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Dibenzothiophene-*S,S*-dioxide – Fluorene Co-oligomers. Stable, Highly-Efficient Blue Emitters with Improved Electron Affinity

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Abstract: Incorporation of dibenzothiophene-*S,S*-dioxide units into conjugated fluorene oligomers changes the frontier orbital energy level and presents an effective way to increase the electron affinity of these materials, which are highly fluorescent with bright blue emission in both solution and solid state.

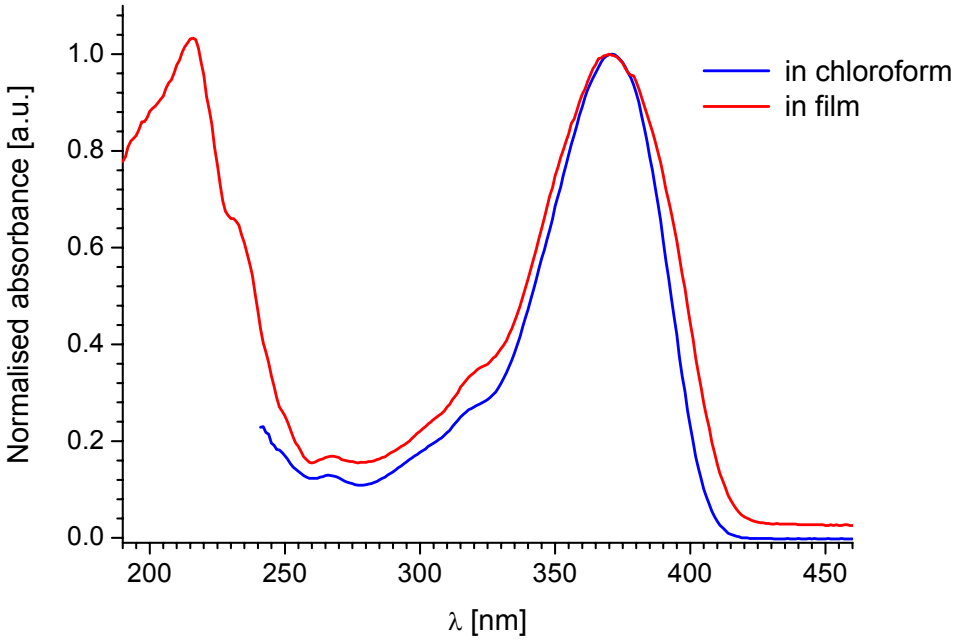


Figure S1. UV-Vis absorption spectra of pentafluorene **FFFFF** in chloroform (λ_{max} = 371 nm) and in film (λ_{max} = 370 nm).

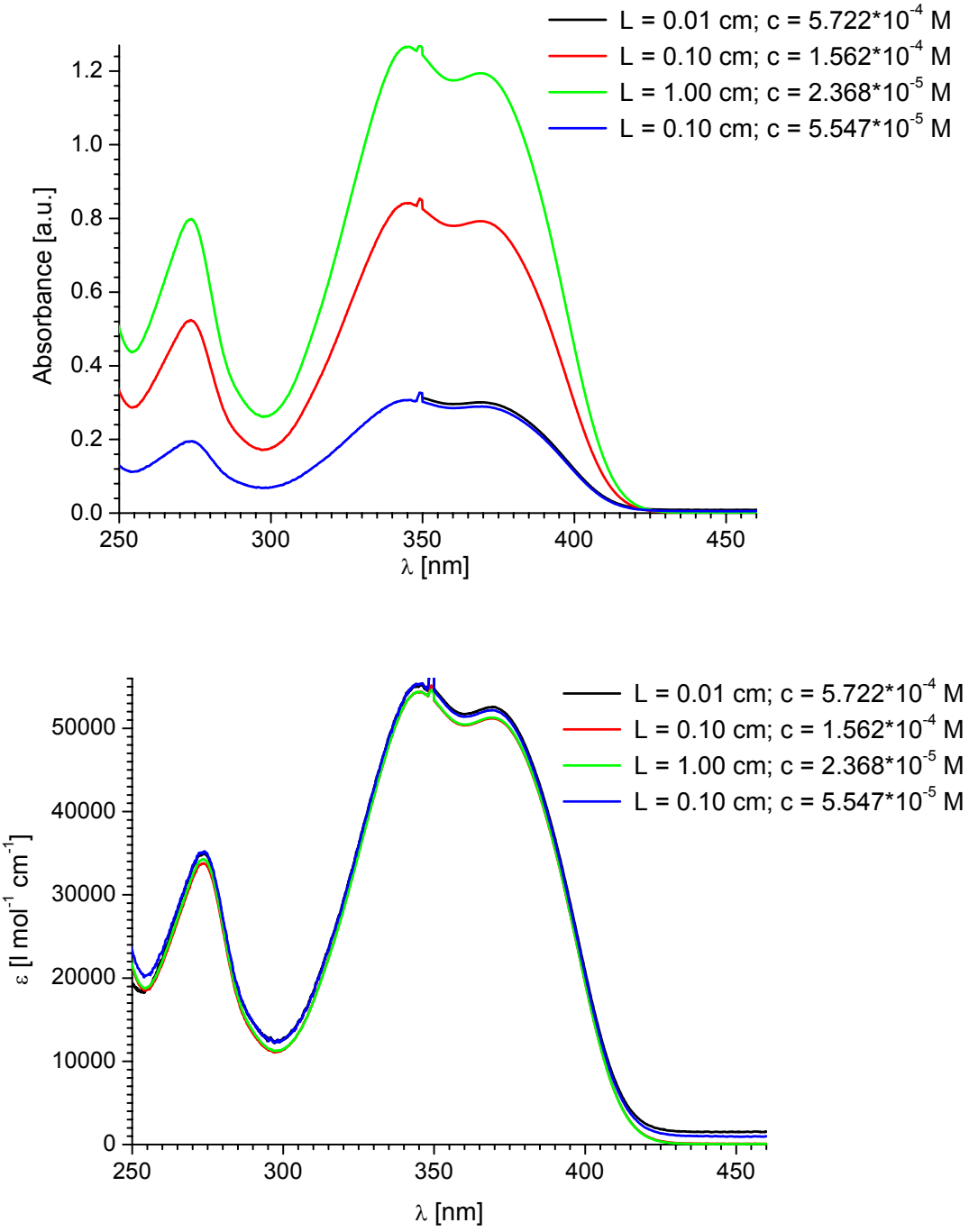


Figure S2. UV-Vis absorption spectra of **FSF** in chloroform.

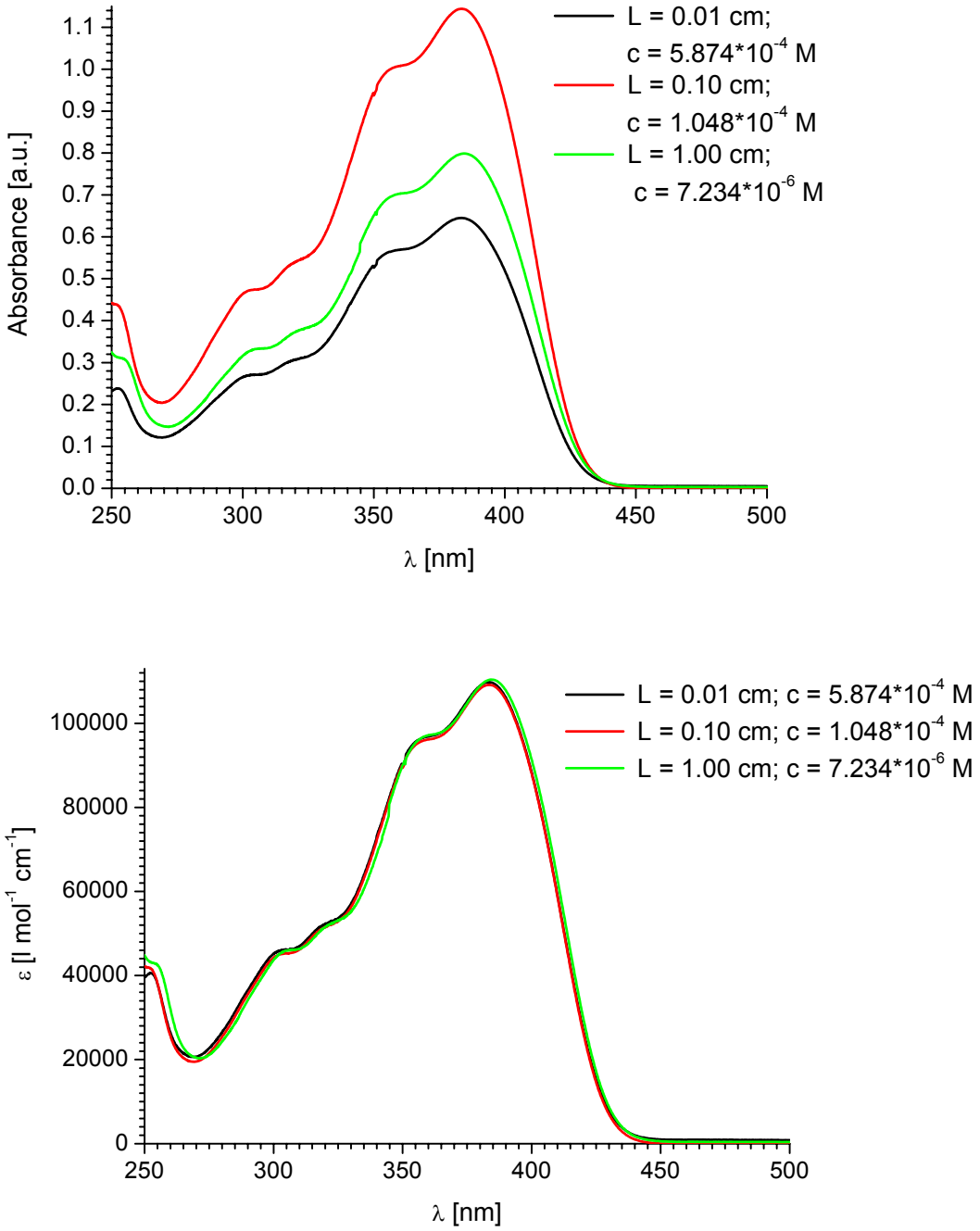


Figure S3. UV-Vis absorption spectra of **FFSFF** in chloroform.

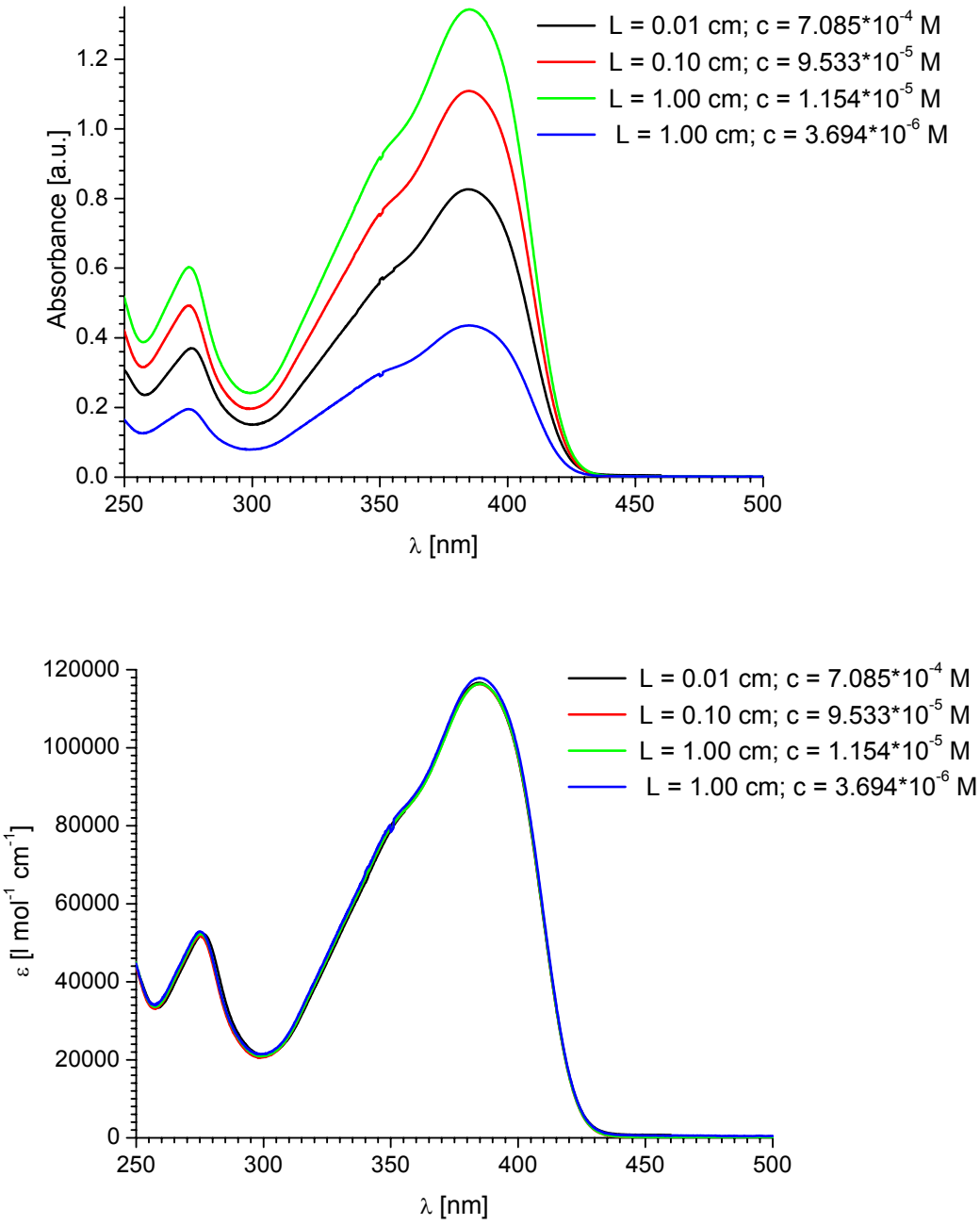


Figure S4. UV-Vis absorption spectra of **FSFSF** in chloroform.

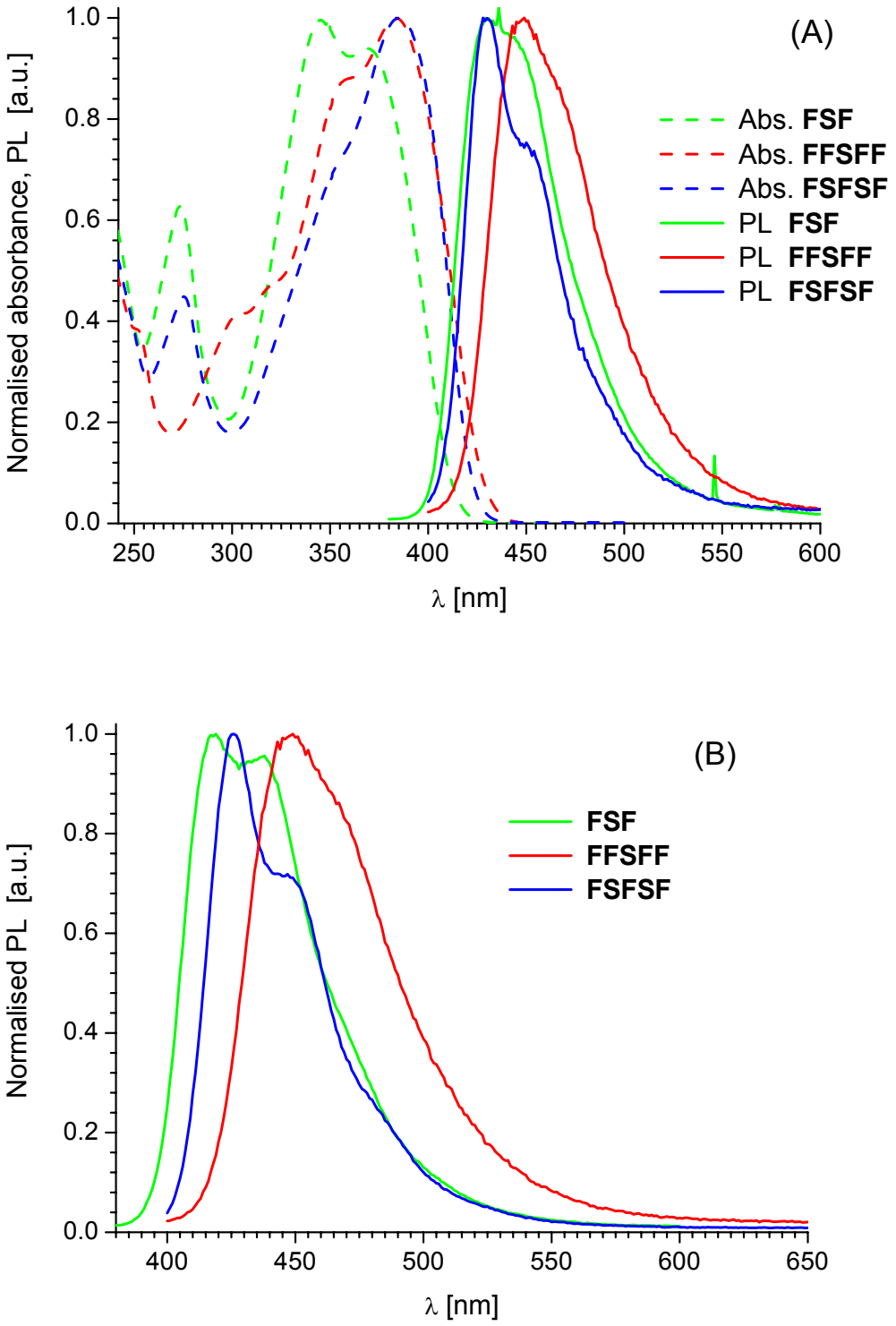


Figure S5. (A) UV-Vis absorption and photoluminescence spectra of **FSF, FFSFF** and **FSFSF** in chloroform. (B) Photoluminescence spectra of **FSF, FFSFF** and **FSFSF** in tetrahydrofuran.

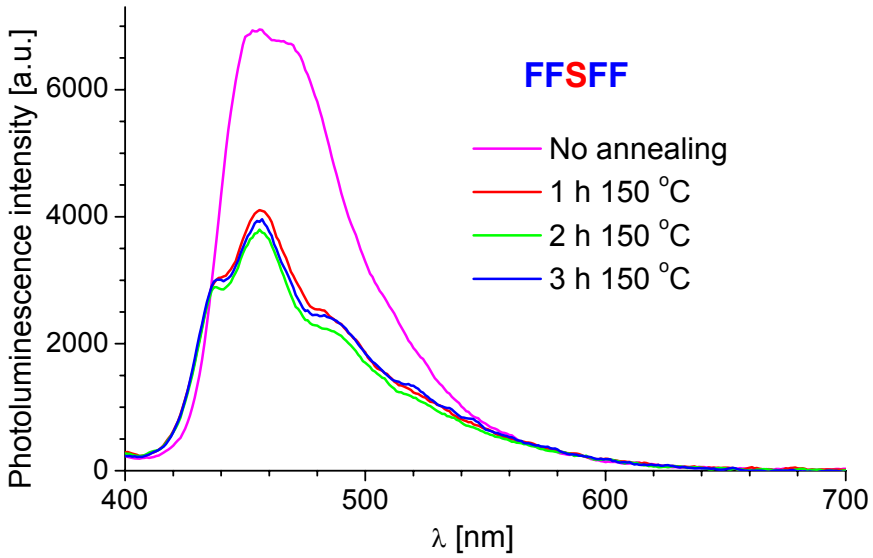


Figure S6. Evolution of the photoluminescence spectra of **FFSFF** films on annealing in an inert atmosphere.

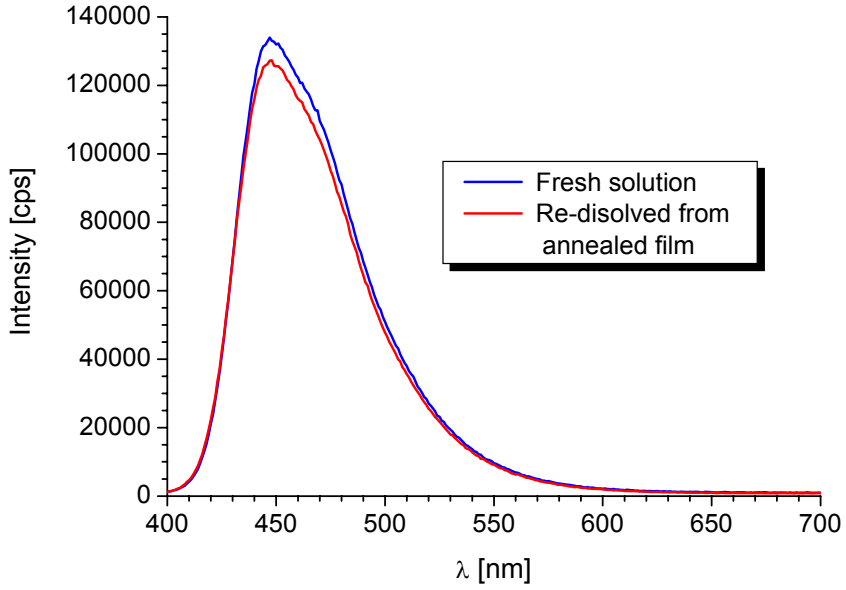


Figure S7. Photoluminescence spectra of **FFSFF** in chloroform solution: (—) fresh solution, λ_{PL} = 449 nm, Φ_{PL} = 67 %; (—) solution of **FFSFF** prepared by dissolution of the film, annealed at 150 °C for 3 h (see Fig. S6) and then stored at ambient temperature in air for 6 months. The spectra are corrected for differences in absorption. Analysis shows that the PL intensity of the re-dissolved film is > 95% of the fresh solution, which is within the accuracy of the experiment.

