance of halogenated functionalized acenes[8]. To perform this step, clean substrates were immersed in a 80 mM solution in room-temperature high purity Ethanol. After 30 minutes treatment, they were rinsed and sonicated in Ethanol for 5 minutes. The organic semiconductor (green in Fig. 3a) was deposited by drop-cast from a dilute Chlorobenzene solution (0.2 wt%), and the sample was placed in a Petri dish, with additional Chlorobenzene. The entire system was covered with a glass cover, and placed in dark. We allowed two-three days for solvent evaporation before we characterized the devices electrically. In Fig.3c (main text), we show the evolution of the drain current (I_D) with the gate-source voltage (V_{GS}) in the saturation regime (drain-source voltage V_{DS} = - 40V) for the device in Fig. 3b. The slope (red) of the curve corresponding to the left axis, plotted with open circles ($\sqrt{I_D}$ versus V_{GS}) was used to estimate the mobility, which for this devices was μ = 0.1 cm^2/Vs. For mobility calculations, only the area of the crystal present in the transistor channel was considered. Then for the device presented in Fig. 3, the channel length was L = 100μm, and channel width was W = 300μm. On the right axis of Fig. 3c we plot in blue the $log(I_D)$ to determine the on/off current ratio, which for this device was 10^5.

Field-Effect Transistor Measurements – compound 3

Field-effect transistors (FETs) of **3** and its blend with high-density polyethylene (HDPE; weight-average molecular weight M_w = 13.6 kg/mol) were fabricated by drop casting solutions in xylene (1 wt% total solid content) onto pre-patterned silicon substrates comprising 230 ± 10 nm thermally oxidised SiO_2 as gate dielectric and patterned 30 nm thick Au S/D electrodes (interdigitated fingers, channel length = 10 μm, channel width = 1 mm) with an indium tin oxide (ITO) adhesion layer. The SiO_2 and Au surfaces were treated with, respectively, octadecyltrichlorosilane (OTS) and perfluorodecanethiol (PFDT). The solution and substrate were kept at 110 °C during the casting. FET fabrication and characterisation were carried out in the same glove box and exposure to light was limited.