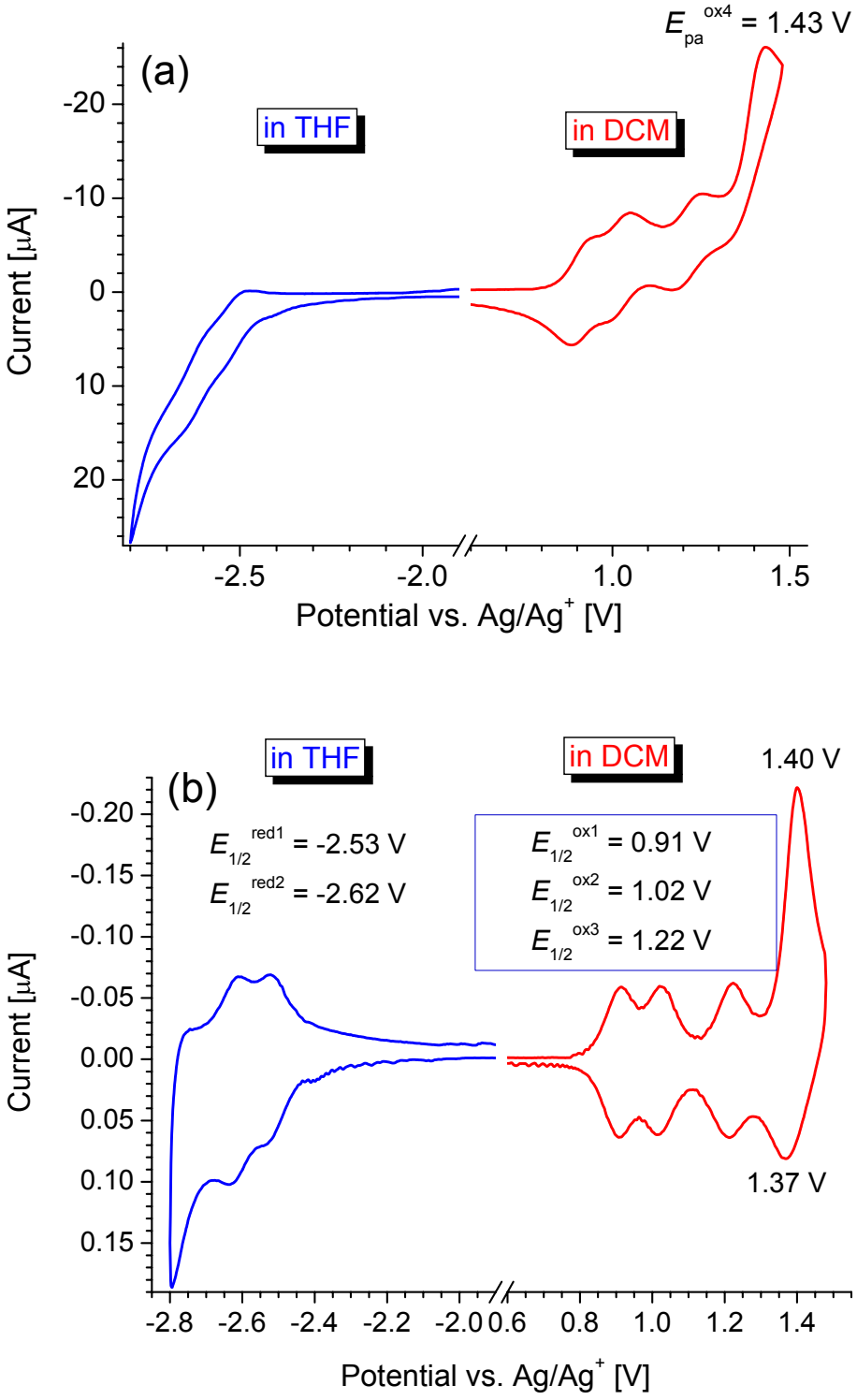


Figure S8. Cyclic voltammetry of **FFFFF** (a) and deconvoluted CV spectra (b); electrolyte 0.2 M Bu_4NPF_6, scan rate 100 mV s^{-1}, 20 °C.

Experimental Part

General

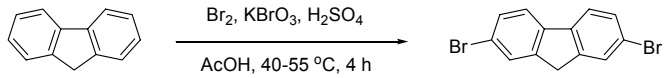
Elemental analyses were obtained on a Carlo-Erba Strumentazione instrument. Melting points were determined in open-end capillaries using a Stuart Scientific melting point apparatus SMP3 and were uncorrected. Solution ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian Unity 300, Bruker Avance 400 and Varian Inova 500 spectrometers operating at (^{1}H) 299.91, 400.13, 499.99 and (^{13}C) 75.42, 100.62, 124.99 MHz, respectively. Chemical shifts are reported in ppm relative to TMS as internal standard. Mass spectra were obtained on a Micromass Autospec instrument operating in EI mode at 70 eV. MALDI-TOF spectra were obtained on an Applied Biosystems Voyager-DE STR operating in reflector mode.

UV-Vis absorption spectra were recorded on Perkin Elmer Lamda 19, Cary 5E and Genesis 10 spectrophotometers. Photoluminescence spectra were recorded on a Jobin Horiba Fluoromax 3, with an excitation at 390 nm, PL quantum yields (Φ_{PL}) in solution were measured using anthracene as a standard, Φ_{PL} = 27% in ethanol solution.[1] Films of dibenzothiophene-*S,S*-dioxide/fluorene co-oligomers were spin-coated onto a quartz substrate from chloroform solution. Φ_{PL} of films were measured with an integrating sphere as described previously.[2]

Synthesis

2,7-Dibromofluorene, 2,7-dibromo-9,9-dihexylfluorene, 2-bromo-9,9-dihexylfluorene, 9,9-dihexylfluorene-2,7-diboronic acid (**2**) and 9,9-dihexylfluorene-2-boronic acid (**3**) have been described in the literature. We performed scale-up syntheses of these known compounds and we present our modified procedures for these widely used intermediates in oligo/polyfluorene chemistry.

2,7-Dibromofluorene.

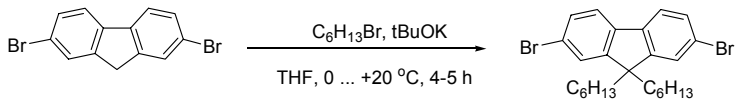


Fluorene (292 g, 1.76 mol) was dissolved in acetic acid (2600 cm^3) at ~70 °C and H_2SO_4 (98%, 25 cm^3) was added slowly to this solution. The reaction mixture was allowed to cool to ~50 °C with stirring, and a solution of bromine (150 cm^3, 2.92 mol) in acetic acid (200 cm^3) was added dropwise for 2–3 h, keeping the temperature at 40–55 °C to avoid crystallization of the fluorene. When ca. 1/3 – 1/2 of bromine was added, 2,7-dibromofluorene started to crystallise. Simultaneously with addition of a second half of bromine, $KBrO_3$ (100 g, 0.60 mol) was added in small portions (***CAUTION: add slowly, exothermic reaction!***) at 40–55 °C with vigorous stirring, which promotes the heavy precipitation of 2,7-dibromofluorene. The mixture was stirred for 3–4 h, then allowed to cool gradually to room temperature. After cooling the mixture to 10 °C, the solid was filtered off, washed with 70% AcOH (500 cm^3) and water until pH 7, and dried affording the crude product as a cream-coloured solid (481 g, 85 %) of > 95% purity (by ^{1}H NMR). To further purify the product it was stirred in AcOH (~ 1000 cm^3) at reflux (no full dissolution) for 4 h, cooled, filtered off, washed with AcOH and dried. Yield 455 g, 80%.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (2H, d, $J_{1\text{-}3}$ = 1.8 Hz, H-1,8), 7.59 (2H, d, $J_{3\text{-}4}$ = 8.0 Hz, H-4,5), 7.50 (2H, dd, $J_{3\text{-}4}$ = 8.0 Hz, $J_{1\text{-}3}$ = 1.8 Hz, H-3,6), 3.89 (2H, s, CH_2).

^{13}C NMR (100 MHz, $CDCl_3$): δ 144.79, 139.69, 130.15, 128.31, 121.19, 120.94, 36.56.

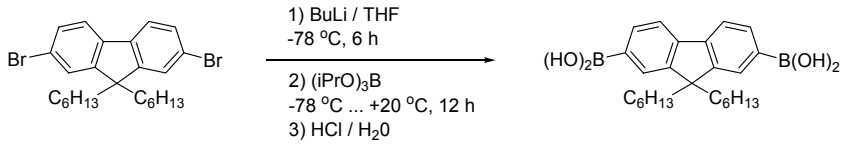
2,7-Dibromo-9,9-dihexylfluorene (adapted from ref. [3]).



Under argon, a 3 L three-neck flask was charged with 2,7-dibromofluorene (130.0 g, 0.40 mol), 1-bromohexane (220 cm^3, 1.57 mol) and dry THF (1000 cm^3). After full dissolution the mixture was cooled to 0 °C and a solution of potassium *tert*-butoxide (100.6 g, 0.90 mol) in dry THF (1000 cm^3) was added dropwise at 0 – +5 °C with vigorous stirring during 1.5 h. Upon adding the *tert*-butoxide solution the reaction mixture became orange (generation of fluorene anion) and then the colour changed to light pink (at the end of *tert*-butoxide addition no orange colour is produced, indicating that the alkylation reaction has been completed). The mixture was stirred at room temperature for 4 h, filtered from the KBr precipitate, and the solid was washed on the filter with DCM. The filtrate was evaporated on a rotavapor, the residue was dissolved in DCM (1500 cm^3), washed with water, dried over $MgSO_4$, and the solvent was evaporated. Excess 1-bromohexane was removed *in vacuo* (80 °C, 1 mbar) yielding crude product (196.7 g, 99.6 %) as yellow

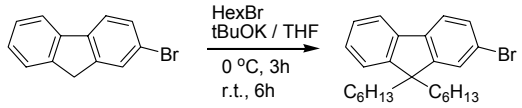
crystals. This was purified by column chromatography (7 × 17 cm column, silica gel, eluent – petrol ether, bp 40–60 °C) to afford 2,7-dibromo-9,9-dihexylfluorene (179.5 g, 91 %) as colourless plates. The material can also be additionally recrystallised from hexane or ethanol.
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.51 (2H, d, J = 7.8 Hz, H-1,8), 7.45 (2H, dd, J = 1.8 Hz and 7.8 Hz, H-3,6), 7.44 (2H, d, J = 1.8 Hz, H-4,5), 1.96–1.87 (4H, m, $CH_2C_5H_{11}$), 1.16–1.08 (4H, m, $CH_2CH_2CH_2C_3H_7$), 1.08–0.98 [8H, m, $(CH_2)_3CH_2CH_2CH_3$], 0.78 (6H, t, J = 7.4 Hz, CH_3), 0.62–0.53 (4H, m, $CH_2CH_2C_4H_9$).

9,9-dihexylfluorene-2,7-diboronic acid (3).



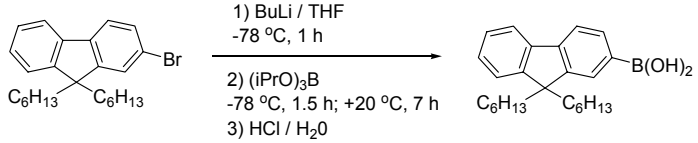
To a stirred solution of 2,7-dibromo-9,9-dihexylfluorene (30.0 g, 60. 9 mmol) in dry THF (1000 cm^3) under argon, a solution of BuLi in hexane (2.5 M; 54 cm^3, 135 mmol) was added dropwise at –78 °C. The mixture was stirred at this temperature for 6 h to give a white suspension. Triisopropylborate (60 cm^3, 258 mmol) was added quickly and the mixture was stirred overnight allowing the temperature to rise gradually to room temperature. Water (300 cm^3) was added and the mixture was stirred at r.t. for 4 h. Organic solvents were removed on a rotavapor (35 °C, 40 mbar), water (1100 cm^3) was added and the mixture was acidified with concentrated HCl. The product was extracted into diethyl ether (7 × 300 cm^3), the organic layer was dried over $MgSO_4$ and solvent was removed on a rotavapor. The residue was dissolved in acetone (110 cm^3) and reprecipitated into a mixture of water (130 cm^3) and concentrated HCl (70 cm^3) affording product **3** (24.3 g, 95 %) as a white powder. The product can be additionally purified by dissolution in acetone (100 cm^3) and addition of hexane (200 cm^3) to this solution.
^{1}H NMR (400 MHz, acetone-d_6): δ 7.99 (2H, dd, H-1,8), 7.90 (2H, dd, $J_{3\text{-}4}$ = 7.6 Hz, $J_{1\text{-}3}$ = 1.3 Hz, H-3,6), 7.80 (2H, dd, $J_{3\text{-}4}$ = 7.6 Hz, $J_{1\text{-}4}$ = 0.6 Hz, H-4,5), 7.19 [4H, s, $B(OH)_2$], 2.12–2.00 (4H, m, $CH_2C_5H_{11}$), 1.2–0.9 [12H, m, $(CH_2)_2(CH_2)_3CH_3$], 0.74 (6H, t, J = 7.2 Hz, CH_3), 0.64–0.54 (4H, m, $CH_2CH_2C_4H_9$).
^{13}C NMR (100 MHz, acetone-d_6): δ 150.87, 144.09, 133.87, 129.39, 119.92, 55.50, 41.09, 32.27, 30.39, 24.57, 23.16, 14.21

2-Bromo-9,9-dihexylfluorene



1-Bromohexane (230 cm^3) was added to a solution of 2-bromofluorene (106 g, 0.43 mol) in dry THF (1000 cm^3) under argon and cooled to 0°C. Potassium *tert*-butoxide (111 g, 0.99 mol) was dissolved in dry THF (1000 cm^3) and added dropwise at –5 °C for 2 h to the above solution. The reaction was left stirring under argon at 0 °C for 3 h and then it was allowed to warm up to room temperature and stirred for another 6 h. The obtained precipitate of KBr was filtered off and washed with DCM. The combined filtrates were evaporated and chromatographed on silica, eluted with petrol ether. 1-Bromohexane was removed under high vacuum (70 °C, 0.9 mbar), followed by another purification by column chromatography on silica to afford 171 g (95%) of the title product as a light yellowish oil.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67–7.63 (1H, m), 7.54 (1H, dd, J = 0.8 and 7.6 Hz, H-3), 7.46–7.42 (2H, m), 7.36–7.29 (3H, m), 2.00–1.86 (4H, m, $–CH_2C_5H_{11}$), 1.16–1.07 (4H, m, $CH_2CH_2CH_2C_3H_7$), 1.07–0.97 [8H, m, $(CH_2)_3CH_2CH_2CH_3$], 0.76 (6H, t, J = 7.6 Hz, CH_3), 0.64–0.55 (4H, m, $CH_2CH_2C_4H_9$).
^{13}C NMR (75 MHz, $CDCl_3$): δ 152.92, 150.26, 140.09, 139.98, 129.82, 127.41, 126.87, 126.61, 126.08, 122.83, 120.98, 119.70, 55.34, 40.27, 31.46, 29.63, 23.64, 22.56, 13.99.

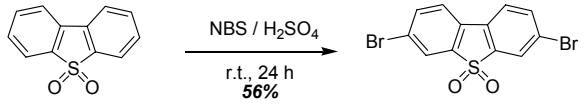
9,9-Dihexylfluorene-2-boronic acid (2).



A 1.6 M solution of *n*-butyllithium in hexane (130 cm^3, 0.208 mol) was added dropwise over 30 min to a solution of 2-bromo-9,9-dihexylfluorene (65.0 g, 0.157 mol) in dry THF (2300 cm^3) at –78 °C under argon and the mixture was stirred for 1 h. Then triisopropylborate (113 cm^3, 0.487 mol) was added dropwise for 60 min at –78 °C and the reaction

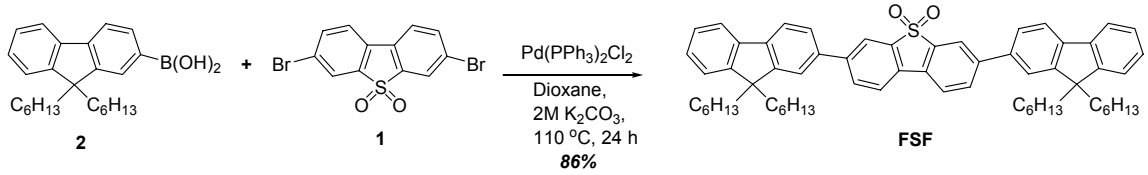
mixture was vigorously stirred under argon at this temperature until the light pink colour of the solution disappeared (*ca*. 1.5 h), then the temperature was allowed to rise gradually to room temperature and the reaction mixture was left stirring under argon for 7 h at room temperature to give a colourless suspension. THF was removed up to *ca*. 500 cm^3 and the solid was washed with water (800 cm^3). 13% HCl (800 cm^3) was added and the mixture was vigorously stirred for 3 h. The product was extracted into diethyl ether, washed with water, dried over $MgSO_4$ and purified by column chromatography on silica, eluting first with petrol ether and then with mixture of petrol ether and toluene (3:1, 1:1 v/v). Yield: 37.09 g (62 %) of a colourless solid.
^{1}H NMR (200 MHz, $CDCl_3$): δ 8.32 (1H, d, J = 7.6 Hz, H-4), 8.22 (1H, s, H-1), 7.90 (1H, d, J = 7.6 Hz, H-5), 7.86–7.77 (1H, m), 7.46–7.32 (3H, m), 2.22–1.96 (4H, m, $-CH_2C_5H_{11}$), 1.20–0.96 [12H, m, $CH_2CH_2(CH_2)_3CH_3$], 0.75 (6H, t, J = 6.4 Hz, CH_3), 0.78–0.58 (4H, m, (4H, m, $CH_2CH_2C_4H_9$).
^{13}C NMR (75 MHz, $CDCl_3$) δ 151.64, 150.12, 145.57, 140.72, 134.61, 129.67, 128.94 (br.), 127.92, 126.83, 123.03, 120.40, 119.26, 55.05, 40.42, 31.53, 29.75, 23.80, 22.58, 14.01.

3,7-Dibromodibenzothiophene-*S,S*-dioxide (1)



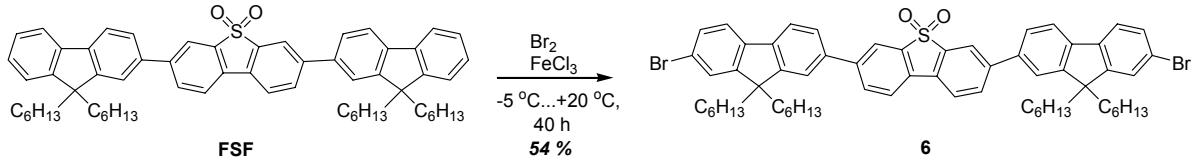
Dibenzothiophene-*S,S*-dioxide (100.0 g, 0.46 mol) was dissolved in concentrated H_2SO_4 (3000 cm^3). *N*-bromosuccinimide (NBS) (82.3 g, 0.46 mol) was added to this solution in several portions and the mixture was stirred at room temperature for 1 h. Additional NBS (82.3 g, 0.46 mol) was added to the mixture, which was then vigorously stirred at room temperature for 24 h. The precipitation started in 2–3 h and a lot of white solid was formed at the end of the process. The solid was filtered off, washed with H_2SO_4 (200 cm^3), then with H_2O until neutral and recrystallised from chlorobenzene to obtain 3,6-dibromodibenzothiophene-*S,S*-dioxide **1** as colourless needles (96 g, 56%), m.p. 317–318 °C. Lit.[4] m.p. 288–290 °C.
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93 (2H, d, J = 1.8 Hz, H-4,6), 7.77 (2H, dd, J = 1.8 and 8.4 Hz, H-2,8), 7.64 (2H, d, J = 8.1 Hz, H-1,9).

3,7-Bis(9,9-di-*n*-hexylfluorene-2-yl)dibenzothiophen-*S,S*-dioxide (FSF).



Under argon, to a mixture of 3,6-dibromodibenzothiophene-*S,S*-dioxide **1** (0.37 g, 1.00 mmol), 9,9-di-*n*-hexylfluorene-2-boronic acid **2** (0.77 g, 2.04 mmol) and dichlorobis(triphenylphosphine)palladium(II) (16 mg, 0.02 mmol), degassed 2 M potassium carbonate aqueous solution (4 cm^3) and 1,4-dioxane (10 cm^3) were added via a syringe. The reaction was stirred under argon with heating at 110 °C (oil bath) for 24 h with protection from the sunlight. The resulting slurry was poured into 5% NaCl-aqueous solution, the product was extracted with dichloromethane (50 cm^3), the organic layer was washed with water until pH 7 and dried over anhydrous magnesium sulphate. After evaporation of the solvent, the residue was purified by column chromatography on silica gel eluting first with petroleum ether to remove by-products and then with petrol ether (PE) – dichloromethane mixture (PE:DCM, 1:1 v/v), to obtain the title product **FSF** (0.76 g, 86%) as a light yellow powder, m.p. 153 °C.
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.16 (2H, d, *J* = 1.6 Hz, H-4,6 dibenzothiophene), 7.96 (2H, dd, *J* = 1.6 and 7.8 Hz, H-2,8 dibenzothiophene), 7.91 (2H, d, *J* = 7.8 Hz, H-1,9 dibenzothiophene), 7.81 (2H, d, *J* = 8.0 Hz, H-4 fluorene), 7.75 (2H, dd, *J* = 1.5 and 7.0 Hz, H-5 fluorene), 7.63 (2H, dd, *J* = 1.8 and 8.0 Hz, H-3 fluorene), 7.61 (2H, s, H-1 fluorene), 7.39–7.33 (6H, m, H-6,7,8 fluorene), 2.06–2.00 (8H, m, $CH_2C_5H_{11}$), 1.16–1.00 [24H, m, $CH_2CH_2(CH_2)_3CH_3$], 0.77 (12H, t, *J* = 7.3 Hz, CH_3), 0.70–0.60 (8H, m, $CH_2CH_2C_4H_9$).
^{13}C NMR (100 MHz, $CDCl_3$): δ 151.89, 151.09, 144.16, 141.82, 140.28, 138.61, 137.44, 132.57, 129.95, 127.56, 126.92, 125.87, 122.96, 121.91, 121.24, 120.64, 120.30, 120.02, 55.34, 40.47, 31.51, 29.70, 23.79, 22.59, 14.01
m/z (ES+): 880 (M^+, 100%). [Exact Mass (calcd):880.5253]
Anal. Calcd for $C_{62}H_{72}O_2S$ (M.W. 881.30): C, 84.50; H, 8.23; S, 3.64. Found: C, 84.45; H, 8.21; S, 3.58

3,7-Bis(2-bromo-9,9-di-*n*-hexylfluorene-7-yl)dibenzothiophene-*S,S*-dioxide (6).



To a solution of **FSF** (0.50 g, 0.57 mmol) in chloroform (4.5 cm^3) containing $FeCl_3$ (14 mg, 0.09 mmol; 0.15 equivalents) a solution of bromine (0.19 g, 1.21 mmol; 2.14 equivalents) in chloroform (1.3 cm^3) was added at –5 °C (*it is important that the reaction proceeds in the dark to avoid bromination of the aliphatic part of the molecule*). The solution was allowed to warm to room temperature and stirred for 40 h. The resulting solution was washed with water and several times with a 0.3 M sodium carbonate aqueous solution. The aqueous layer was additionally extracted with chloroform and the combined organic solution was dried over anhydrous magnesium sulfate. Removing the solvent afforded crude product (0.49 g, 83%), which was recrystallised from acetone to yield compound **6** (0.32 g, 54%) as a light yellow powder, m.p. 241–242.5 °C.

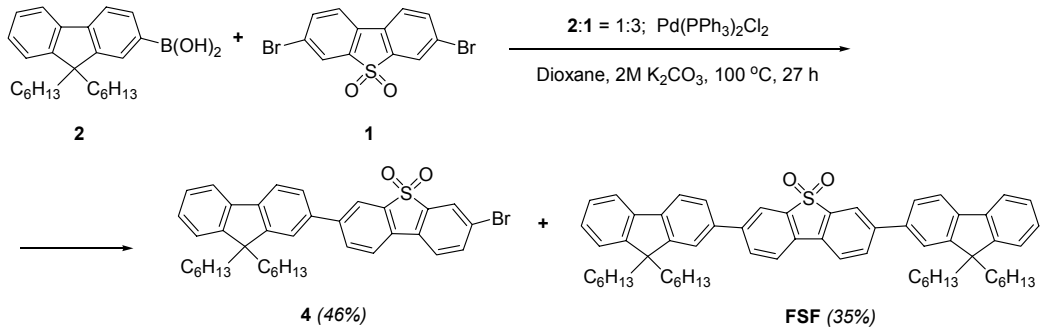
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.14 (2H, s.br., H-4,6 dibenzothiophene), 7.96 (2H, dd, *J* = 1.5 and 8.1 Hz, H-2,8 dibenzothiophene), 7.91 (2H, d, *J* = 8.1 Hz, H-1,9 dibenzothiophene), 7.78 (2H, d, *J* = 8.1 Hz, H-4 fluorene), 7.65–7.58 (6H, m), 7.51–7.48 (4H, m), 2.07–1.96 (8H, m, $CH_2C_5H_{11}$), 1.20–1.00 [24H, m, $CH_2CH_2(CH_2)_3CH_3$], 0.78 (12H, t, J = 6.9 Hz, CH_3), 0.69–0.57 (8H, m, $CH_2CH_2C_4H_9$).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.31, 151.54, 143.99, 140.72, 139.32, 138.65, 137.93, 132.62, 130.17, 130.05, 126.27, 126.10, 121.99, 121.64, 121.38, 121.27, 120.69, 120.45, 55.70, 40.37, 31.50, 29.63, 23.76, 22.60, 14.01.

m/z (EI): 1036 (M^+, 45%, ^{79}Br, ^{79}Br), 1038 (M^+, 100%, , ^{79}Br, ^{81}Br), 1040 (M^+, 67%, ^{81}Br, ^{81}Br). [Exact Mass (calcd): 1036.3463].

Anal. Calcd for $C_{62}H_{70}Br_2O_2S$ (M.W. 1039.09): C, 71.66; H, 6.79; Br, 15.38; S, 3.09. Found: C, 71.49; H, 6.87; Br, 15.13; S, 3.19

3-Bromo-7-(9,9-di-*n*-hexylfluorene-2-yl)dibenzothiophene-*S,S*-dioxide (4)



The flask with 3,6-dibromodibenzothiophene-*S,S*-dioxide **1** (11.92 g, 31.86 mmol) and 9,9-di-n-hexyl-2-fluoreneboronic acid **2** (4.02 g, 10.62 mmol) was flushed with argon. Anhydrous 1,4-dioxane (350 cm^3), degassed 2.3 M potassium carbonate aqueous solution (30 cm^3) and dichlorobis(triphenylphosphine)palladium(II) (0.09 g, 0.13 mmol) were added. The reaction mixture was stirred under argon with heating at 100 °C (oil bath) for 27 h with protection from the sunlight. The resulting solution was concentrated and the product was extracted with dichloromethane (250 cm^3), washed with water until pH 7 and dried over anhydrous magnesium sulphate. After evaporation of the solvent, the residue was purified by column chromatography on silica gel eluting first with PE to remove by-products. Further elution with a mixture of PE:DCM (1:1 v/v) yielded first compound **FSF** (1.64 g, 35%) and then compound **4** (3.06 g, 46%) as a yellowish powder, m.p. 177.5–178.5 °C.

Compound **4**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (1H, d, *J* = 1.6 Hz, H-6 benzothiophene), 7.97 (1H, d, *J* = 1.6 Hz, H-4 benzothiophene), 7.93 (1H, dd, *J* = 1.6 and 8.0 Hz, H-8 benzothiophene), 7.84 (1H, d, *J* = 8.0 Hz, H-9 benzothiophene), 7.79 (1H, d, *J* = 8.0 Hz), 7.78 (1H, dd, *J* = 1.6 and 8.4 Hz, H-2 benzothiophene), 7.76–7.72 (1H, m), 7.70 (1H, d, *J* = 8.4 Hz, H-1 benzothiophene), 7.60 (1H, dd, *J* = 1.8 and 7.8 Hz), 7.58 (1H, m), 7.39–7.34 (3H, m), 2.06–1.99 (4H, m, $CH_2C_5H_{11}$), 1.16–0.99 [12H, m, $CH_2CH_2(CH_2)_3CH_3$], 0.76 (6H, t, J = 7.0 Hz, CH_3), 0.69–0.59 (4H, m, $CH_2CH_2C_4H_9$).

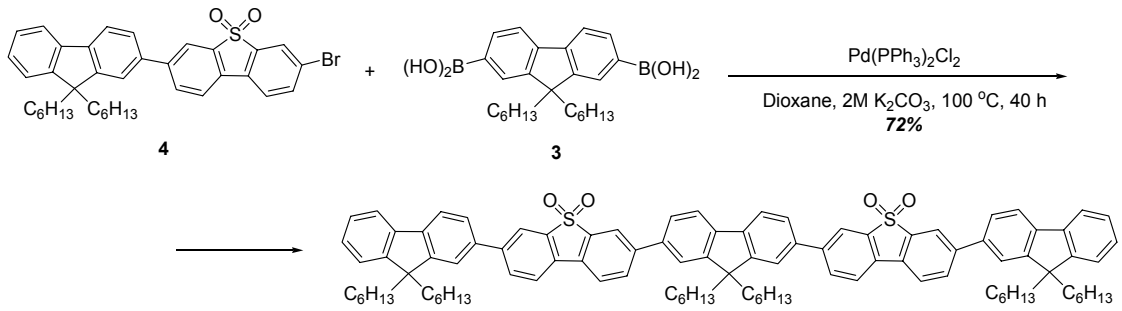
^{13}C NMR (100 MHz, $CDCl_3$) δ 151.93, 151.08, 144.75, 141.98, 140.21, 139.36, 138.17, 137.20, 136.97, 132.67, 130.48, 129.01, 127.62, 126.94, 125.89, 125.51, 123.96, 122.97, 122.89, 121.92, 121.23, 120.65, 120.32, 120.05, 55.34, 40.43, 31.49, 29.68, 23.77, 22.57, 13.99.

m/z (EI): 626 (M^+, 96%, ^{79}Br), 628 (M^+, 100%, ^{81}Br). [Exact Mass (calcd): 626.1854].

Anal. Calcd for $C_{37}H_{39}BrO_2S$ (M.W. 627.67): C, 70.80; H, 6.26; Br, 12.73; S, 5.11. Found: C, 70.92; H, 6.33; Br, 12.60, S, 5.13.

*In spite of the high excess of dibromide **1** over boronic acid **2** in this synthesis (**1:2** = 3 mol : 1 mol), a substantial amount of **FSF** was formed in the reaction, probably due to the high reactivity of **4** compared to that for **1**. When the ratio of **1:2** was increased to 1:7, this did not increase the yield of compound **4** due to the low solubility of 3,6-dibromodibenzothiophene-S,S-dioxide **1**, which does not completely dissolve in the mixture.*

2,7-Bis[7-(9,9-di-*n*-hexylfluorene-2-yl)dibenzothiophene-*S,S*-dioxide-3-yl]-9,9-di-*n*-hexylfluorene (FSFSF).



4 **3**

FSFSF

To a flask containing compound **4** (0.51 g, 0.81 mmol), 9,9-di-*n*-hexylfluorene-2,7-diboronic acid (0.14 g, 0.33 mmol) and dichlorobis(triphenylphosphine)palladium(II) (11 mg, 0.02 mmol), degassed 2 M potassium carbonate aqueous solution (1.5 cm^3) and 1,4-dioxane (4 cm^3) were added via syringe. The reaction mixture was stirred under argon with heating on an oil bath at 100 °C for *ca.* 40 h under protection from light. Filtration, washing with dioxane (*ca.* 1 cm^3), n-hexane (*ca.* 3.5 cm^3) and water (to remove inorganic salts) afforded crude product (0.42 g), which was purified by column chromatography on silica gel eluting with a mixture PE:DCM, 1:1 to afford the title product **FSFSF** (0.33 g, 72%), as a light yellow powder, m.p. > 270 °C.

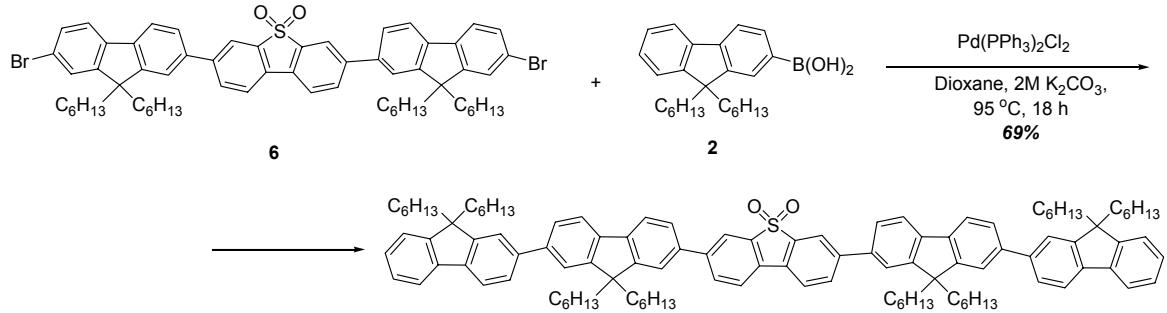
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.17 (4H, dd, *J* = 1.5 and 6.0 Hz), 8.02–7.95 (4H, m), 7.93 (2H, d, J = 8.0 Hz), 7.92 (2H, d, J = 8.0 Hz), 7.86 (2H, d, *J* = 8.0 Hz), 7.81 (2H, d, *J* = 7.5 Hz), 7.76 (2H, dd, *J* = 1.5 and 6.0 Hz), 7.69–7.60 (8H, m), 7.41–7.33 (6H, m), 2.16–2.09 [4H, m, $CH_2C_5H_{11}$ (central fluorene)], 2.08–2.00 [8H, m, $CH_2C_5H_{11}$ (terminal fluorenes)], 1.18–1.00 [36H, m, $CH_2CH_2(CH_2)_3CH_3$], 0.782 [6H, t, J = 7.0 Hz, CH_3 (central fluorene)], 0.773 [12H, t, J = 7.0 Hz, CH_3 (terminal fluorenes)], 0.74–0.60 (12H, m, $CH_2CH_2C_4H_9$).

^{13}C NMR (75 MHz, $CDCl_3$) δ 152.28, 151.89, 151.08, 144.20, 143.93, 141.83, 140.96, 140.26, 138.63, 138.60, 137.99, 137.39, 132.62, 132.61, 130.11, 129.89, 127.58, 126.93, 126.12, 125.87, 122.97, 121.97 (×2), 121.31, 121.22, 120.71, 120.66, 120.62, 120.31, 120.03, 55.69, 55.34, (40.47, 40.49), (31.54, 31.51), 29.71, (23.91, 23.80), (22.62, 22.60), 14.02.

m/z (MALDI-TOF, dithranol matrix/THF): 1426.78 (93%), 1427.78 (100%), 1428.78 (71%), 1429.78 (34%). [Exact Mass (calcd): 1426.7846. Calculated MS: m/z 1427.79 (100.0%), 1426.78 (93.4%), 1428.79 (53.0%), 1429.79 (18.5%), 1429.78 (9.0%), 1428.78 (8.4%)].

Anal. Calcd for $C_{99}H_{110}O_4S_2$ (M.W. 1428.06): C, 83.26; H, 7.76; S, 4.49. Found: C, 83.07; H, 7.93; S, 4.39

3,7-Bis[7-(9,9-di-*n*-hexylfluorene-2-yl)-9,9-di-*n*-hexylfluorene-2-yl]dibenzothiophene-*S,S*-dioxide (FFSFF).



6 **2**

FFSFF

To a flask containing compound **6** (0.20 g, 0.19 mmol), 9,9-di-*n*-hexyl-2-fluoreneboronic acid (0.22 g, 0.58 mmol) and dichlorobis(triphenylphosphine)palladium(II) (9 mg, 0.01 mmol), degassed 2 M potassium carbonate aqueous solution (0.9 cm^3) and 1,4-dioxane (5 cm^3) were added via syringe. The reaction mixture was stirred under argon with heating on

an oil bath at 95 °C for 18 h with protection from light. After removing the solvent, the product was extracted with dichloromethane (50 cm^3), washed with water and dried over anhydrous magnesium sulphate. After evaporation of the solvent, the residue was purified by column chromatography on silica gel eluting first with cyclohexane to remove by-products and then with mixture of cyclohexane and dichloromethane (cHex:DCM=3:1 v/v) to obtain the title product, **FFSFF** (0.21 g, 69%), as a light yellow powder, m.p. 225.6–226.3 °C.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.18 (2H, d, *J* = 1.5 Hz, H-4,6 dibenzothiophene), 7.99 (2H, dd, *J* = 1.5 and 8.0 Hz, H-2,8 dibenzothiophene), 7.93 (2H, d, *J* = 8.0 Hz, H-1,9 dibenzothiophene), 7.85 (2H, d, *J* = 7.0 Hz), 7.83 (2H, d, *J* = 8.0 Hz), 7.80 (2H, d, *J* = 7.5 Hz), 7.75 (2H, d, *J* = 7.0 Hz), 7.70–7.63 (12H, m), 7.39–7.31 (6H, m), 2.16–2.08 [8H, m, $CH_2C_5H_{11}$ (inner fluorene)], 2.08–1.98 [8H, m, $CH_2C_5H_{11}$ (terminal fluorene)], 1.18–1.02 [48H, m, $CH_2CH_2(CH_2)_3CH_3$], 0.778 [12H, t, J = 7.0 Hz, CH_3 (inner fluorene)], 0.773 [12H, t, J = 7.0 Hz, CH_3 (terminal fluorene)], 0.78–0.66 (16H, m, $CH_2CH_2C_4H_9$).

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.20, 151.87, 151.51, 151.00, 144.16, 141.53, 141.11, 140.73, 140.46, 140.31, 139.44, 138.65, 137.42, 132.58, 129.98, 127.05, 126.80, 126.28, 126.08, 125.99, 122.93, 121.94, 121.50, 121.43, 121.31, 120.65, 120.37, 120.27, 119.92, 119.75, 55.50, 55.17, (40.54, 40.37), (31.49, 31.47), 29.68, (23.85, 23.78), (22.59, 22.56), 14.02.

m/z (MALDI-TOF, dithranol matrix/THF): 1544.92 (95%), 1545.92 (100%), 1546.92 (88%), 1547.91 (62%), 1548.91 (27%).

[Exact Mass (calcd): 1545.0261. Calculated MS: m/z 1546.03 (100.0%), 1545.03 (82.6%), 1547.03 (60.0%), 1548.04 (23.8%), 1549.04 (7.0%), 1548.03 (4.5%), 1547.02 (3.7%)].

Anal. Calcd for $C_{112}H_{136}O_2S$ (M.W. 1546.34): C, 86.99; H, 8.86; S, 2.07. Found: C, 86.89; H, 8.91; S, 2.15

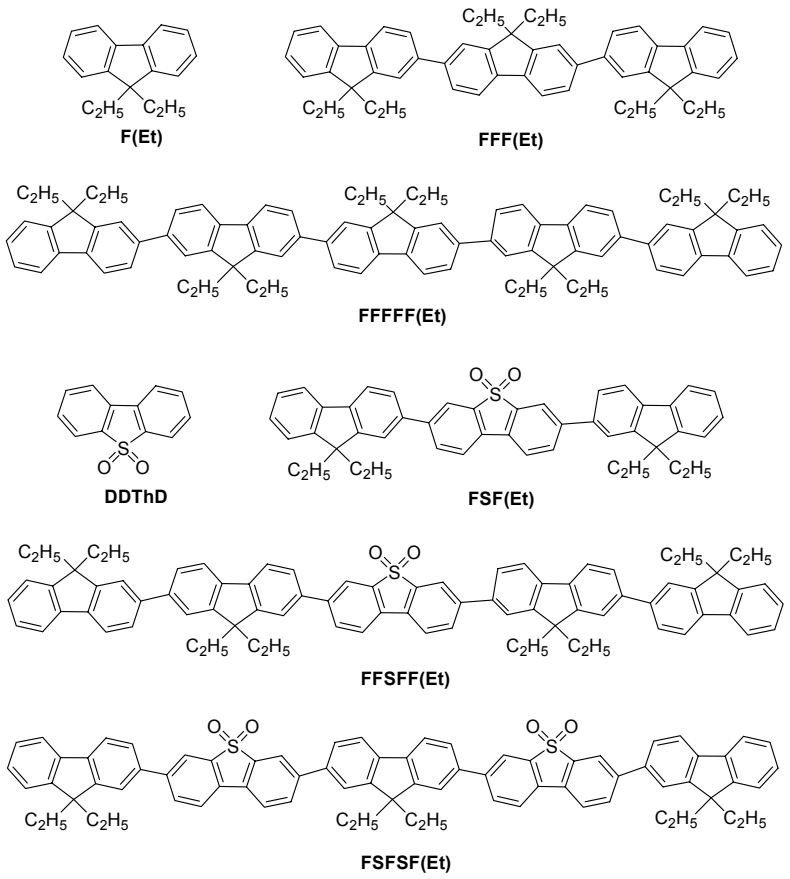
Cyclic voltammetry and Spectroelectrochemistry.

Cyclic voltammetry experiments were performed on a BAS-CV50W electrochemical workstation with *iR* compensation at 100 mV s^{-1}, using Ag/Ag^+ (0.01 M $AgNO_3$ in dry acetonitrile), platinum disk (Ø = 1.6 mm or 2.0 mm) and platinum wire as the reference, working and counter electrodes, respectively. Oxidation potentials were measured in dichloromethane and reduction potentials were measured in dry tetrahydrofuran solution under argon at room temperature. The solutions contained the substrate in concentrations *ca.* 2–5 × 10^{-4} M, together with *n*-Bu_4NPF_6 (0.2 M) as the supporting electrolyte.

Spectroelectrochemical measurements were performed on a Varian Cary 5E spectrophotometer in a 1 mm quartz cell using a Pt grid as the working electrode and Pt wire as the counter and reference electrodes, in DCM solution with 0.1 M Bu_4NPF_6 as the supporting electrolyte.

Computational Procedures

The *ab initio* computations were performed for compounds with 9,9-diethyl substituents on the fluorene ring (instead of the 9,9-dihexylfluorene derivatives studied experimentally) to decrease the computation time. The optimisation of the geometries of dibenzothiophene-*S,S*-dioxide (**S**), 9,9-diethylfluorene **F(Et)**, its trimer **FFF(Et)** and pentamer **FFFFF(Et)**, as well as compounds **FSF(Et)**, **FFSFF(Et)**, and **FSFSF(Et)** were carried out with the Gaussian 98[5] package of programs at density-functional theory (DFT) level using Pople's 6-31G split valence basis set supplemented by *d*-polarisation functions on heavy atoms. DFT calculations were carried out using Becke's three-parameter hybrid exchange functional[6] with Lee–Yang–Parr gradient-corrected correlation functional (B3LYP).[7] Thus, optimization of the geometries and calculation of electronic structures were performed at B3LYP/6-31G(d) level of theory. Contours of HOMO and LUMO orbitals were visualised using Molekel v.4.3 program.[8] No constraints of bonds/angles/dihedral angles were applied in the calculations and all the atoms were free to optimise.