Crystallographic analysis of 3

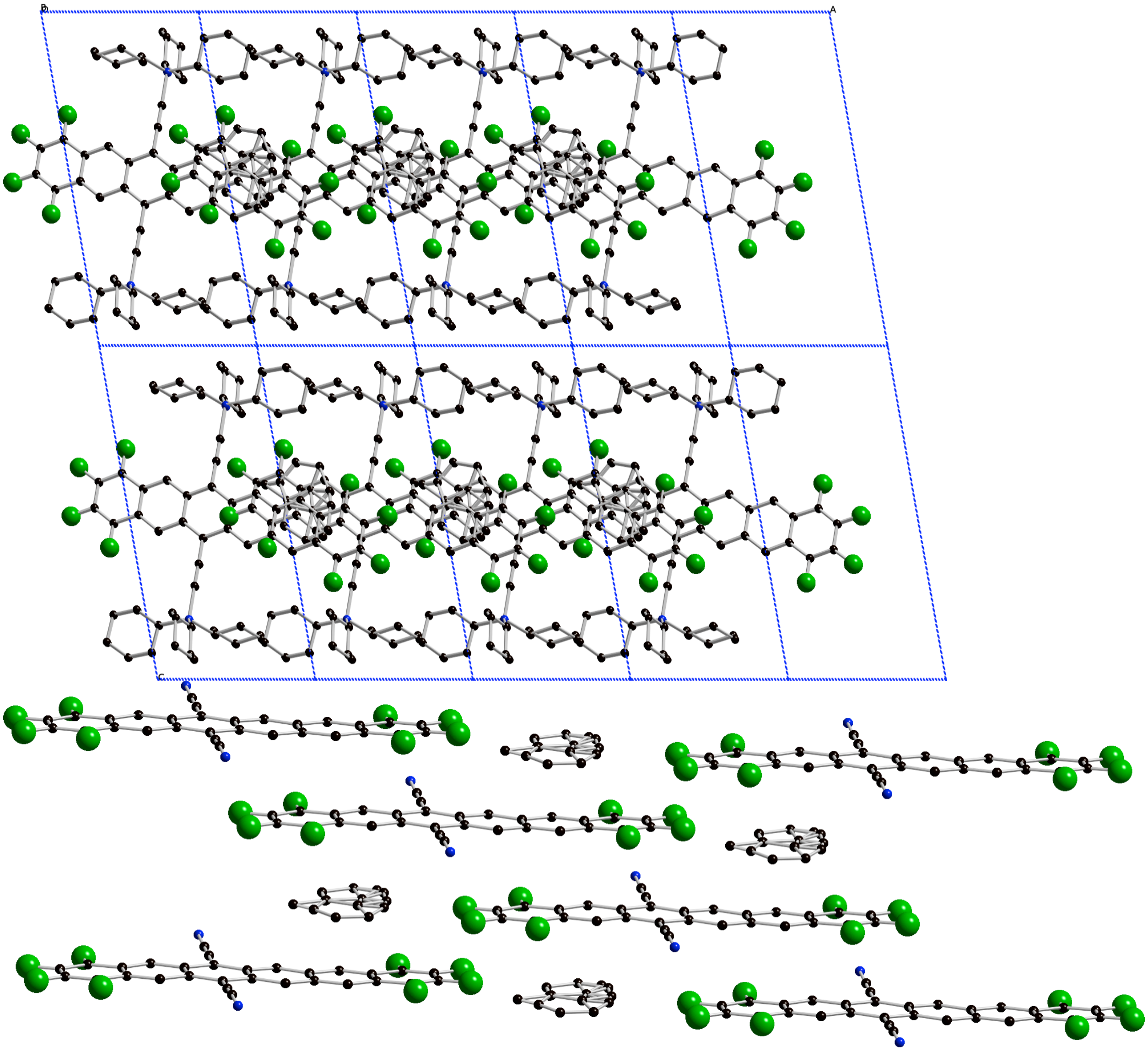


Figure S4: Crystal packing of hexacene **3**, showing layered (top) two-dimensional π-stacking (bottom) along with incorporated solvent.

X-ray data were collected on a Bruker-Nonius X8 Proteum CCD diffractometer using CuK(alpha) radiation. The structures were solved using SHELXS and refined using SHELXL from the SHELX-97 (Sheldrick, 2008) program package. Molecular fragment editing was performed using the XP program of SHELXTL (Sheldrick, 2008). All non-hydrogen atoms were refined with anisotropic displacement parameters. H atoms were found in difference Fourier maps and subsequently placed in idealized positions within constrained distances of the attached atom.

To ensure satisfactory refinement of the disordered parts of the structure, a combination of constraints and restraints were needed. The constraints (SHELXL97 command

EADP) was used to make the coordinates and/or displacement parameters of closely proximate or pseudo-centrosymmetrically related atoms equal. The restraints (SHELXL97 commands SAME, DELU, FLAT) were used to ensure similar geometries and displacement parameters of closely proximate chemically similar groups, and to ensure reasonable flatness for the minor component toluene.

The largest difference map peaks are consistent with a type of disorder in which the whole molecule is flipped to superimpose the long and short ends of the acene ring system, but without shifting the tricyclohexyl-silylethynyl groups. Indeed, this sort of disorder had been anticipated from the outset, as the first model of the structure was obtained using space group P=\1. The overall fit for the P1 model is vastly superior to the centrosymmetric model (which could only have been an average structure in any case). Inversion twinning was tested, but it does not seem to have been a problem with this particular crystal. Data were obtained from a second flat plate-shaped crystal (with ostensibly the same unit cell) using CuK\a radiation, and that one does appear to have been an inversion twin. Whether the difference was caused (at least in part) by the difference in wavelength is not known.