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B3LYP/6-31(d) optimised geometries of F(Et), FFF(Et), FFFF(Et), S, FSF(Et), FFSFF(Et) and FSFSF(Et)

9,9-Diethylfluorene **F(Et)**

E = −658.6761028 Hartree

Dipole moment: 0.3637 Debye.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.460451	0.538079	0.000117
2	6	0	3.015416	1.863983	0.000018
3	6	0	1.648977	2.154080	-0.000015
4	6	0	0.734657	1.098842	0.000067
5	6	0	1.180882	-0.238250	0.000114
6	6	0	2.542993	-0.519937	0.000156
7	6	0	-0.734588	1.098852	-0.000050
8	6	0	-1.180862	-0.238225	-0.000138
9	6	0	0.000023	-1.208909	-0.000004
10	6	0	-1.648879	2.154116	0.000065
11	6	0	-3.015329	1.864058	0.000014
12	6	0	-3.460401	0.538169	-0.000140
13	6	0	-2.542971	-0.519878	-0.000208
14	6	0	0.000395	-2.123093	-1.260299
15	6	0	-0.000042	-1.403528	-2.612432
16	6	0	-0.000287	-2.123112	1.260285
17	6	0	-0.000360	-1.403593	2.612441
18	1	0	4.526572	0.327008	0.000170
19	1	0	3.738656	2.675247	-0.000048
20	1	0	1.307951	3.186443	-0.000127
21	1	0	2.899903	-1.547510	0.000243
22	1	0	-1.307822	3.186468	0.000201
23	1	0	-3.738547	2.675342	0.000098
24	1	0	-4.526528	0.327126	-0.000197
25	1	0	-2.899918	-1.547438	-0.000324
26	1	0	0.878037	-2.781219	-1.198775
27	1	0	-0.876501	-2.782218	-1.198805
28	1	0	0.000128	-2.133117	-3.430287
29	1	0	-0.885500	-0.770125	-2.729340
30	1	0	0.884924	-0.769485	-2.729589
31	1	0	-0.877610	-2.781644	1.198569
32	1	0	0.876917	-2.781849	1.198976
33	1	0	-0.000586	-2.133215	3.430269
34	1	0	0.884944	-0.770014	2.729583
35	1	0	-0.885473	-0.769731	2.729425

FFF(Et)

HF=-1973.6464711 Hartree

Dipole moment: 0.1697 Debye

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.729096	0.791568	-0.073076
2	6	0	0.729158	0.791531	0.072480
3	6	0	1.174266	-0.545209	0.121834
4	6	0	-0.000027	-1.516443	-0.000254
5	6	0	-1.174284	-0.545145	-0.122326
6	6	0	-2.525537	-0.831409	-0.252725
7	6	0	-3.468906	0.213647	-0.337062
8	6	0	-3.005068	1.542669	-0.287760
9	6	0	-1.649204	1.838507	-0.157346
10	6	0	1.649266	1.838460	0.156725
11	6	0	3.005123	1.542591	0.287242
12	6	0	3.468873	0.213559	0.336679
13	6	0	2.525507	-0.831497	0.252360
14	6	0	-0.130203	-2.430502	1.253577
15	6	0	0.130123	-2.430447	-1.254133
16	6	0	-4.916749	-0.082318	-0.467483
17	6	0	4.916756	-0.082408	0.467300
18	6	0	-5.363107	-1.162699	-1.253084
19	6	0	-6.718428	-1.463196	-1.378287
20	6	0	-7.655026	-0.674160	-0.708360

21	6	0	-7.228036	0.412774	0.080319
22	6	0	-5.876954	0.706370	0.199581
23	6	0	5.876989	0.706199	-0.199799
24	6	0	7.228079	0.412675	-0.080320
25	6	0	7.654978	-0.674097	0.708617
26	6	0	6.718338	-1.463062	1.378568
27	6	0	5.363015	-1.162655	1.253130
28	6	0	-9.118712	-0.753380	-0.642646
29	6	0	-9.583395	0.283034	0.193011
30	6	0	-8.419922	1.117194	0.728892
31	6	0	8.420026	1.116998	-0.728859
32	6	0	9.583459	0.283067	-0.192552
33	6	0	9.118694	-0.753238	0.643196
34	6	0	-10.015360	-1.639874	-1.242995
35	6	0	-11.382369	-1.483273	-1.003092
36	6	0	-11.845692	-0.455960	-0.174664
37	6	0	-10.945996	0.432632	0.427578
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40	6	0	11.382338	-1.482879	1.004216
41	6	0	10.015293	-1.639558	1.243869
42	6	0	8.524254	2.607717	-0.291897
43	6	0	8.342500	1.073486	-2.283491
44	6	0	8.233841	-0.319624	-2.910835
45	6	0	8.612872	2.860792	1.216192
46	6	0	-8.342103	1.074158	2.283509
47	6	0	-8.233362	-0.318772	2.911239
48	6	0	-8.524299	2.607790	0.291490
49	6	0	-8.613348	2.860397	-1.216642
50	6	0	-0.267080	-1.709270	2.597882
51	6	0	0.266731	-1.709161	-2.598434
52	1	0	-2.872060	-1.861885	-0.261584
53	1	0	-3.720036	2.355268	-0.380393
54	1	0	-1.320262	2.874410	-0.130822
55	1	0	1.320316	2.874356	0.130108
56	1	0	3.720140	2.355151	0.379789
57	1	0	2.872039	-1.861965	0.261346
58	1	0	-0.998168	-3.086859	1.103044
59	1	0	0.747676	-3.090597	1.281089
60	1	0	0.998214	-3.086666	-1.103721
61	1	0	-0.747659	-3.090675	-1.281546
62	1	0	-4.633767	-1.759257	-1.793612
63	1	0	-7.033464	-2.299358	-1.997626
64	1	0	-5.544975	1.526410	0.831577
65	1	0	5.545033	1.526115	-0.831962
66	1	0	7.033360	-2.299075	1.998113
67	1	0	4.633605	-1.759201	1.793567
68	1	0	-9.660281	-2.440369	-1.887298
69	1	0	-12.091893	-2.165496	-1.463898
70	1	0	-12.912156	-0.346012	0.003278
71	1	0	-11.316929	1.228054	1.070183
72	1	0	11.317099	1.228098	-1.069518
73	1	0	12.912235	-0.345652	-0.002026
74	1	0	12.091823	-2.164972	1.465275
75	1	0	9.660160	-2.439977	1.888235
76	1	0	9.404468	3.041640	-0.785878
77	1	0	7.654691	3.140771	-0.700437
78	1	0	7.481341	1.680719	-2.594493
79	1	0	9.231399	1.583449	-2.679515
80	1	0	8.177773	-0.240631	-4.002473
81	1	0	9.101999	-0.939746	-2.664295
82	1	0	7.336550	-0.844347	-2.566797
83	1	0	8.690516	3.935414	1.416928
84	1	0	7.726678	2.486158	1.739115
85	1	0	9.491422	2.374307	1.652384
86	1	0	-7.480875	1.681463	2.594177
87	1	0	-9.230905	1.584272	2.679565
88	1	0	-8.177192	-0.239503	4.002852
89	1	0	-9.101533	-0.938964	2.664934
90	1	0	-7.336099	-0.843585	2.567256
91	1	0	-9.404379	3.041845	0.785597
92	1	0	-7.654617	3.140946	0.699640
93	1	0	-8.690921	3.934967	-1.417688
94	1	0	-7.727360	2.485504	-1.739732
95	1	0	-9.492102	2.373885	-1.652388
96	1	0	-0.353997	-2.437511	3.412232
97	1	0	0.603337	-1.077901	2.804906
98	1	0	-1.157835	-1.072963	2.621835
99	1	0	0.353774	-2.437375	-3.412795
100	1	0	-0.603857	-1.078009	-2.805395
101	1	0	1.157327	-1.072634	-2.622440

FFFFF(Et)

HF=-3288.6168836 Hartree

Dipole moment: 0.0487 Debye

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.730910	0.052002	0.892746
2	6	0	0.730937	-0.052265	0.892730
3	6	0	1.177206	-0.089522	-0.444054
4	6	0	-0.000007	-0.000087	-1.415498
5	6	0	-1.177203	0.089293	-0.444027
6	6	0	-2.531432	0.183316	-0.730312
7	6	0	-3.476853	0.241446	0.314698
8	6	0	-3.012172	0.202815	1.643769
9	6	0	-1.653206	0.109562	1.939651
10	6	0	1.653254	-0.109850	1.939616
11	6	0	3.012214	-0.203089	1.643705
12	6	0	3.476870	-0.241691	0.314626
13	6	0	2.531430	-0.183543	-0.730367
14	6	0	-4.927267	0.336128	0.018241
15	6	0	4.927281	-0.336329	0.018154
16	6	0	-5.391561	1.113808	-1.060506
17	6	0	-6.749061	1.208368	-1.361268
18	6	0	-7.670091	0.514042	-0.574436
19	6	0	-7.225062	-0.268284	0.510588
20	6	0	-5.871790	-0.355908	0.804702
21	6	0	5.871778	0.355773	0.804587
22	6	0	7.225051	0.268202	0.510469
23	6	0	7.670110	-0.514137	-0.574534
24	6	0	6.749106	-1.208531	-1.361339
25	6	0	5.391603	-1.114022	-1.060573
26	6	0	-9.129763	0.414249	-0.653290
27	6	0	-9.576977	-0.439418	0.375516
28	6	0	-8.402082	-0.946891	1.212572
29	6	0	8.402038	0.946914	1.212406
30	6	0	9.576956	0.439434	0.375386
31	6	0	9.129777	-0.414284	-0.653395
32	6	0	-10.048660	0.997497	-1.527869
33	6	0	-11.405840	0.723593	-1.368574
34	6	0	-11.872173	-0.127019	-0.347400
35	6	0	-10.929982	-0.707194	0.527450
36	6	0	10.929952	0.707255	0.527322
37	6	0	11.872168	0.127084	-0.347505
38	6	0	11.405870	-0.723574	-1.368657
39	6	0	10.048700	-0.997530	-1.527950
40	6	0	8.520174	0.512621	2.702956
41	6	0	8.285933	2.498874	1.168510
42	6	0	8.158759	3.121999	-0.224913
43	6	0	8.646495	-0.992727	2.956034
44	6	0	-8.286049	-2.498862	1.168814
45	6	0	-8.158856	-3.122142	-0.224539
46	6	0	-8.520202	-0.512482	2.703086
47	6	0	-8.646427	0.992894	2.956055
48	6	0	-13.321484	-0.405836	-0.196370
49	6	0	13.321473	0.405930	-0.196451
50	6	0	-14.278186	0.606728	-0.416510
51	6	0	-15.631286	0.332946	-0.275830
52	6	0	-16.064316	-0.957584	0.088541
53	6	0	-15.130905	-1.970896	0.313444
54	6	0	-13.773467	-1.688606	0.169600
55	6	0	13.773421	1.688690	0.169598
56	6	0	15.130848	1.970991	0.313522
57	6	0	16.064284	0.957705	0.088614
58	6	0	15.631292	-0.332809	-0.275862
59	6	0	14.278202	-0.606605	-0.416614
60	6	0	17.529853	0.956352	0.160482
61	6	0	17.989859	-0.338522	-0.156051
62	6	0	16.820530	-1.276294	-0.456033
63	6	0	-16.820499	1.276462	-0.455998
64	6	0	-17.989859	0.338679	-0.156178
65	6	0	-17.529890	-0.956220	0.160307
66	6	0	-19.353224	0.612993	-0.163181
67	6	0	-20.258437	-0.409678	0.147166
68	6	0	-19.799838	-1.693216	0.461541
69	6	0	-18.432122	-1.976040	0.470575
70	6	0	18.432051	1.976161	0.470886

71	6	0	19.799771	1.693352	0.461934
72	6	0	20.258407	0.409841	0.147505
73	6	0	19.353228	-0.612819	-0.162977
74	6	0	16.767420	-2.473081	0.539372
75	6	0	16.891650	-1.851926	-1.900757
76	6	0	16.957215	-0.820630	-3.031243
77	6	0	16.688528	-2.106653	2.024404
78	6	0	-16.891510	1.852220	-1.900677
79	6	0	-16.767439	2.473149	0.539527
80	6	0	-16.956944	0.821019	-3.031259
81	6	0	-16.688648	2.106554	2.024523
82	6	0	-0.095018	-1.257007	-2.329400
83	6	0	0.094979	1.256885	-2.329328
84	6	0	0.193790	2.604707	-1.608480
85	6	0	-0.193799	-2.604874	-1.608632
86	1	0	-2.878148	0.184145	-1.760777
87	1	0	-3.729648	0.274748	2.456281
88	1	0	-1.323716	0.091100	2.975553
89	1	0	1.323784	-0.091412	2.975525
90	1	0	3.729705	-0.275035	2.456202
91	1	0	2.878127	-0.184341	-1.760839
92	1	0	-4.674740	1.672811	-1.655222
93	1	0	-7.078424	1.822659	-2.195614
94	1	0	-5.525101	-0.981604	1.623537
95	1	0	5.525065	0.981482	1.623404
96	1	0	7.078492	-1.822838	-2.195663
97	1	0	4.674803	-1.673080	-1.655262
98	1	0	-9.717694	1.650267	-2.331808
99	1	0	-12.120218	1.152883	-2.065179
100	1	0	-11.278062	-1.343607	1.337415
101	1	0	11.278005	1.343700	1.337273
102	1	0	12.120271	-1.152871	-2.065234
103	1	0	9.717759	-1.650345	-2.331862
104	1	0	9.388630	1.028169	3.135327
105	1	0	7.641601	0.899669	3.237250
106	1	0	7.418723	2.788762	1.777485
107	1	0	9.165966	2.916860	1.676339
108	1	0	8.078403	4.212208	-0.147394
109	1	0	9.030285	2.893908	-0.847420
110	1	0	7.267885	2.757004	-0.746370
111	1	0	8.728846	-1.191129	4.030699
112	1	0	7.773834	-1.537820	2.581171
113	1	0	9.536209	-1.406697	2.470436
114	1	0	-7.418872	-2.788731	1.777843
115	1	0	-9.166117	-2.916760	1.676656
116	1	0	-8.078524	-4.212343	-0.146891
117	1	0	-9.030359	-2.894112	-0.847101
118	1	0	-7.267958	-2.757227	-0.746010
119	1	0	-9.388690	-1.027947	3.135490
120	1	0	-7.641655	-0.899543	3.237415
121	1	0	-8.728753	1.191381	4.030705
122	1	0	-7.773734	1.537902	2.581139
123	1	0	-9.536118	1.406890	2.470436
124	1	0	-13.943062	1.609093	-0.671362
125	1	0	-15.449973	-2.973488	0.587254
126	1	0	-13.046885	-2.482932	0.314840
127	1	0	13.046820	2.482993	0.314862
128	1	0	15.449887	2.973570	0.587415
129	1	0	13.943103	-1.608962	-0.671527
130	1	0	-19.720393	1.607664	-0.406279
131	1	0	-21.325600	-0.204115	0.143569
132	1	0	-20.513779	-2.477047	0.700456
133	1	0	-18.080745	-2.975362	0.715225
134	1	0	18.080645	2.975462	0.715582
135	1	0	20.513686	2.477176	0.700956
136	1	0	21.325573	0.204290	0.143972
137	1	0	19.720426	-1.607468	-0.406123
138	1	0	15.902593	-3.095635	0.271708
139	1	0	17.655195	-3.095986	0.363953
140	1	0	17.768362	-2.511661	-1.957784
141	1	0	16.016118	-2.499054	-2.048395
142	1	0	16.998608	-1.324915	-4.003432
143	1	0	16.077947	-0.167958	-3.029983
144	1	0	17.846105	-0.187061	-2.945038
145	1	0	16.650543	-3.014071	2.637776
146	1	0	17.560510	-1.524862	2.340876
147	1	0	15.792504	-1.516822	2.243888
148	1	0	-17.768232	2.511941	-1.957721
149	1	0	-16.015978	2.499379	-2.048179
150	1	0	-15.902583	3.095715	0.271984
151	1	0	-17.655192	3.096086	0.364117

152	1	0	-16.998255	1.325387	-4.003409
153	1	0	-16.077658	0.168372	-3.029966
154	1	0	-17.845824	0.187417	-2.945195
155	1	0	-16.650678	3.013900	2.638002
156	1	0	-17.560664	1.524746	2.340874
157	1	0	-15.792653	1.516674	2.243993
158	1	0	-0.966810	-1.131089	-2.985878
159	1	0	0.783236	-1.259830	-2.989586
160	1	0	0.966750	1.131005	-2.985842
161	1	0	-0.783295	1.259752	-2.989488
162	1	0	0.255225	3.421011	-2.337129
163	1	0	-0.681119	2.786198	-0.975497
164	1	0	1.084669	2.655381	-0.973921
165	1	0	-0.255239	-3.421133	-2.337330
166	1	0	0.681125	-2.786394	-0.975676
167	1	0	-1.084665	-2.655599	-0.974059

Dibenzothiophene-*S,S*-dioxide **S**
E = -1010.6677122 Hartree
Dipole moment: 5.5106 Debye

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.739396	0.954552	0.000036
2	6	0	-0.739398	0.954551	0.000031
3	6	0	-1.291507	-0.334065	-0.000103
4	16	0	0.000001	-1.589902	0.000073
5	6	0	1.291506	-0.334064	-0.000101
6	6	0	2.657404	-0.569394	-0.000223
7	6	0	3.511578	0.538248	-0.000148
8	6	0	2.985258	1.833660	0.000011
9	6	0	1.604886	2.050675	0.000078
10	6	0	-1.604888	2.050674	0.000060
11	6	0	-2.985259	1.833659	-0.000014
12	6	0	-3.511579	0.538246	-0.000144
13	6	0	-2.657404	-0.569395	-0.000211
14	8	0	0.000021	-2.335388	-1.267246
15	8	0	-0.000018	-2.334828	1.267732
16	1	0	3.049302	-1.581898	-0.000366
17	1	0	4.587284	0.389568	-0.000229
18	1	0	3.658462	2.686251	0.000080
19	1	0	1.214004	3.064117	0.000183
20	1	0	-1.214006	3.064116	0.000153
21	1	0	-3.658464	2.686249	0.000031
22	1	0	-4.587285	0.389566	-0.000205
23	1	0	-3.049302	-1.581900	-0.000328

FSF(Et)
HF=-2325.6383698 Hartree
Dipole moment: 5.7212 Debye

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.734237	0.437726	-0.066638
2	6	0	0.734183	0.437728	0.063396
3	6	0	1.285960	-0.850136	0.120445
4	16	0	-0.000093	-2.105708	-0.000802
5	6	0	-1.286103	-0.850146	-0.122640
6	6	0	-2.642369	-1.089985	-0.241855
7	6	0	-3.525139	0.005847	-0.314661
8	6	0	-2.978714	1.302938	-0.258905
9	6	0	-1.607880	1.525619	-0.135873
10	6	0	1.607871	1.525620	0.132049
11	6	0	2.978653	1.302952	0.255678
12	6	0	3.524977	0.005868	0.312644
13	6	0	2.642171	-1.089965	0.240313
14	8	0	-0.118191	-2.851432	1.261589
15	8	0	0.117984	-2.851978	-1.262871
16	6	0	-4.986565	-0.205343	-0.444700
17	6	0	4.986326	-0.205281	0.443631
18	6	0	-5.490551	-1.249991	-1.242585
19	6	0	-6.861107	-1.463625	-1.377802

20	6	0	-7.750234	-0.624840	-0.703478
21	6	0	-7.262491	0.423062	0.103322
22	6	0	-5.897041	0.633544	0.230029
23	6	0	5.897227	0.633046	-0.231217
24	6	0	7.262601	0.422745	-0.103376
25	6	0	7.749837	-0.624414	0.704695
26	6	0	6.860281	-1.462705	1.379069
27	6	0	5.489809	-1.249256	1.242717
28	6	0	-9.216350	-0.611043	-0.650879
29	6	0	-9.621232	0.440946	0.196040
30	6	0	-8.412286	1.187840	0.758480
31	6	0	8.412820	1.187065	-0.758324
32	6	0	9.621418	0.440896	-0.194173
33	6	0	9.215993	-0.610460	0.653273
34	6	0	-10.161046	-1.429695	-1.273543
35	6	0	-11.517261	-1.188586	-1.044331
36	6	0	-11.921696	-0.145364	-0.204630
37	6	0	-10.973879	0.674618	0.420074
38	6	0	10.974213	0.674599	-0.417278
39	6	0	11.921644	-0.144720	0.208881
40	6	0	11.516672	-1.187329	1.049083
41	6	0	10.160305	-1.428463	1.277370
42	6	0	8.416805	2.690927	-0.357310
43	6	0	8.352052	1.102291	-2.312653
44	6	0	8.339568	-0.307760	-2.910610
45	6	0	8.474952	2.986622	1.144565
46	6	0	-8.350193	1.104643	2.312817
47	6	0	-8.336992	-0.304813	2.912163
48	6	0	-8.416848	2.691316	0.355931
49	6	0	-8.476364	2.985488	-1.146184
50	1	0	-3.024059	-2.106059	-0.252600
51	1	0	-3.645146	2.156446	-0.339554
52	1	0	-1.228004	2.542938	-0.104865
53	1	0	1.228060	2.542938	0.100187
54	1	0	3.645105	2.156482	0.335917
55	1	0	3.023795	-2.106053	0.251981
56	1	0	-4.797112	-1.885306	-1.786328
57	1	0	-7.223403	-2.271781	-2.007843
58	1	0	-5.519158	1.424228	0.873759
59	1	0	5.519752	1.423166	-0.875874
60	1	0	7.222181	-2.270314	2.010038
61	1	0	4.796025	-1.884140	1.786523
62	1	0	-9.851153	-2.241915	-1.926243
63	1	0	-12.264599	-1.816628	-1.521779
64	1	0	-12.980693	0.030331	-0.035363
65	1	0	-11.300082	1.482457	1.071178
66	1	0	11.300825	1.481961	-1.068770
67	1	0	12.980753	0.031008	0.040355
68	1	0	12.263708	-1.814876	1.527653
69	1	0	9.850009	-2.240215	1.930462
70	1	0	9.271184	3.169056	-0.855483
71	1	0	7.518588	3.156497	-0.786036
72	1	0	7.456831	1.646138	-2.644365
73	1	0	9.209920	1.659937	-2.712626
74	1	0	8.290323	-0.254286	-4.003995
75	1	0	9.243130	-0.865679	-2.643709
76	1	0	7.474205	-0.883175	-2.565645
77	1	0	8.471674	4.068653	1.318386
78	1	0	7.614873	2.560790	1.672146
79	1	0	9.383412	2.578019	1.599056
80	1	0	-7.454758	1.648936	2.643219
81	1	0	-9.207792	1.662566	2.712977
82	1	0	-8.286578	-0.250250	4.005441
83	1	0	-9.240805	-0.863067	2.646803
84	1	0	-7.471966	-0.880526	2.566848
85	1	0	-9.270870	3.169810	0.854369
86	1	0	-7.518326	3.157462	0.783392
87	1	0	-8.473283	4.067344	-1.321098
88	1	0	-7.616747	2.559161	-1.674118
89	1	0	-9.385223	2.576390	-1.599425

FFSFF

HF=-3640.6088025 Hartree

Dipole moment: 5.6270 Debye

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.734056	-0.174462	0.352944
2	6	0	0.737589	-0.182755	0.273078
3	6	0	1.283016	1.068583	-0.047751
4	16	0	-0.014456	2.302747	-0.245150
5	6	0	-1.296426	1.084274	0.097036
6	6	0	-2.658162	1.321805	0.099542
7	6	0	-3.537050	0.256296	0.379921
8	6	0	-2.978959	-1.009499	0.647288
9	6	0	-1.602817	-1.231922	0.633503
10	6	0	1.619818	-1.249126	0.462936
11	6	0	2.991540	-1.043368	0.323375
12	6	0	3.532268	0.216775	-0.000511
13	6	0	2.640291	1.292752	-0.183219
14	8	0	-0.087658	2.759721	-1.641385
15	8	0	0.049315	3.303370	0.831136
16	6	0	-5.004430	0.464590	0.383811
17	6	0	4.994118	0.406599	-0.154793
18	6	0	-5.557278	1.670951	0.854926
19	6	0	-6.933648	1.888682	0.854223
20	6	0	-7.781006	0.887680	0.374772
21	6	0	-7.244705	-0.328385	-0.096546
22	6	0	-5.873836	-0.538577	-0.092645
23	6	0	5.903760	-0.297888	0.660933
24	6	0	7.269434	-0.118853	0.497318
25	6	0	7.759896	0.769551	-0.481835
26	6	0	6.872134	1.476162	-1.295592
27	6	0	5.501635	1.289676	-1.127274
28	6	0	-9.239175	0.835550	0.242107
29	6	0	-9.593668	-0.408565	-0.317263
30	6	0	-8.353485	-1.263669	-0.579347
31	6	0	8.418343	-0.774948	1.263437
32	6	0	9.629004	-0.135551	0.582552
33	6	0	9.223870	0.755724	-0.431403
34	6	0	-10.229034	1.766153	0.564546
35	6	0	-11.563969	1.447371	0.323729
36	6	0	-11.938625	0.209100	-0.234605
37	6	0	-10.925431	-0.719545	-0.551449
38	6	0	10.977209	-0.344086	0.836683
39	6	0	11.955578	0.334991	0.081443
40	6	0	11.530556	1.223366	-0.926178
41	6	0	10.178925	1.438193	-1.187584
42	6	0	8.411633	-2.324025	1.100583
43	6	0	8.365784	-0.447166	2.784218
44	6	0	8.367918	1.040073	3.150588
45	6	0	8.463616	-2.848099	-0.337686
46	6	0	-8.199734	-1.615919	-2.088198
47	6	0	-8.147228	-0.426913	-3.052398
48	6	0	-8.383413	-2.593364	0.230382
49	6	0	-8.532731	-2.450781	1.747929
50	6	0	-13.365618	-0.109146	-0.486385
51	6	0	13.400343	0.115432	0.336918
52	6	0	-14.370292	0.321556	0.404796
53	6	0	-15.701655	0.019589	0.156160
54	6	0	-16.064206	-0.721712	-0.986298
55	6	0	-15.082653	-1.156538	-1.878460
56	6	0	-13.747732	-0.847519	-1.623268
57	6	0	13.883406	-0.057967	1.648452
58	6	0	15.237514	-0.267143	1.905219
59	6	0	16.134916	-0.305643	0.836593
60	6	0	15.669922	-0.134867	-0.482608
61	6	0	14.320751	0.073199	-0.730671
62	6	0	17.587979	-0.506886	0.797365
63	6	0	18.006957	-0.464404	-0.548465
64	6	0	16.821321	-0.228452	-1.483656
65	6	0	-16.934235	0.380224	0.985622
66	6	0	-18.047257	-0.254243	0.152049
67	6	0	-17.521555	-0.891790	-0.990545
68	6	0	-19.417506	-0.266317	0.389670
69	6	0	-20.263333	-0.917716	-0.516771
70	6	0	-19.739468	-1.550184	-1.649045
71	6	0	-18.364601	-1.541773	-1.894534
72	6	0	18.511520	-0.713541	1.824370
73	6	0	19.859578	-0.876715	1.497316
74	6	0	20.277438	-0.834650	0.163117
75	6	0	19.350848	-0.628349	-0.866557
76	6	0	16.626010	-1.406900	-2.482880
77	6	0	16.981738	1.082792	-2.307693
78	6	0	17.188809	2.364418	-1.494953
79	6	0	16.447597	-2.793604	-1.857546
80	6	0	-17.112776	1.921521	1.117832
81	6	0	-16.867408	-0.223329	2.419314