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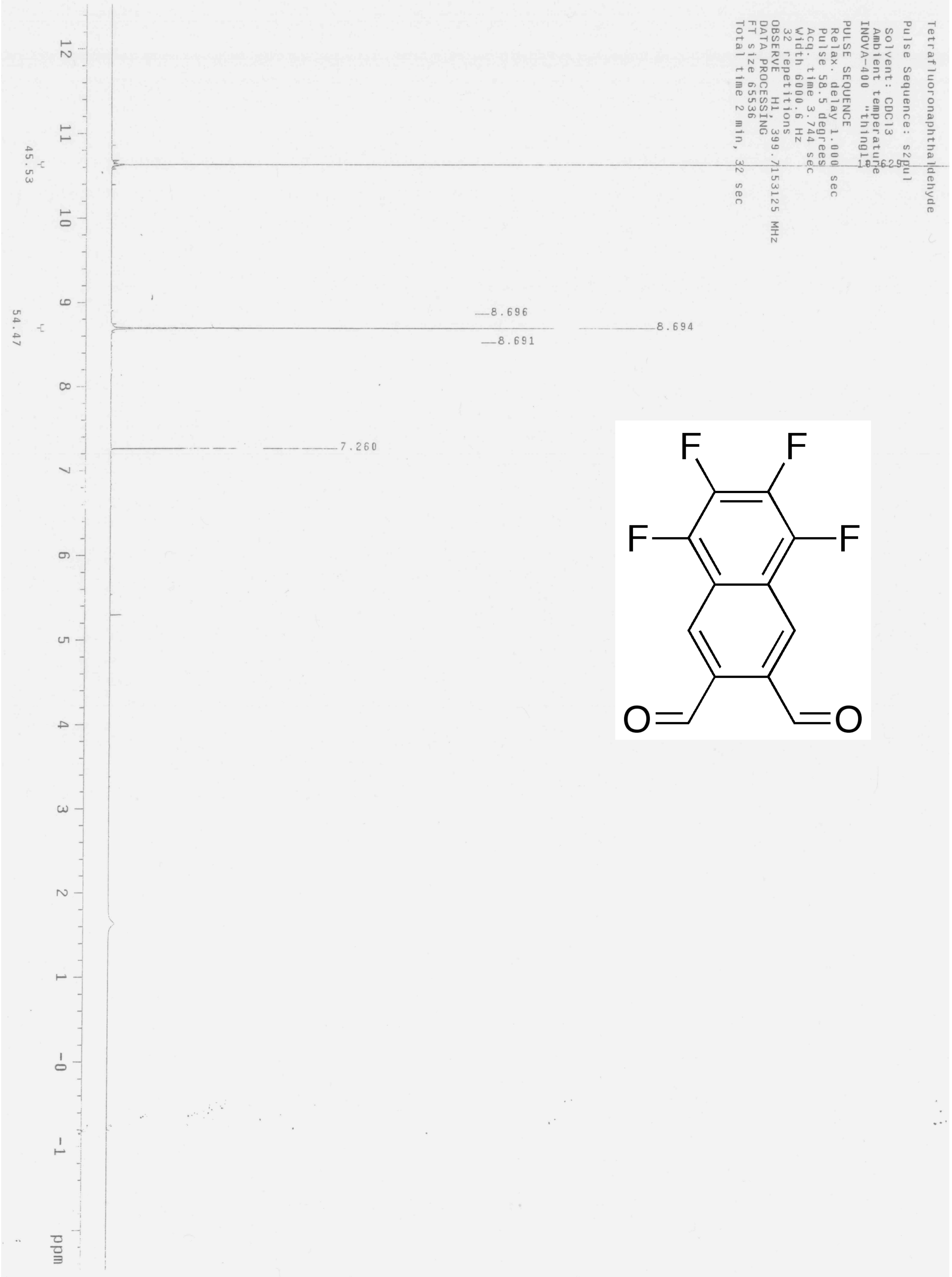