82	6	0	-17.196263	2.702874	-0.196986
83	6	0	-16.688611	-1.742372	2.500216
84	1	0	-3.045103	2.307327	-0.139359
85	1	0	-3.641596	-1.833916	0.892831
86	1	0	-1.215340	-2.223718	0.849068
87	1	0	1.245687	-2.240191	0.703864
88	1	0	3.663205	-1.888271	0.441235
89	1	0	3.013810	2.287317	-0.405495
90	1	0	-4.899192	2.438481	1.251873
91	1	0	-7.333524	2.826897	1.229883
92	1	0	-5.458836	-1.462709	-0.487332
93	1	0	5.525503	-0.960358	1.435574
94	1	0	7.236039	2.156856	-2.060765
95	1	0	4.811212	1.814511	-1.781115
96	1	0	-9.970097	2.733698	0.987217
97	1	0	-12.333276	2.181439	0.545070
98	1	0	-11.200775	-1.689917	-0.957044
99	1	0	11.291177	-1.052862	1.598876
100	1	0	12.275819	1.772326	-1.494490
101	1	0	9.881119	2.135742	-1.966401
102	1	0	9.264538	-2.725181	1.664757
103	1	0	7.511689	-2.710844	1.598358
104	1	0	7.468069	-0.924169	3.200914
105	1	0	9.221262	-0.942199	3.263777
106	1	0	8.332943	1.162306	4.238980
107	1	0	9.270619	1.541559	2.786443
108	1	0	7.501183	1.559528	2.728707
109	1	0	8.450150	-3.943851	-0.343168
110	1	0	7.606341	-2.499696	-0.923238
111	1	0	9.375082	-2.522357	-0.849269
112	1	0	-7.287906	-2.217976	-2.202874
113	1	0	-9.033966	-2.274538	-2.365847
114	1	0	-8.036946	-0.779745	-4.083948
115	1	0	-9.061779	0.172912	-2.999842
116	1	0	-7.300109	0.230886	-2.832265
117	1	0	-9.206564	-3.206971	-0.160242
118	1	0	-7.460982	-3.146151	0.004536
119	1	0	-8.533974	-3.437999	2.223675
120	1	0	-7.709457	-1.872165	2.179982
121	1	0	-9.470120	-1.951121	2.013109
122	1	0	-14.088144	0.869344	1.300499
123	1	0	-15.347850	-1.720391	-2.769321
124	1	0	-12.985833	-1.158370	-2.332254
125	1	0	13.187279	0.000732	2.480343
126	1	0	15.582818	-0.388085	2.928963
127	1	0	13.957865	0.177461	-1.750217
128	1	0	-19.835491	0.221605	1.267308
129	1	0	-21.335300	-0.931930	-0.338617
130	1	0	-20.407829	-2.052034	-2.343710
131	1	0	-17.962452	-2.034588	-2.776220
132	1	0	18.191626	-0.746854	2.862903
133	1	0	20.589789	-1.037487	2.286026
134	1	0	21.329585	-0.963185	-0.076741
135	1	0	19.686925	-0.597684	-1.900600
136	1	0	15.754157	-1.175194	-3.109899
137	1	0	17.491187	-1.420569	-3.159775
138	1	0	17.827839	0.946998	-2.995216
139	1	0	16.091411	1.192730	-2.942072
140	1	0	17.289500	3.226421	-2.164189
141	1	0	16.343053	2.557060	-0.826542
142	1	0	18.094883	2.308266	-0.882790
143	1	0	16.325868	-3.550303	-2.640883
144	1	0	17.315595	-3.074892	-1.252203
145	1	0	15.561990	-2.832259	-1.214731
146	1	0	-18.019603	2.106274	1.709820
147	1	0	-16.276553	2.306471	1.717722
148	1	0	-16.044022	0.269280	2.954444
149	1	0	-17.786603	0.063783	2.948059
150	1	0	-17.313756	3.773671	0.004618
151	1	0	-16.290472	2.572771	-0.798258
152	1	0	-18.050400	2.380835	-0.801757
153	1	0	-16.657892	-2.065325	3.547006
154	1	0	-17.514443	-2.269459	2.011267
155	1	0	-15.755867	-2.062315	2.024080

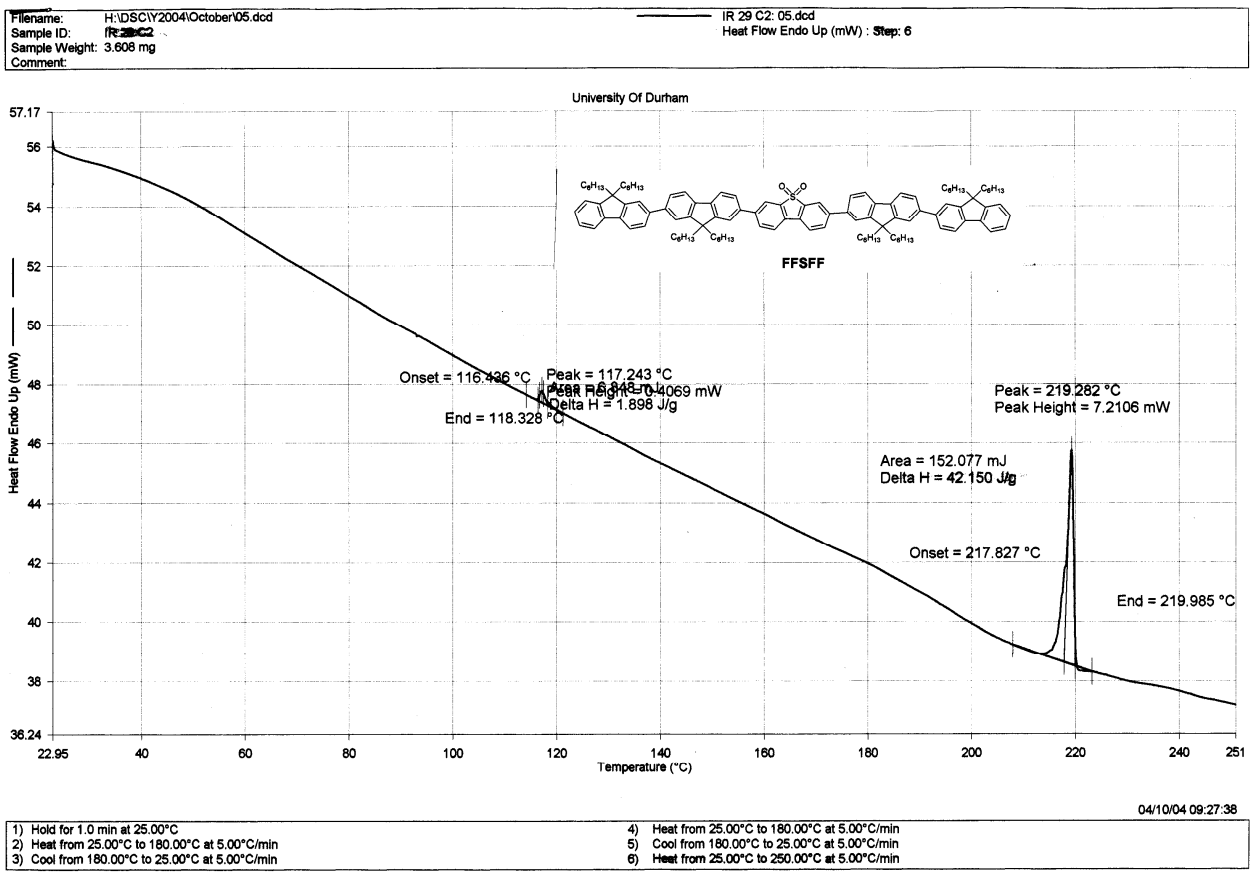
FSFSF

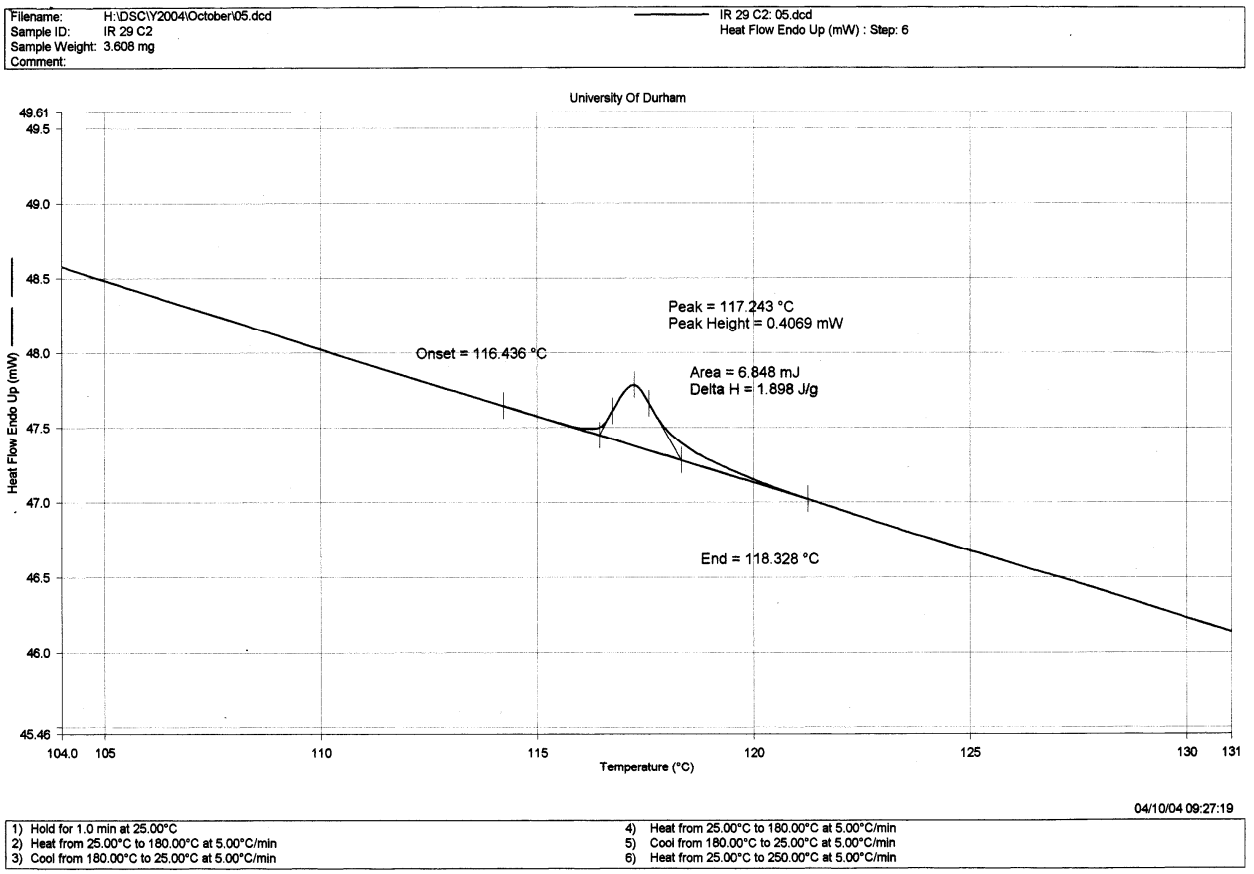
HF=-3992.6004057 Hartree

Dipole moment: 8.7453 Debye

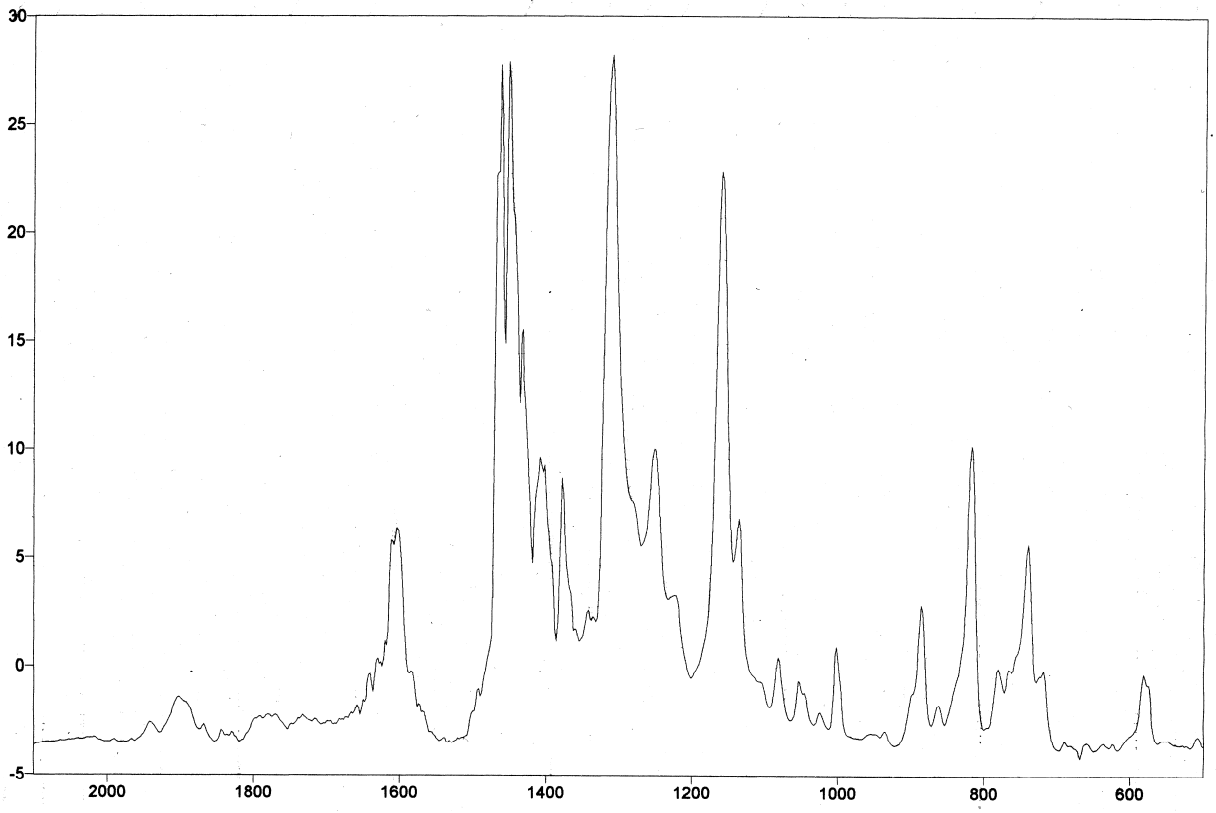
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.732158	-1.169860	-0.021637
2	6	0	-0.732091	-1.169613	0.026383
3	6	0	-1.179241	0.167278	0.041965
4	6	0	0.000124	1.139163	-0.005870
5	6	0	1.179423	0.166839	-0.046527
6	6	0	2.536714	0.450848	-0.090439
7	6	0	3.478568	-0.598209	-0.107591
8	6	0	3.014006	-1.927319	-0.080940
9	6	0	1.652413	-2.219867	-0.039469
10	6	0	-1.652425	-2.219388	0.051790
11	6	0	-3.013979	-1.926435	0.091541
12	6	0	-3.478431	-0.597140	0.109030
13	6	0	-2.536501	0.451703	0.084250
14	6	0	4.931895	-0.309374	-0.150931
15	6	0	-4.931746	-0.308017	0.150758
16	6	0	5.439073	0.765213	-0.907389
17	6	0	6.801778	1.054731	-0.963116
18	6	0	7.706861	0.261783	-0.253345
19	6	0	7.193810	-0.805646	0.497452
20	6	0	5.846215	-1.105857	0.566792
21	6	0	-5.846237	-1.109673	-0.560975
22	6	0	-7.193838	-0.809131	-0.493306
23	6	0	-7.706736	0.263566	0.250043
24	6	0	-6.801493	1.061640	0.953846
25	6	0	-5.438776	0.771865	0.899733
26	6	0	9.173594	0.382253	-0.168545
27	6	0	9.762969	-0.586732	0.656156
28	16	0	8.515373	-1.686921	1.347426
29	16	0	-8.515691	-1.697088	-1.335842
30	6	0	-9.763107	-0.591756	-0.652480
31	6	0	-9.173506	0.383245	0.164941
32	6	0	10.014114	1.309940	-0.788556
33	6	0	11.389790	1.248268	-0.570675
34	6	0	11.974273	0.271638	0.259471
35	6	0	11.124781	-0.665397	0.880870
36	6	0	-11.125005	-0.672224	-0.876039
37	6	0	-11.974392	0.269186	-0.261118
38	6	0	-11.389649	1.251911	0.561633
39	6	0	-10.013896	1.315324	0.778493
40	8	0	-8.661601	-3.053424	-0.786026
41	8	0	8.411128	-1.501890	2.802896
42	8	0	8.661751	-3.047542	0.808435
43	6	0	13.439945	0.228431	0.476645
44	6	0	-13.440157	0.224154	-0.477248
45	6	0	14.332097	0.522383	-0.574993
46	6	0	15.701765	0.478634	-0.358484
47	6	0	16.211849	0.144728	0.912438
48	6	0	15.341276	-0.149394	1.963294
49	6	0	13.966576	-0.106887	1.738556
50	6	0	-13.967410	-0.121471	-1.736114
51	6	0	-15.342222	-0.165829	-1.959821
52	6	0	-16.212293	0.136889	-0.910991
53	6	0	-15.701572	0.481236	0.356879
54	6	0	-14.331804	0.526749	0.572355
55	6	0	-17.677636	0.170969	-0.849410
56	6	0	-18.059635	0.530773	0.459168
57	6	0	-16.834787	0.753187	1.346035
58	6	0	16.835487	0.741992	-1.349338
59	6	0	18.059867	0.527070	-0.460058
60	6	0	17.677220	0.178257	0.851305
61	6	0	19.407169	0.630827	-0.789313
62	6	0	20.372098	0.385518	0.195370
63	6	0	19.989780	0.038971	1.495701
64	6	0	18.639061	-0.067614	1.833557
65	6	0	-18.639944	-0.083186	-1.829091
66	6	0	-19.990504	0.026233	-1.491504
67	6	0	-20.372194	0.383691	-0.193953
68	6	0	-19.406786	0.637256	0.788175
69	6	0	-16.802807	-0.235737	2.549171
70	6	0	-16.778713	2.203264	1.909804
71	6	0	-16.805582	3.328992	0.871636
72	6	0	-16.855873	-1.725080	2.195870
73	6	0	16.780016	2.187020	-1.925853
74	6	0	16.803856	-0.257681	-2.543737
75	6	0	16.804891	3.321682	-0.897375
76	6	0	16.857094	-1.743727	-2.176890
77	6	0	0.047101	2.057091	1.250998

78	6	0	-0.046774	2.047754	-1.269522
79	6	0	-0.095448	1.323153	-2.618099
80	6	0	0.094929	1.342501	2.604931
81	8	0	-8.412200	-1.523548	-2.792780
82	1	0	2.884805	1.480836	-0.081144
83	1	0	3.731374	-2.741902	-0.121555
84	1	0	1.320556	-3.254726	-0.028944
85	1	0	-1.320660	-3.254325	0.048453
86	1	0	-3.731385	-2.740663	0.138068
87	1	0	-2.884508	1.481633	0.067888
88	1	0	4.748881	1.372045	-1.485867
89	1	0	7.150940	1.888352	-1.565898
90	1	0	5.495479	-1.926330	1.184901
91	1	0	-5.495631	-1.934520	-1.173315
92	1	0	-7.150536	1.899481	1.550822
93	1	0	-4.748439	1.382855	1.473641
94	1	0	9.604749	2.085132	-1.430232
95	1	0	12.029615	1.992050	-1.035983
96	1	0	11.535828	-1.451833	1.505967
97	1	0	-11.536176	-1.463265	-1.495231
98	1	0	-12.029303	1.999052	1.021773
99	1	0	-9.604389	2.095268	1.414297
100	1	0	13.938007	0.753499	-1.561708
101	1	0	15.720989	-0.401537	2.949983
102	1	0	13.287084	-0.308412	2.561741
103	1	0	-13.288322	-0.329703	-2.557961
104	1	0	-15.722411	-0.426039	-2.944228
105	1	0	-13.937243	0.766115	1.556909
106	1	0	19.715947	0.898591	-1.797185
107	1	0	21.427095	0.464433	-0.053074
108	1	0	20.750176	-0.148992	2.248945
109	1	0	18.346628	-0.337393	2.845208
110	1	0	-18.347984	-0.361482	-2.838571
111	1	0	-20.751257	-0.168065	-2.242778
112	1	0	-21.427069	0.464662	0.054347
113	1	0	-19.715112	0.913394	1.793919
114	1	0	-15.892510	-0.030794	3.129264
115	1	0	-17.644805	0.012547	3.209595
116	1	0	-17.621926	2.327263	2.602914
117	1	0	-15.870083	2.291887	2.521243
118	1	0	-16.761573	4.304766	1.368577
119	1	0	-15.954050	3.264437	0.185969
120	1	0	-17.721604	3.300040	0.272623
121	1	0	-16.823010	-2.332026	3.107615
122	1	0	-17.776136	-1.977427	1.658933
123	1	0	-16.008272	-2.019579	1.568358
124	1	0	17.624366	2.305062	-2.618625
125	1	0	15.872388	2.270120	-2.539565
126	1	0	15.893564	-0.058044	-3.125657
127	1	0	17.645881	-0.015144	-3.206242
128	1	0	16.761645	4.293158	-1.402725
129	1	0	15.952117	3.262792	-0.212742
130	1	0	17.719804	3.297977	-0.296430
131	1	0	16.824368	-2.359058	-3.083005
132	1	0	17.777326	-1.991011	-1.637562
133	1	0	16.009484	-2.032528	-1.546747
134	1	0	0.922260	2.714117	1.155344
135	1	0	-0.830587	2.717156	1.217359
136	1	0	-0.921599	2.705871	-1.178491
137	1	0	0.831242	2.707608	-1.241046
138	1	0	-0.123630	2.050035	-3.437551
139	1	0	0.784036	0.687576	-2.765115
140	1	0	-0.985179	0.690799	-2.703063
141	1	0	0.122843	2.075428	3.418993
142	1	0	-0.784764	0.708209	2.756221
143	1	0	0.984473	0.710606	2.695064

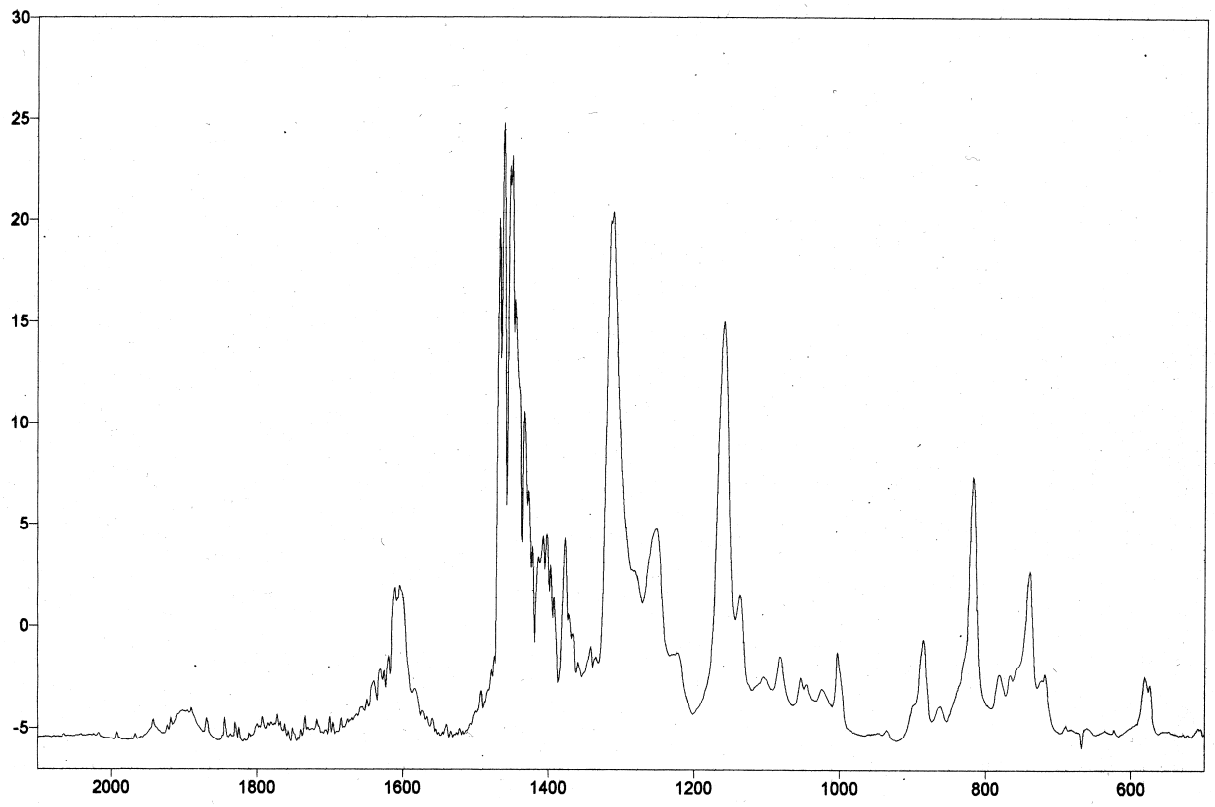




Differential scanning calorimetry of **FFSFF**

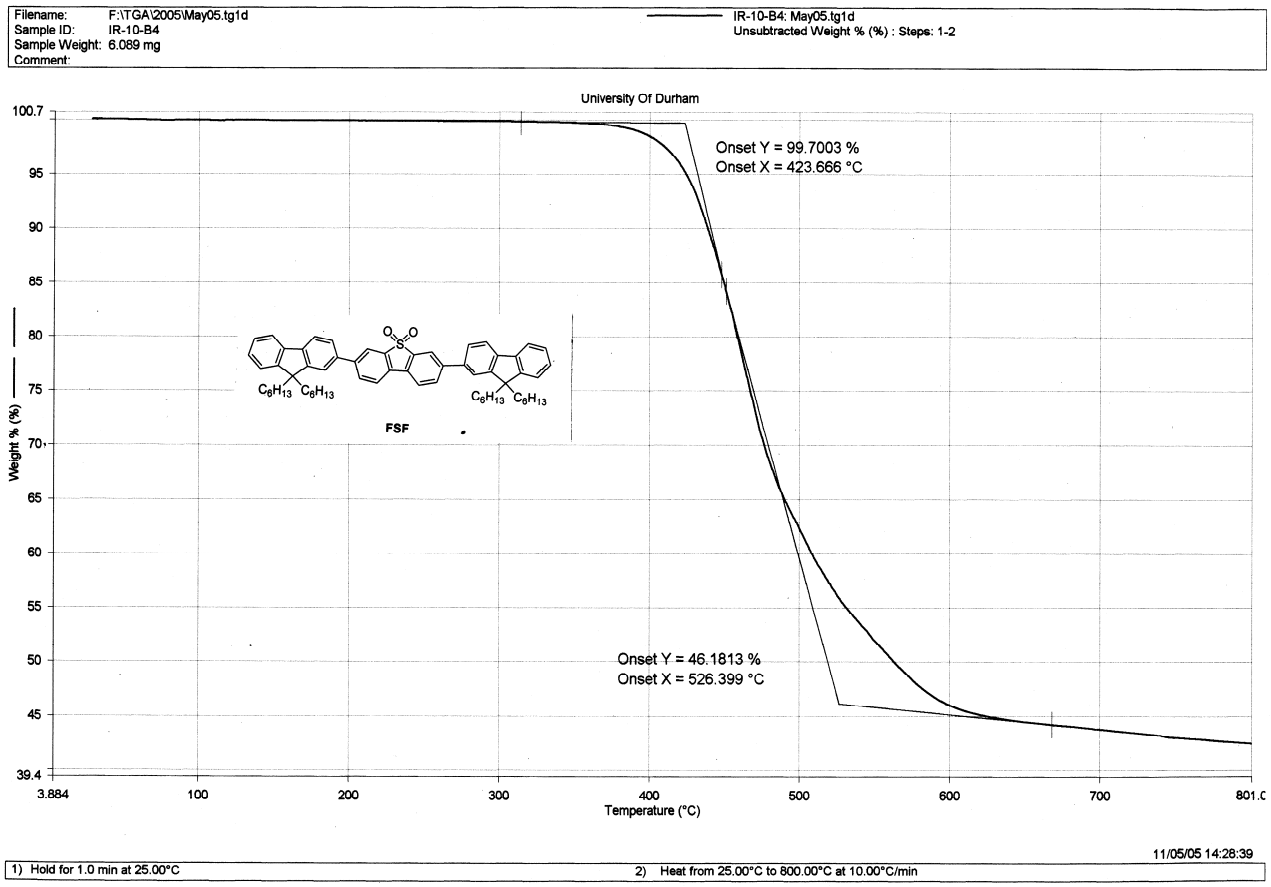


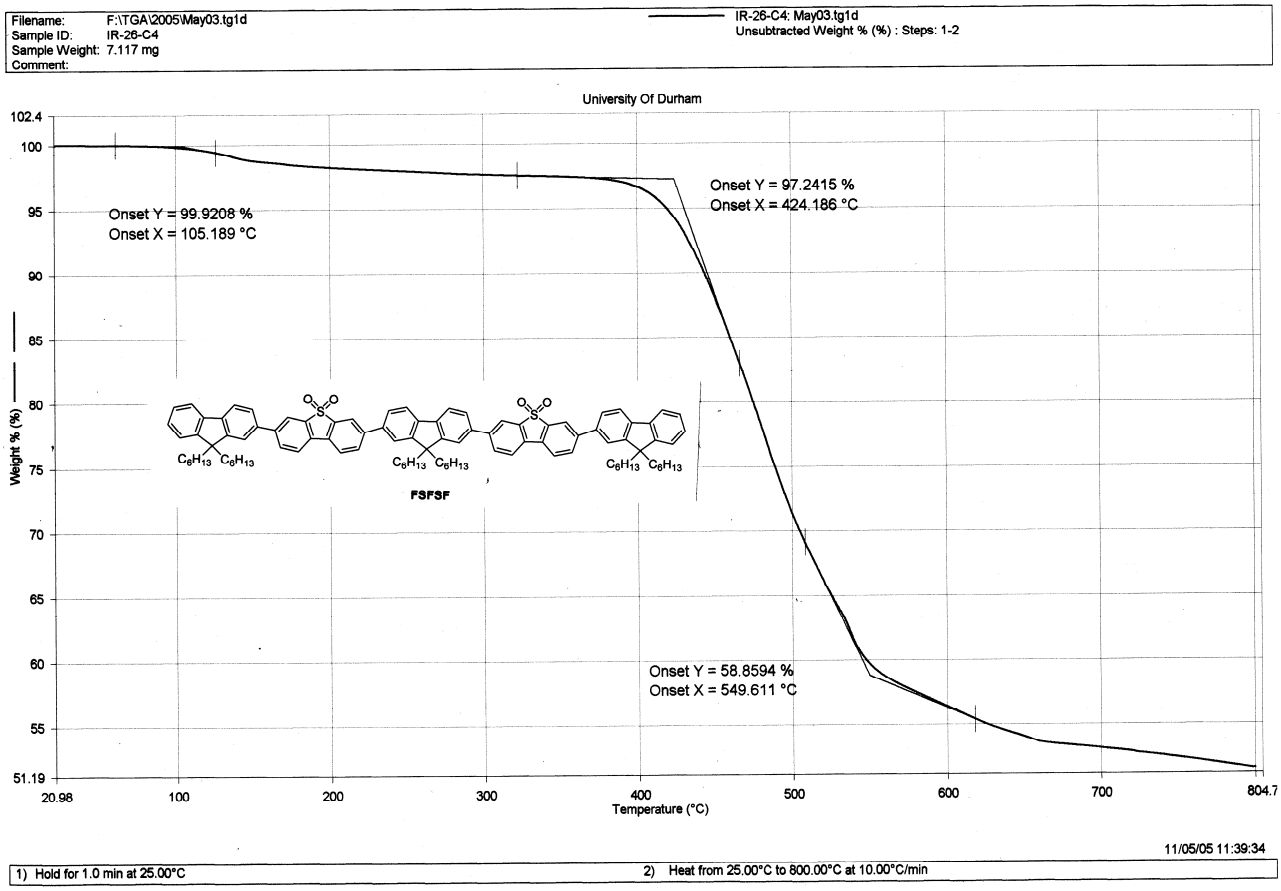
FTIR spectrum of pristine **FFSFF** (in KBr).

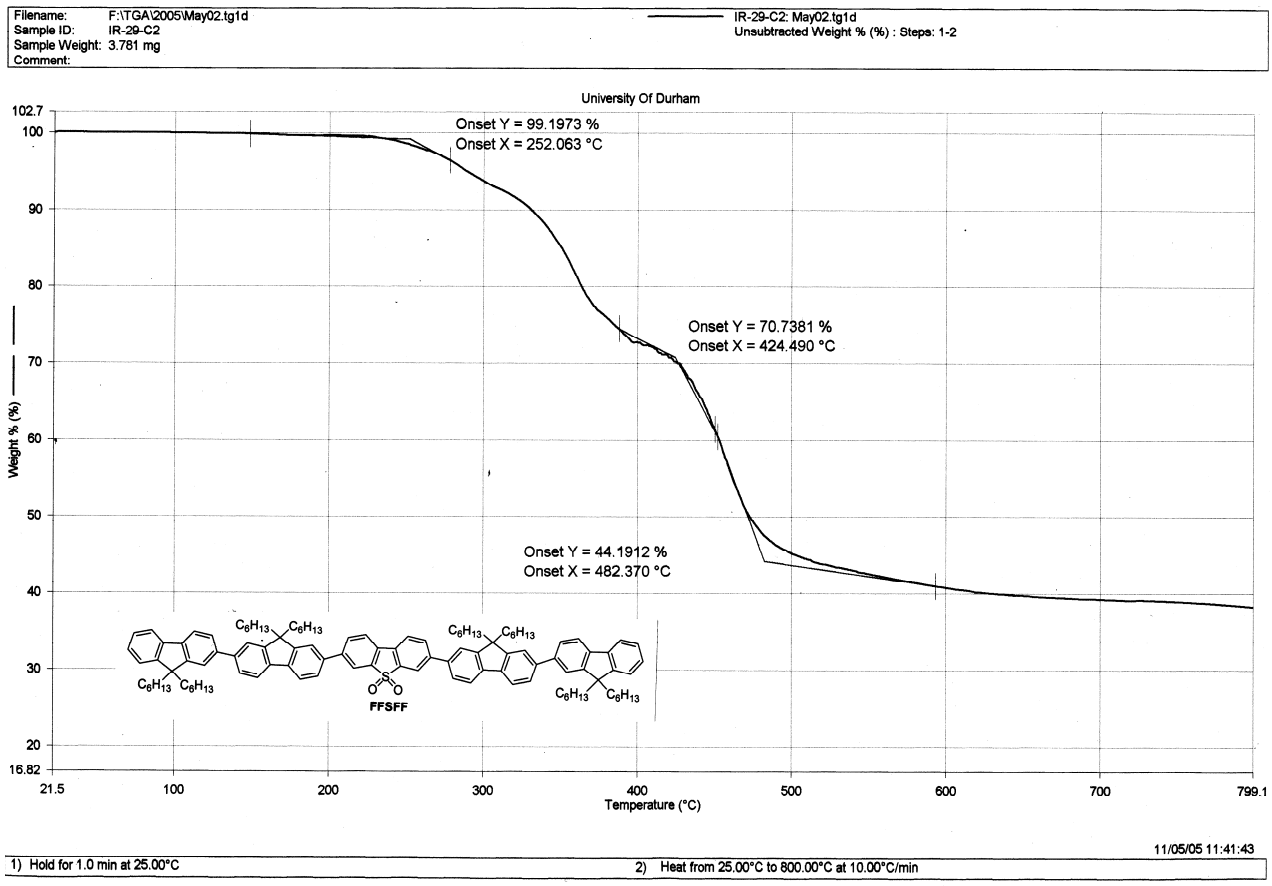


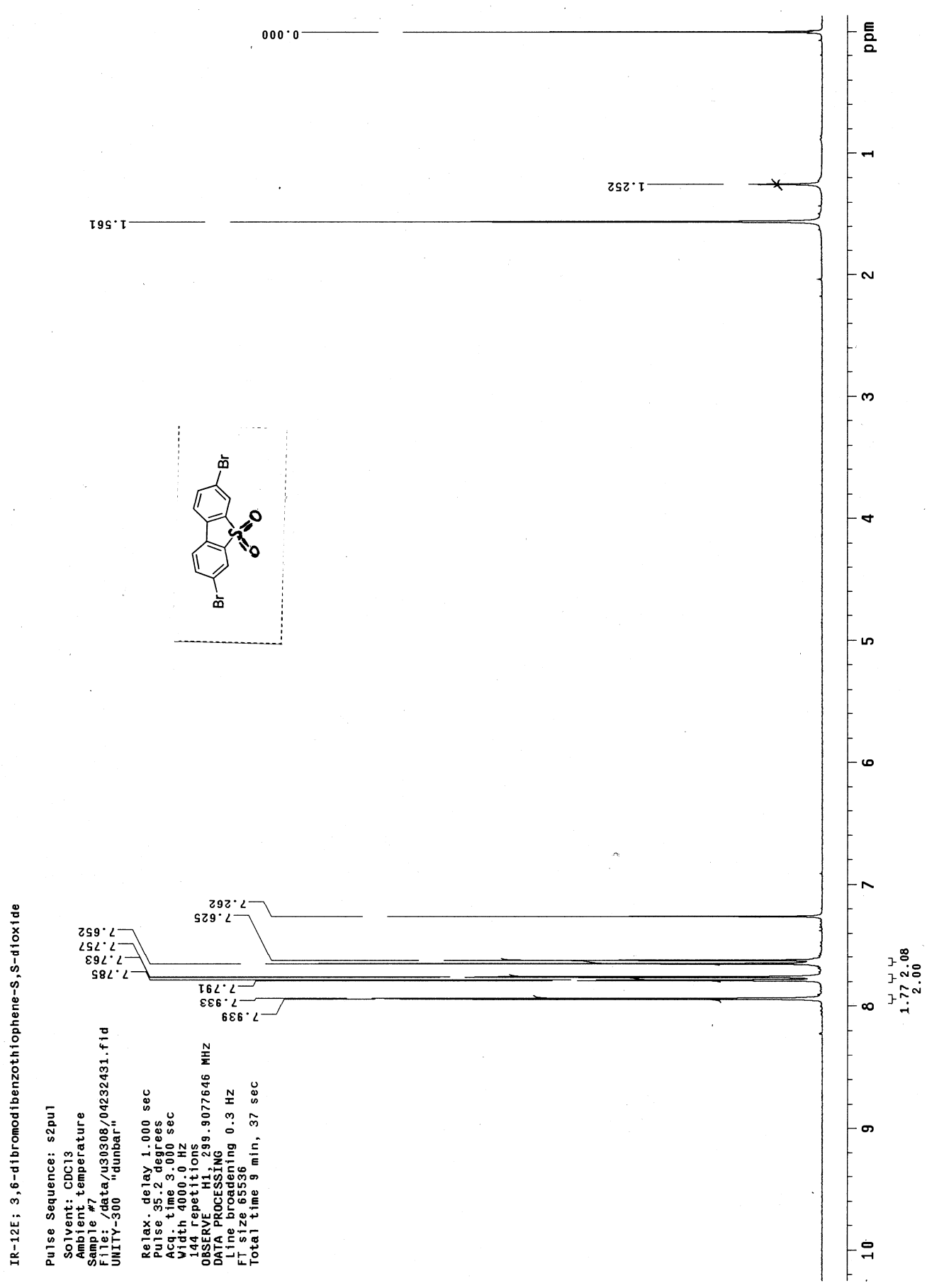
FTIR spectrum of **FFSFF** after annealing (in KBr).

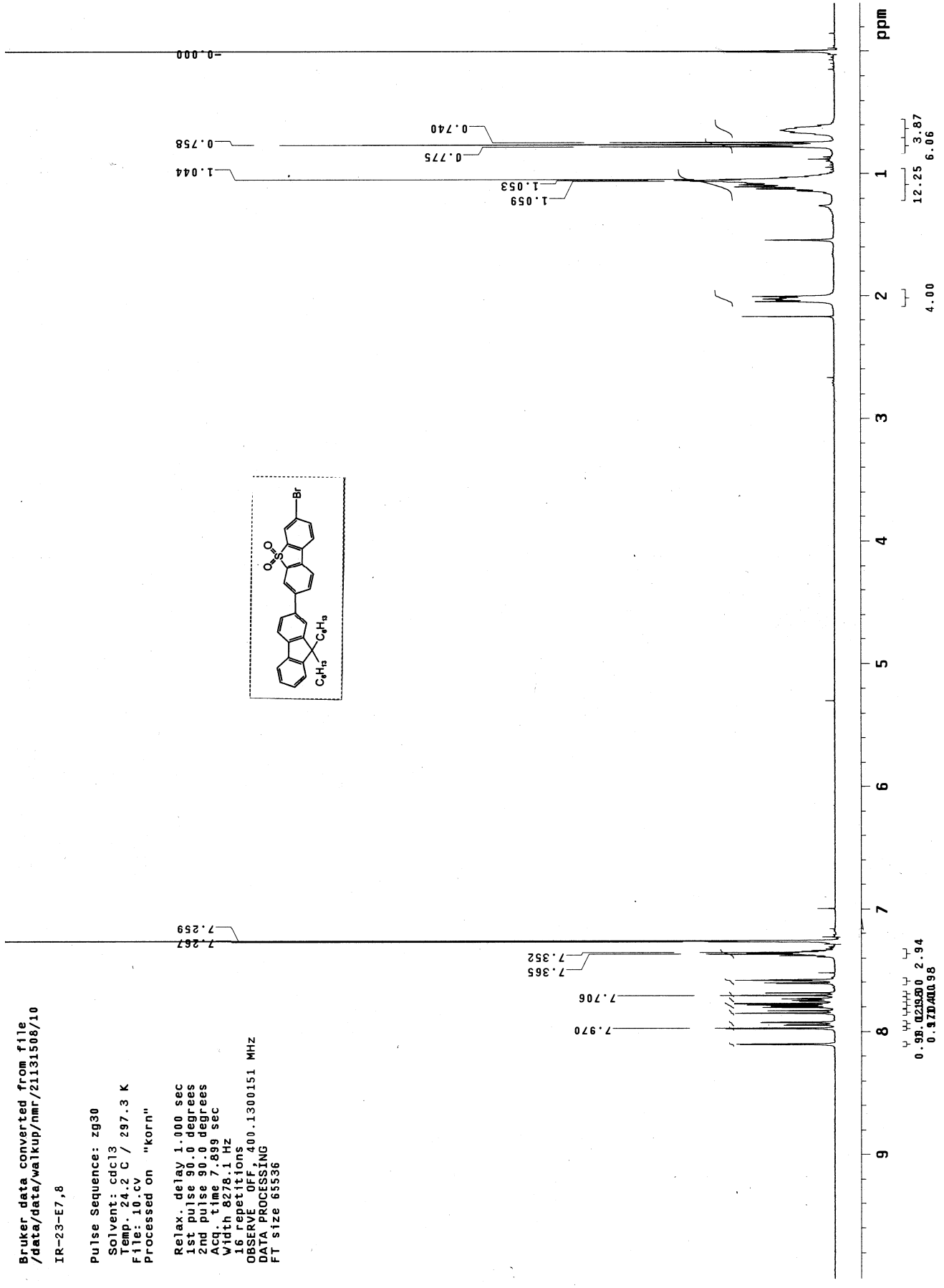
[The film of **FFSFF** was drop-casted from chloroform on quartz plate and annealed at 180 °C for 24 h in air. Then it was re-dissolved in dichloromethane, the solvent was evaporated and the IR spectrum of **FFSFF** in KBr was recorded.]