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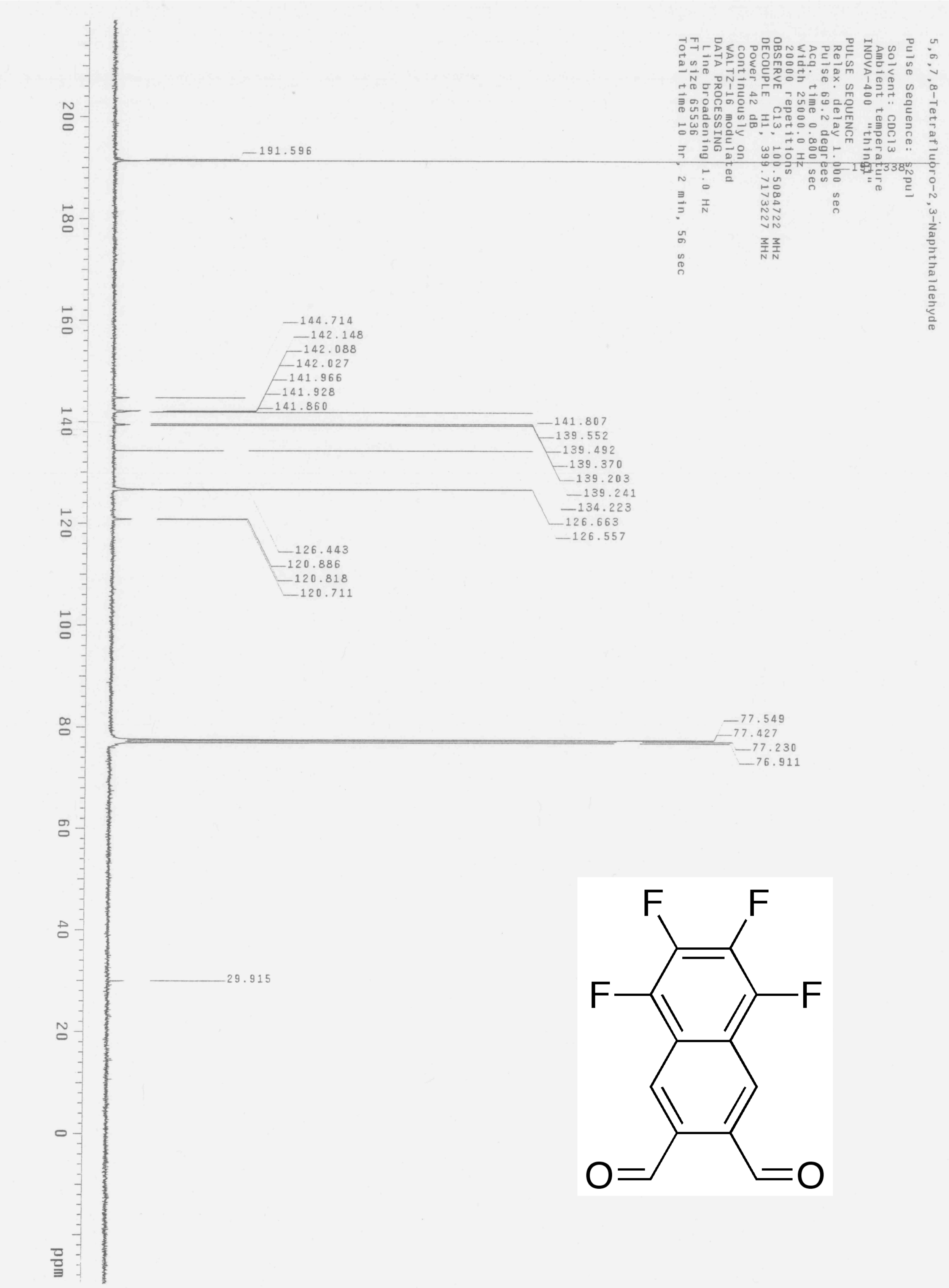