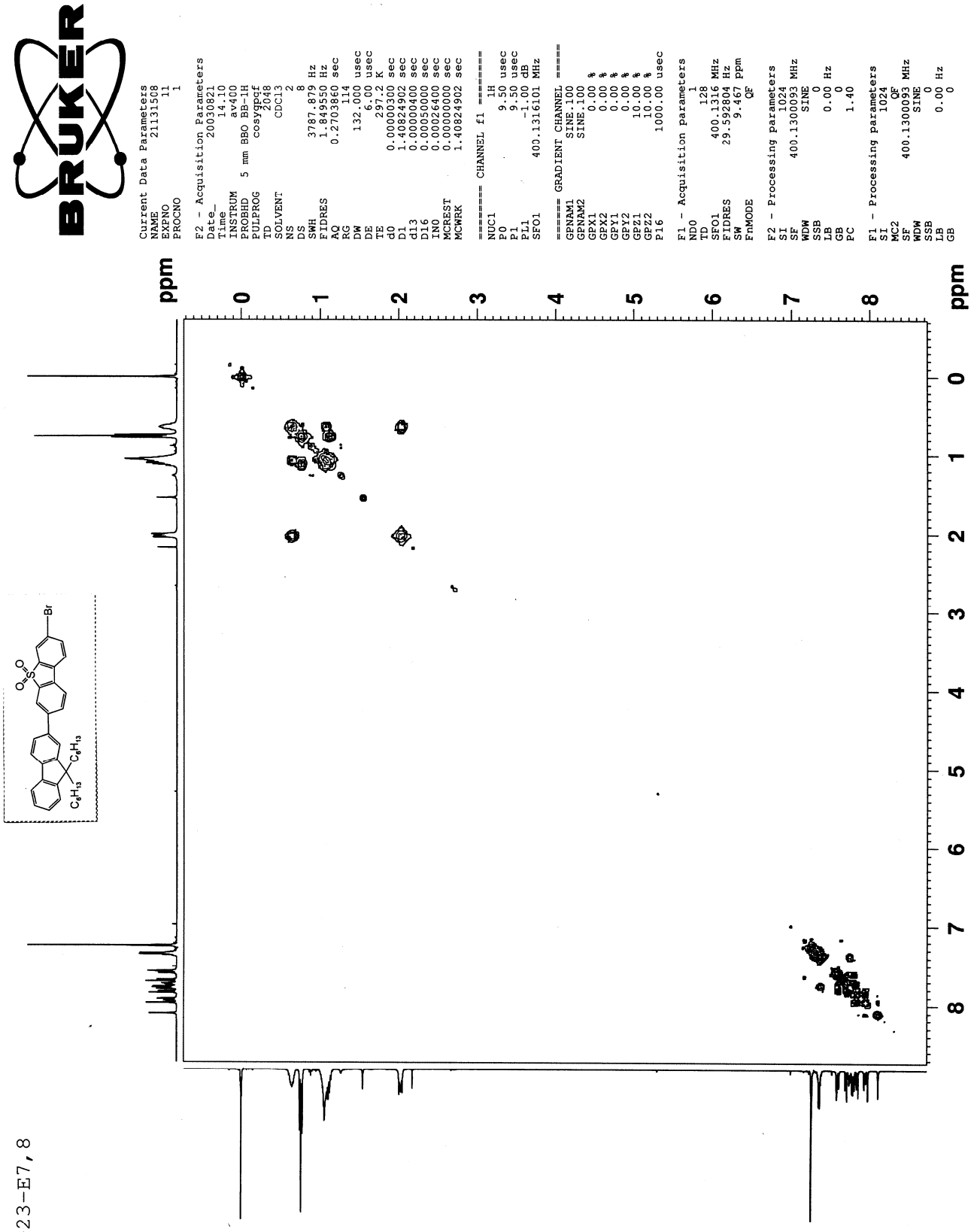

Filename: F:\TGA\2005\May05.tg1d
Sample ID: IR-10-B4
Sample Weight: 6.089 mg
Comment:
IR-10-B4: May05.tg1d
Unsubtracted Weight % (%) : Steps: 1-2
University Of Durham
Onset Y = 99.7003 %
Onset X = 423.666 °C
Onset Y = 46.1813 %
Onset X = 526.399 °C
FSF
Weight % (%)
Temperature (°C)
11/05/05 14:28:39
1) Hold for 1.0 min at 25.00°C
2) Heat from 25.00°C to 800.00°C at 10.00°C/min

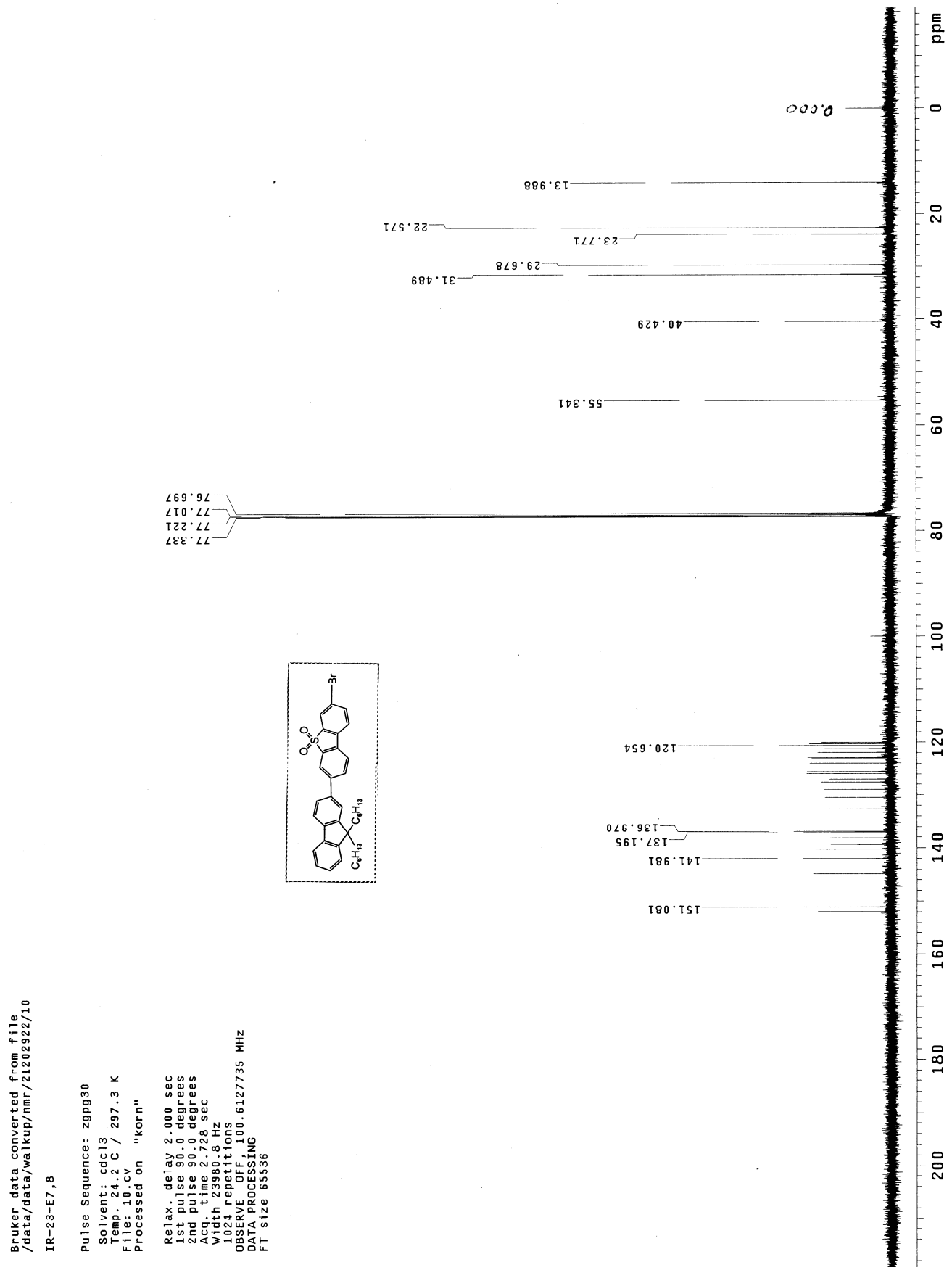

Filename: F:\TGA\2005\May03.tg1d
Sample ID: IR-26-C4
Sample Weight: 7.117 mg
Comment:
IR-26-C4: May03.tg1d
Unsubtracted Weight % (%) : Steps: 1-2
University Of Durham
Onset Y = 99.9208 %
Onset X = 105.189 °C
Onset Y = 97.2415 %
Onset X = 424.186 °C
Onset Y = 58.8594 %
Onset X = 549.611 °C
FSFSF
Weight % (%)
Temperature (°C)
11/05/05 11:39:34
1) Hold for 1.0 min at 25.00°C
2) Heat from 25.00°C to 800.00°C at 10.00°C/min

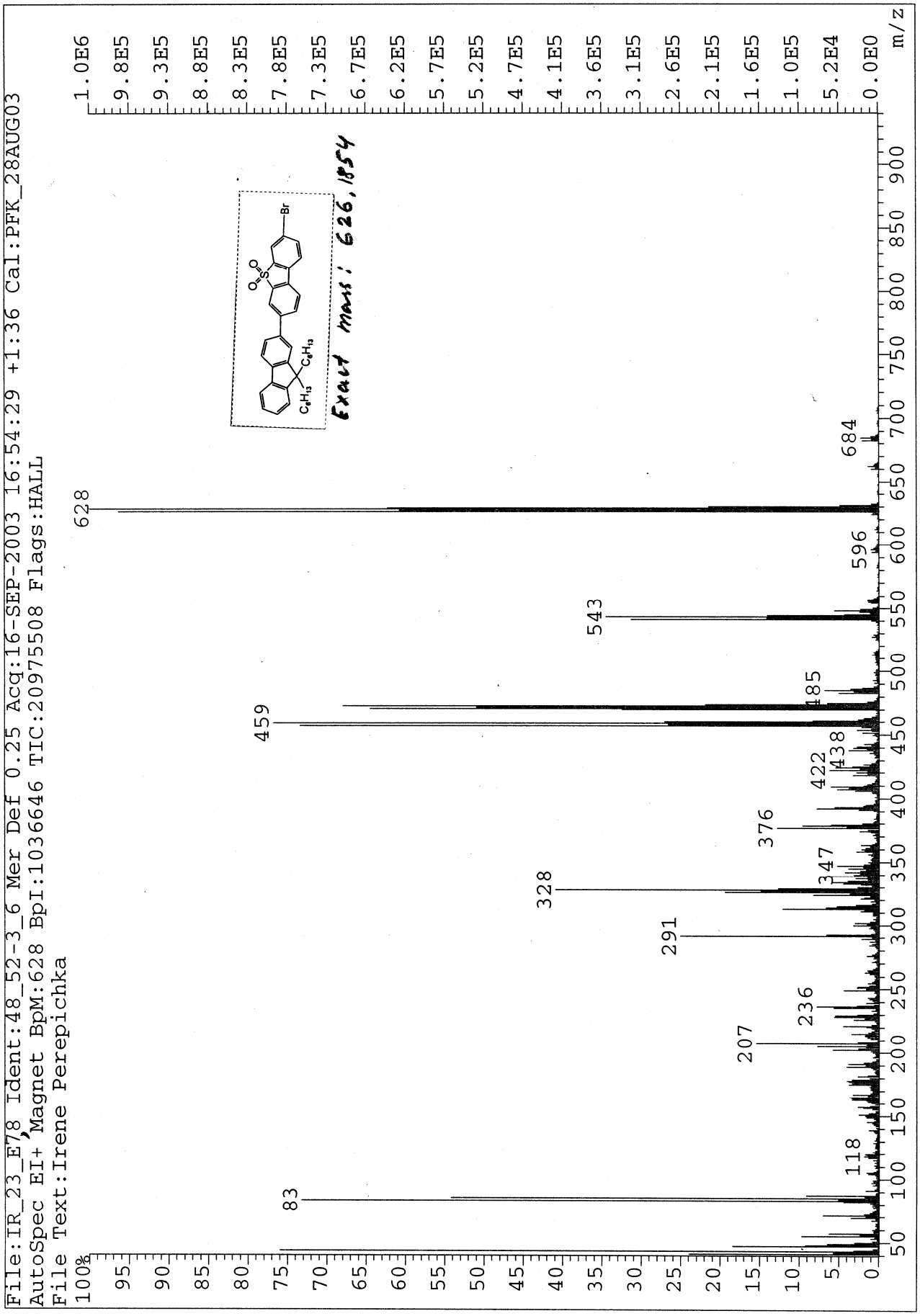

Filename: F:\TGA\2005\May02.tg1d
Sample ID: IR-29-C2
Sample Weight: 3.781 mg
Comment:
IR-29-C2: May02.tg1d
Unsubtracted Weight % (%) : Steps: 1-2
University Of Durham
Onset Y = 99.1973 %
Onset X = 252.063 °C
Onset Y = 70.7381 %
Onset X = 424.490 °C
Onset Y = 44.1912 %
Onset X = 482.370 °C
FFSFF
Weight % (%)
Temperature (°C)
102.7
100
90
80
70
60
50
40
30
20
16.82
21.5
100
200
300
400
500
600
700
799.1
11/05/05 11:41:43
1) Hold for 1.0 min at 25.00°C
2) Heat from 25.00°C to 800.00°C at 10.00°C/min

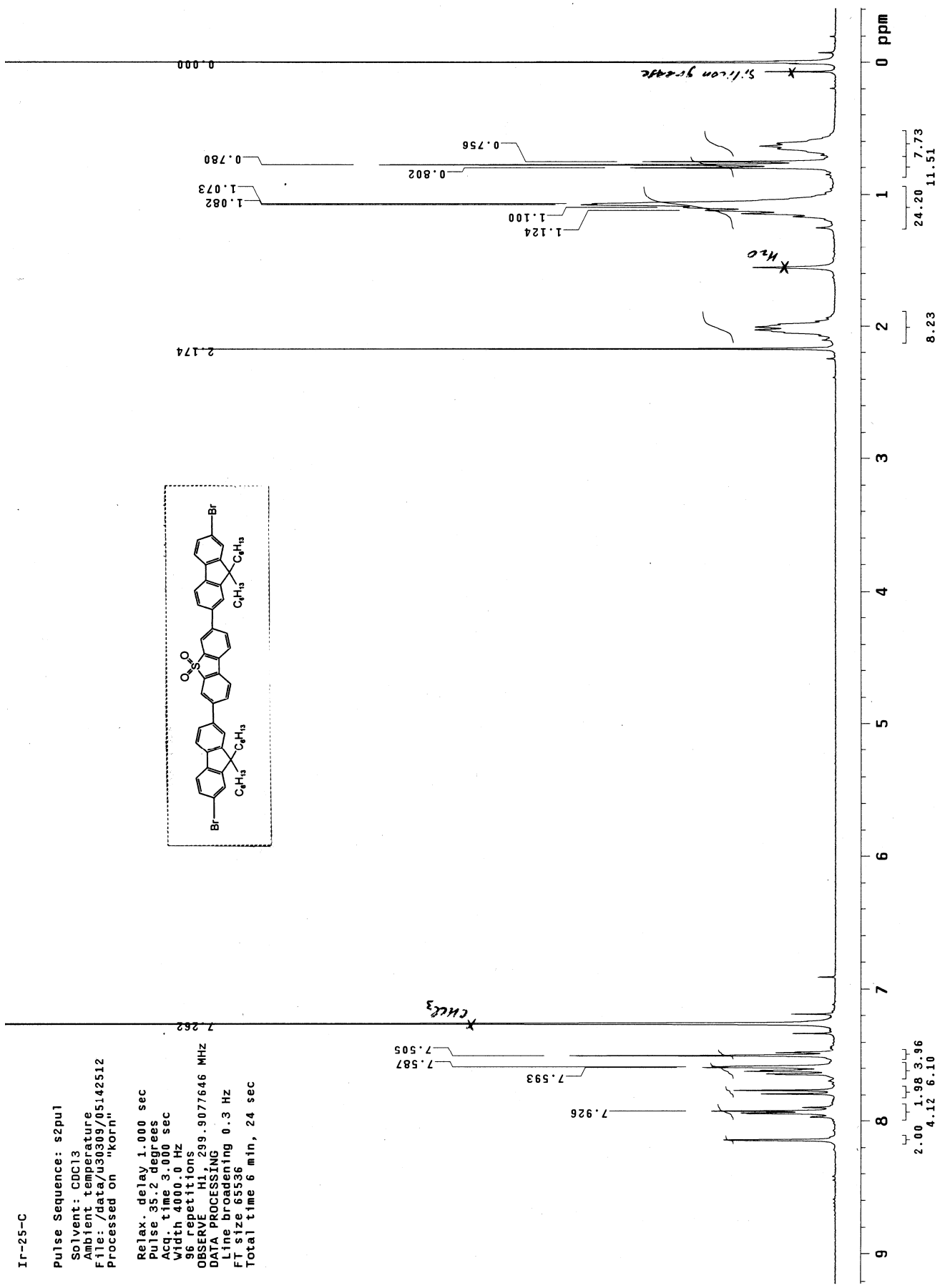

IR-12E; 3,6-dibromodibenzothiophene-S,S-dioxide
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Sample #7
File: /data/u30308/04232431.fid
UNITY-300 "dunbar"
Relax. delay 1.000 sec
Pulse 35.2 degrees
Acq. time 3.000 sec
Width 4000.0 Hz
144 repetitions
OBSERVE H1, 299.9077646 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 9 min, 37 sec
0.000
1.252
1.561
7.262
7.625
7.652
7.757
7.763
7.785
7.791
7.933
7.939
1.77 2.08
2.00
ppm
Br
Br
O
O
S

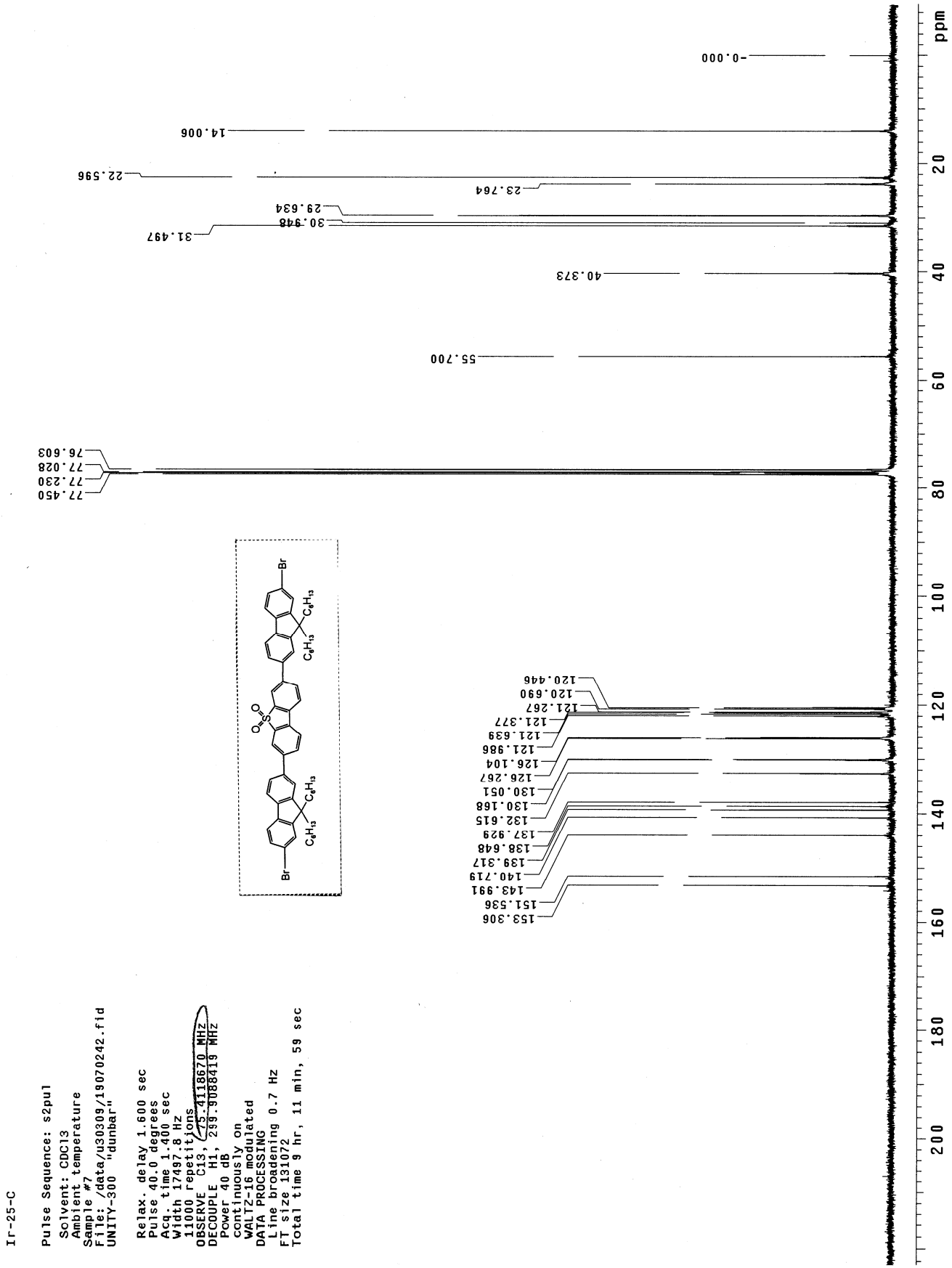

Bruker data converted from file
/data/data/walkup/nmr/21131508/10
IR-23-E7,8
Pulse Sequence: zg30
Solvent: cdcl3
Temp. 24.2 C / 297.3 K
File: 10.cv
Processed on "korn"
Relax. delay 1.000 sec
1st pulse 90.0 degrees
2nd pulse 90.0 degrees
Acq. time 7.899 sec
Width 8278.1 Hz
16 repetitions
OBSERVE OFF, 400.1300151 MHz
DATA PROCESSING
FT size 65536
0.000
0.758
1.044
0.740
0.775
1.053
1.059
7.259
7.267
7.352
7.365
7.706
7.970
ppm
Br
C_6H_{13}
C_6H_{13}