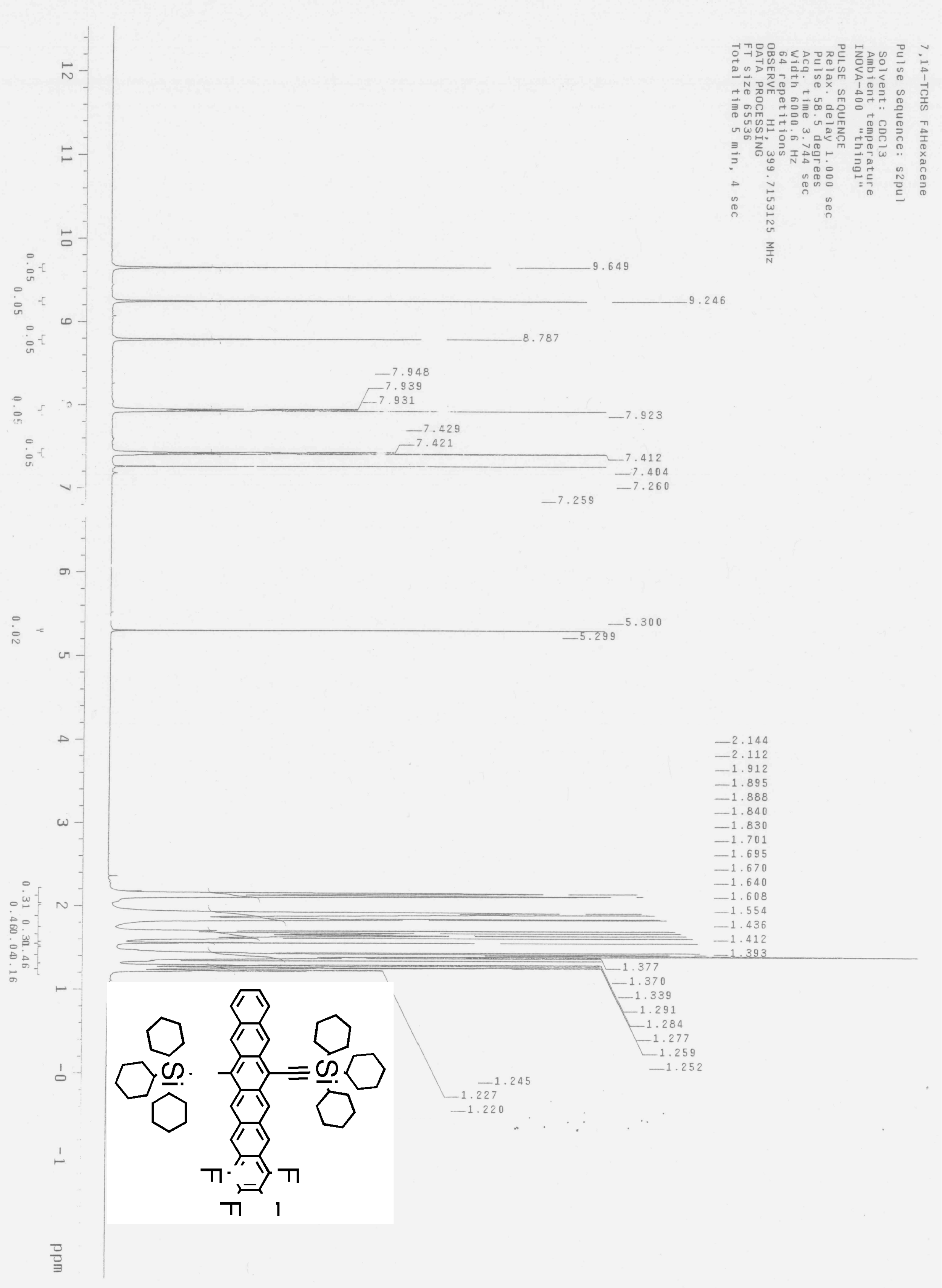
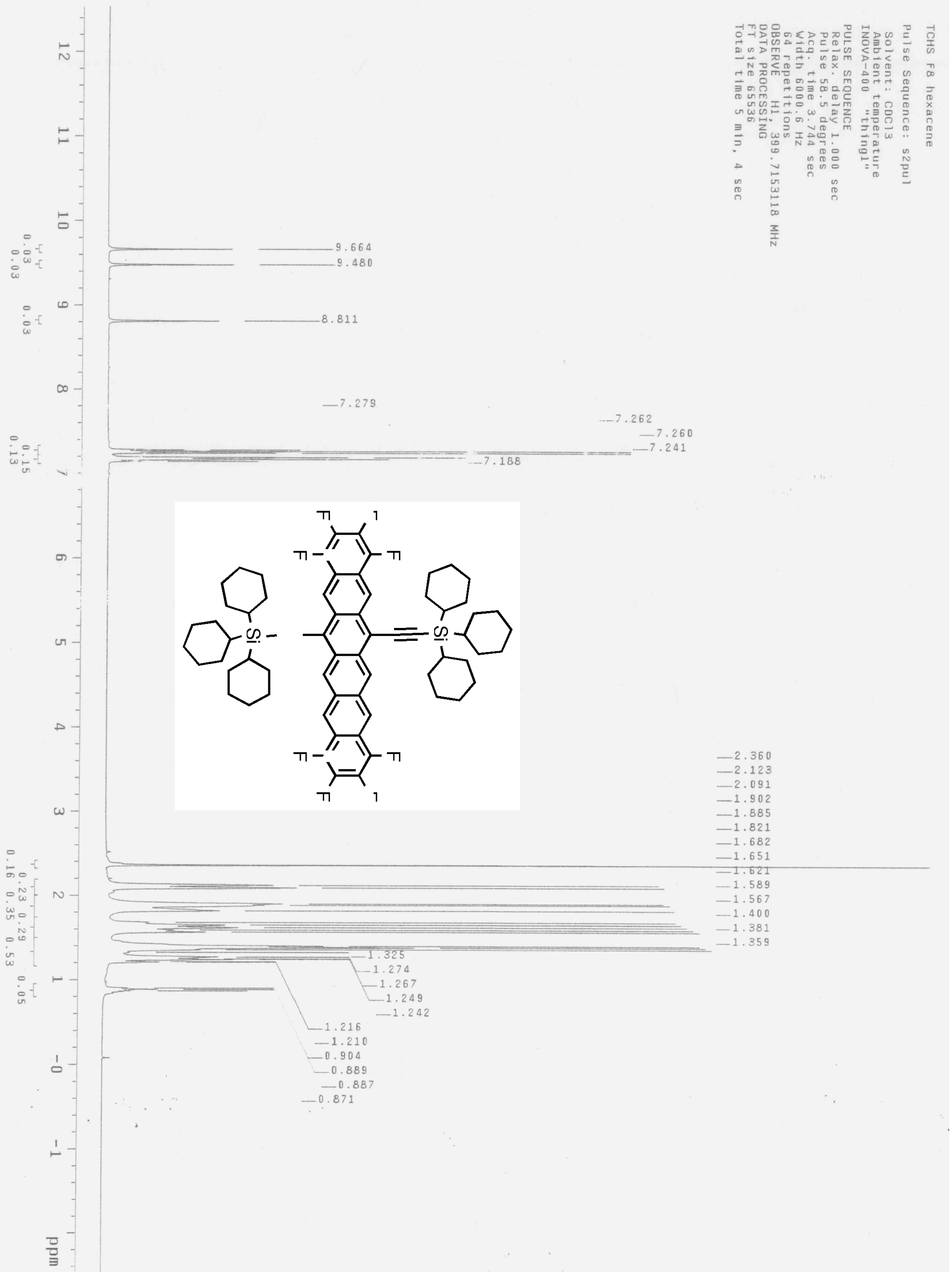
O
O


5,6,7,8-Tetrafluoro-2,3-Naphthaldehyde
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-400 "thing1"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 69.2 degrees
Acq. time 0.800 sec
Width 25000.0 Hz
20000 repetitions
OBSERVE C13, 100.5084722 MHz
DECOUPLE H1, 399.7173227 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 10 hr, 2 min, 56 sec
191.338
191.596
144.714
142.148
142.088
142.027
141.966
141.928
141.860
141.807
139.552
139.492
139.370
139.203
139.241
134.223
126.663
126.557
126.443
120.886
120.818
120.711
77.549
77.427
77.230
76.911
29.915
200
180
160
140
120
100
80
60
40
20
0
ppm
F
F
F
F
O
O


7,14-TCHS F4Hexacene
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-400 "thing1"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 58.5 degrees
Acq. time 3.744 sec
Width 6000.6 Hz
64 repetitions
OBSERVE H1, 399.7153125 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 4 sec
9.649
9.246
8.787
7.948
7.939
7.931
7.923
7.429
7.421
7.412
7.404
7.260
7.259
5.300
5.299
2.144
2.112
1.912
1.895
1.888
1.840
1.830
1.701
1.695
1.670
1.640
1.608
1.554
1.436
1.412
1.393
1.377
1.370
1.339
1.291
1.284
1.277
1.259
1.252
1.245
1.227
1.220
0.05
0.05
0.05
0.05
0.05
0.02
0.31
0.30
1.46
0.46
0.04
0.16
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
Si
Si
F
F
F
F


TCHS F8 hexacene
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-400 "thing1"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 58.5 degrees
Acq. time 3.744 sec
Width 6000.6 Hz
64 repetitions
OBSERVE H1, 399.7153118 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 4 sec
9.664
9.480
8.811
7.279
7.262
7.260
7.241
7.188
2.360
2.123
2.091
1.902
1.885
1.821
1.682
1.651
1.621
1.589
1.567
1.400
1.381
1.359
1.325
1.274
1.267
1.249
1.242
1.216
1.210
0.904
0.889
0.887
0.871
0.03
0.03
0.03
0.15
0.13
0.23
0.29
0.16
0.35
0.53
0.05
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
F
F
F
F
F
F
F
F
Si
Si