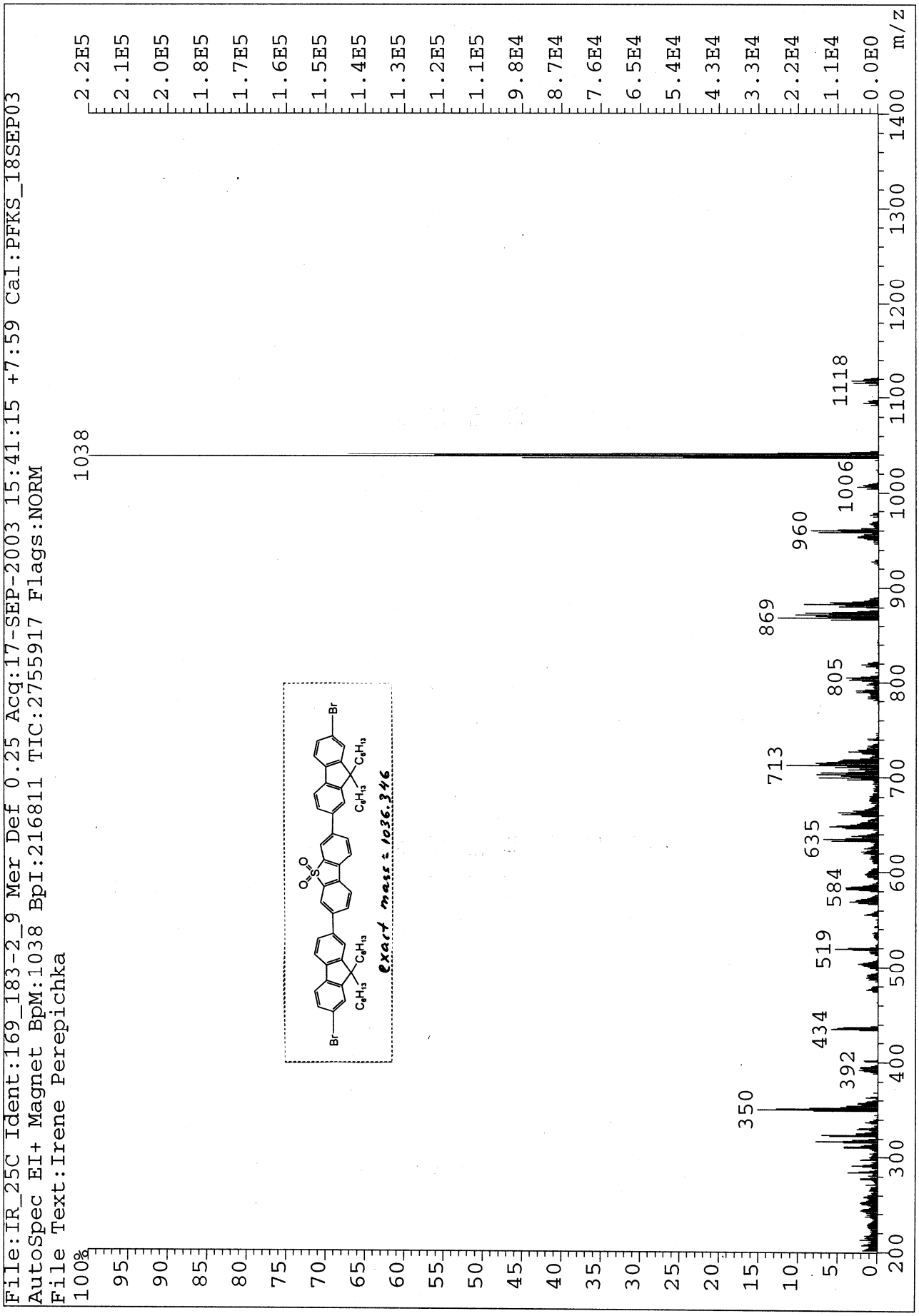

BRUKER
Current Data Parameters
NAME 21131508
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030821
Time_ 14.10
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG cosygpqf
TD 2048
SOLVENT CDCl3
NS 2
DS 8
SWH 3787.879 Hz
FIDRES 1.849550 Hz
AQ 0.2703860 sec
RG 114
DW 132.000 usec
DE 6.00 usec
TE 297.2 K
d0 0.00000300 sec
D1 1.40824902 sec
d13 0.00000400 sec
D16 0.00050000 sec
IN0 0.00026400 sec
MCREST 0.00000000 sec
MCWRK 1.40824902 sec
======== CHANNEL f1 ========
NUC1 1H
P0 9.50 usec
P1 9.50 usec
PL1 -1.00 dB
SFO1 400.1316101 MHz
====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec
F1 - Acquisition parameters
NDO 1
TD 128
SFO1 400.1316 MHz
FIDRES 29.592804 Hz
SW 9.467 ppm
FnMODE QF
F2 - Processing parameters
SI 1024
SF 400.1300093 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300093 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
ppm
ppm
IR-23-E7,8

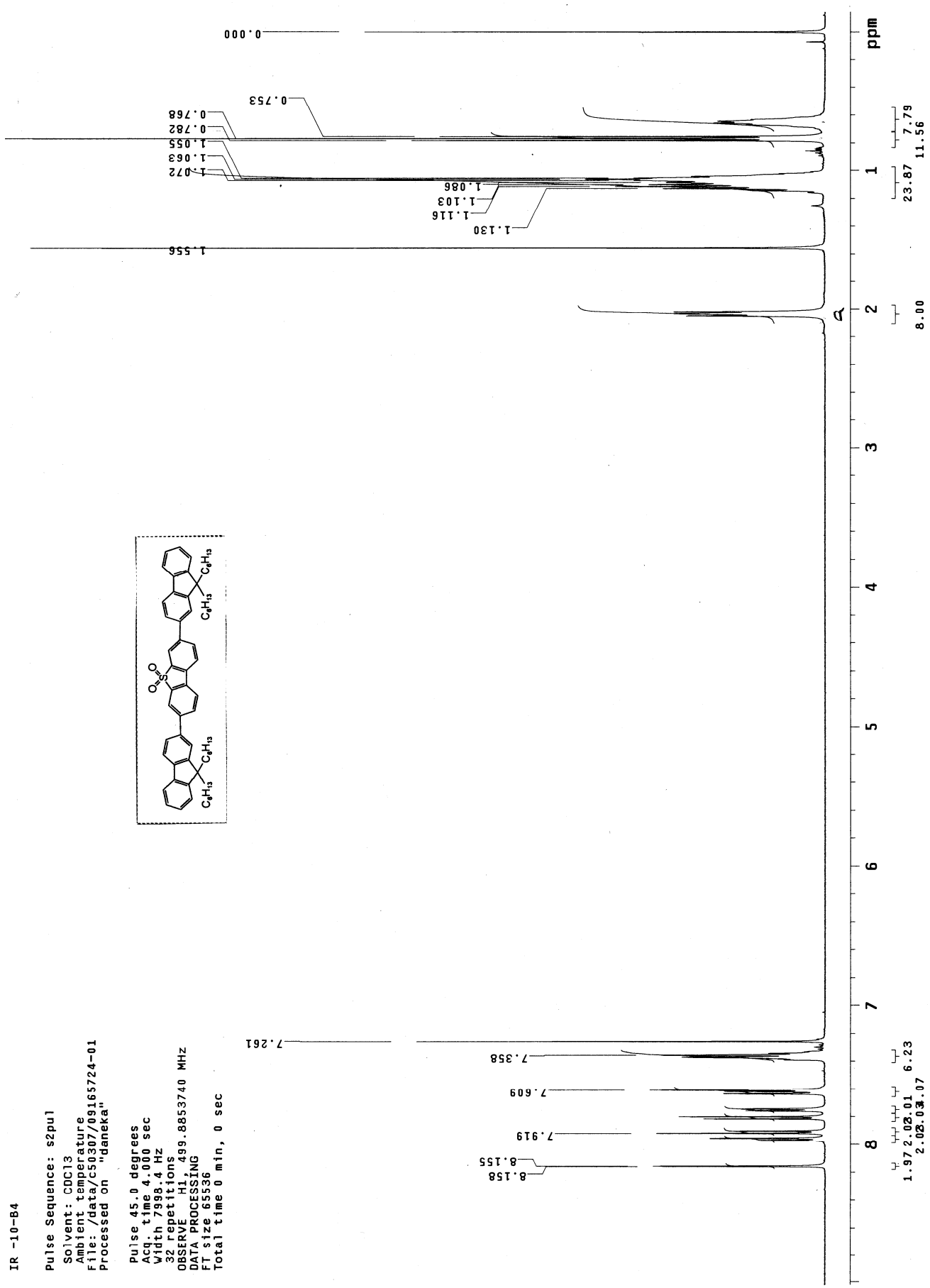

Bruker data converted from file
/data/data/walkup/nmr/21202922/10
IR-23-E7,8
Pulse Sequence: zgpg30
Solvent: cdcl3
Temp. 24.2 C / 297.3 K
File: 10.cv
Processed on "korn"
Relax. delay 2.000 sec
1st pulse 90.0 degrees
2nd pulse 90.0 degrees
Acq. time 2.728 sec
Width 23980.8 Hz
1024 repetitions
OBSERVE OFF, 100.6127735 MHz
DATA PROCESSING
FT size 65536
0.000
13.988
22.571
23.771
29.678
31.489
40.429
55.341
76.697
77.017
77.221
77.337
120.654
136.970
137.195
141.981
151.081
Br
O
O
S
C_6H_{13}
C_6H_{13}
ppm
0
20
40
60
80
100
120
140
160
180
200

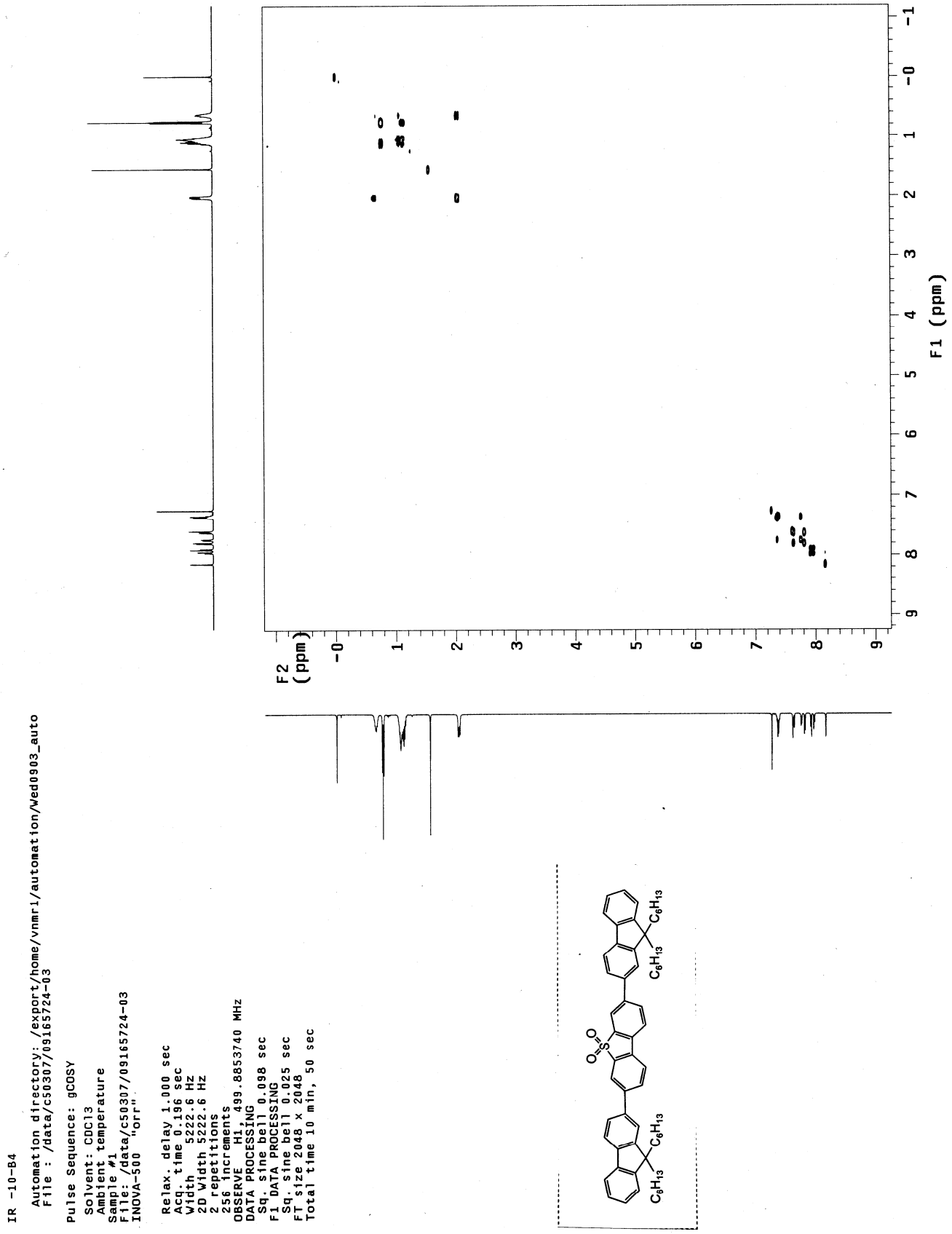

File:IR_23_E78 Ident:48_52-3_6 Mer Def 0.25 Acq:16-SEP-2003 16:54:29 +1:36 Cal:PFK_28AUG03
AutoSpec EI+ Magnet BpM:628 BpI:1036646 TIC:20975508 Flags:HALL
File Text:Irene Perepichka
Exact mass: 626,1854
m/z
100%
628
684
596
543
459
485
438
422
376
347
328
291
236
207
118
83

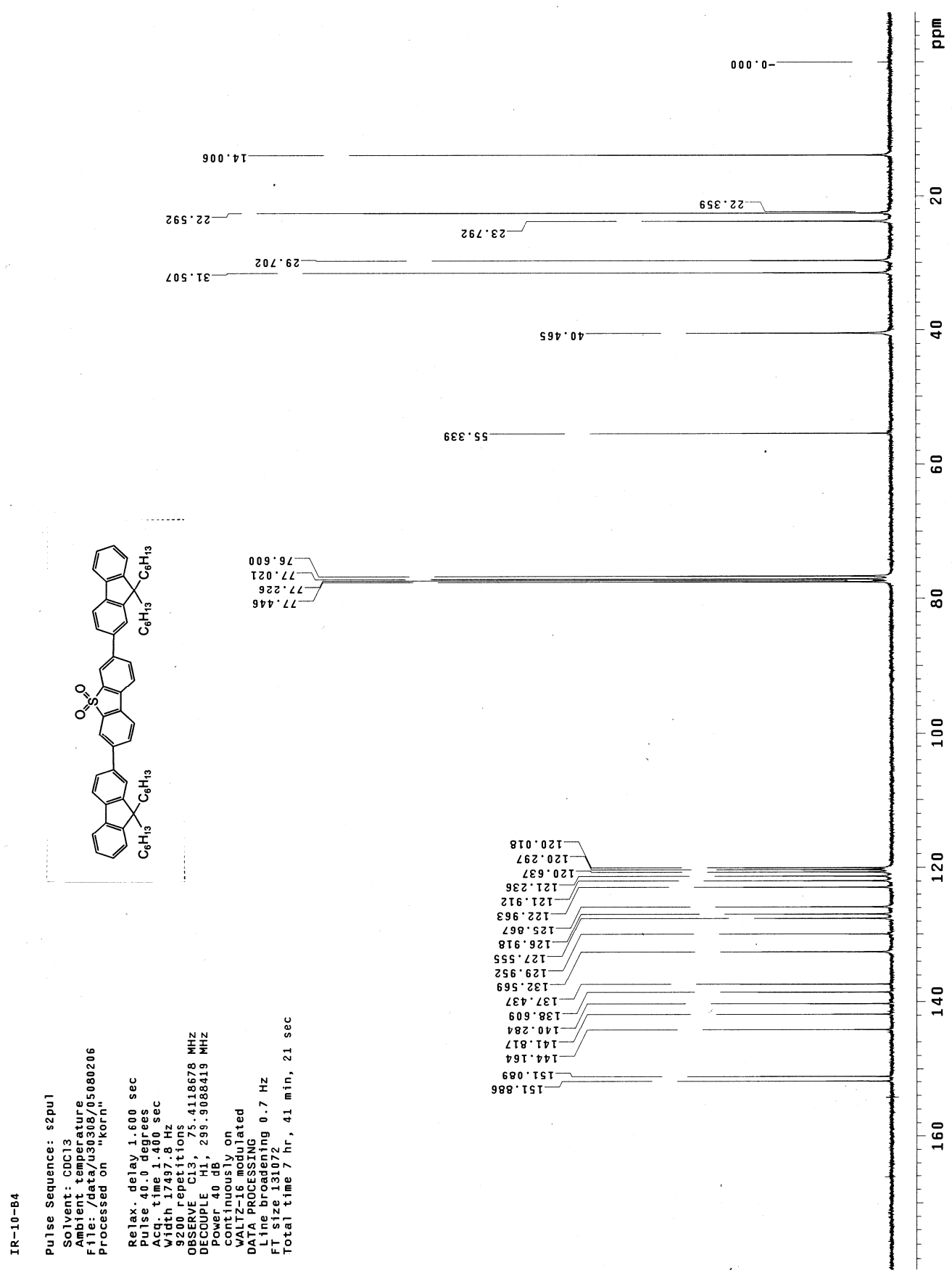

Ir-25-C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: /data/u30309/05142512
Processed on "korn"
Relax. delay 1.000 sec
Pulse 35.2 degrees
Acq. time 3.000 sec
Width 4000.0 Hz
96 repetitions
OBSERVE H1, 299.9077646 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 6 min, 24 sec
0.000
0.756
0.780
0.802
1.073
1.082
1.100
1.124
2.174
7.262
7.505
7.587
7.593
7.926
0 ppm
7.73
11.51
24.20
8.23
2.00
1.98
3.96
4.12
6.10
Br
C_6H_{13}
C_6H_{13}
C_6H_{13}
C_6H_{13}
Br

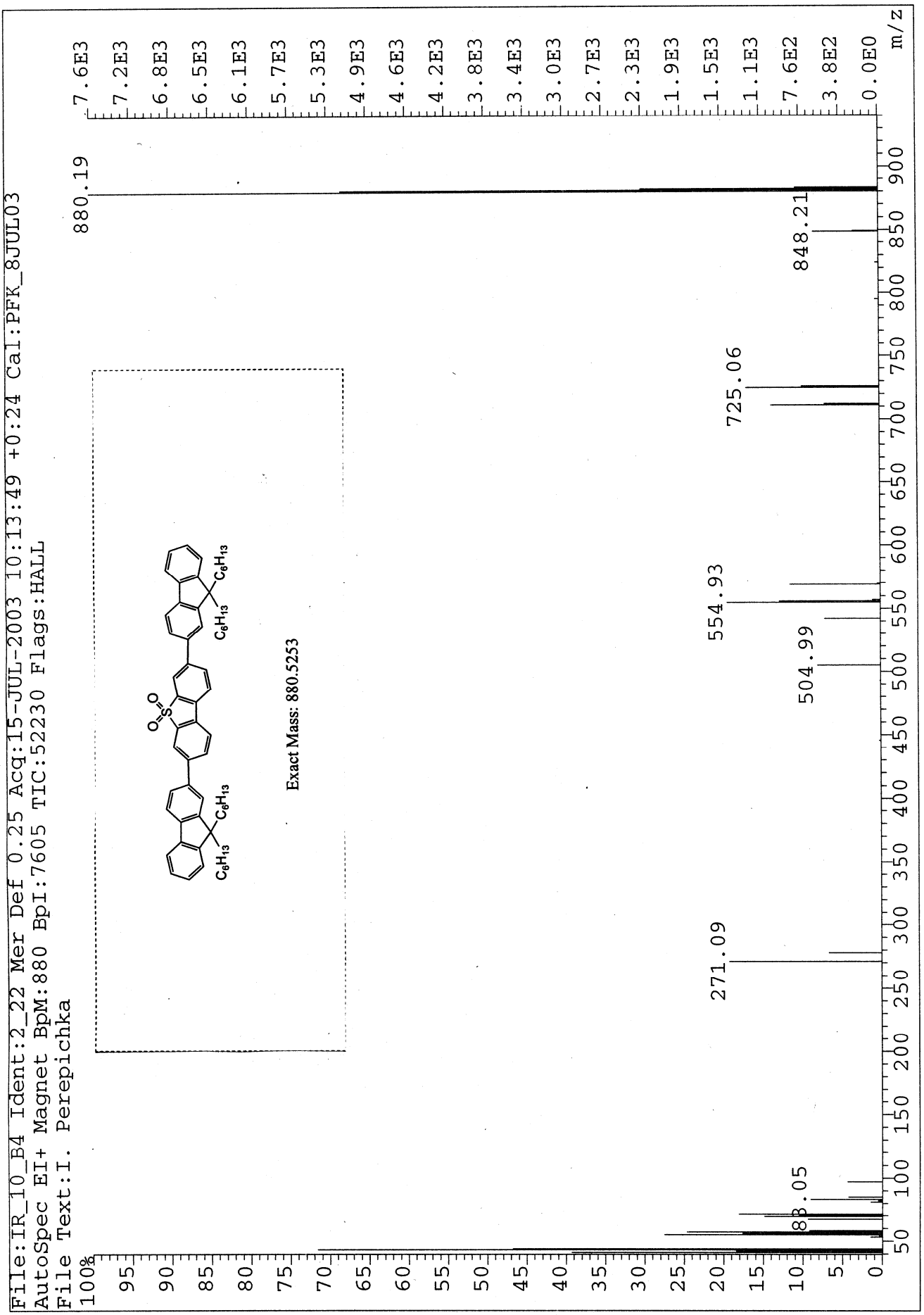

Ir-25-C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Sample #7
File: /data/u030309/19070242.fid
UNITY-300 "dunbar"
Relax. delay 1.600 sec
Pulse 40.0 degrees
Acq. time 1.400 sec
Width 17497.8 Hz
11000 repetitions
OBSERVE C13, 75.4118670 MHz
DECOUPLE H1, 299.9088419 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.7 Hz
FT size 131072
Total time 9 hr, 11 min, 59 sec
ppm
-0.000
14.006
22.596
23.764
29.634
30.948
31.497
40.373
55.700
76.603
77.028
77.230
77.450
120.446
120.690
121.267
121.377
121.639
121.986
126.104
126.267
130.051
130.168
132.615
137.929
138.648
139.317
140.719
143.991
151.536
153.306
Br
C_6H_{13}
C_6H_{13}
C_6H_{13}
C_6H_{13}
Br

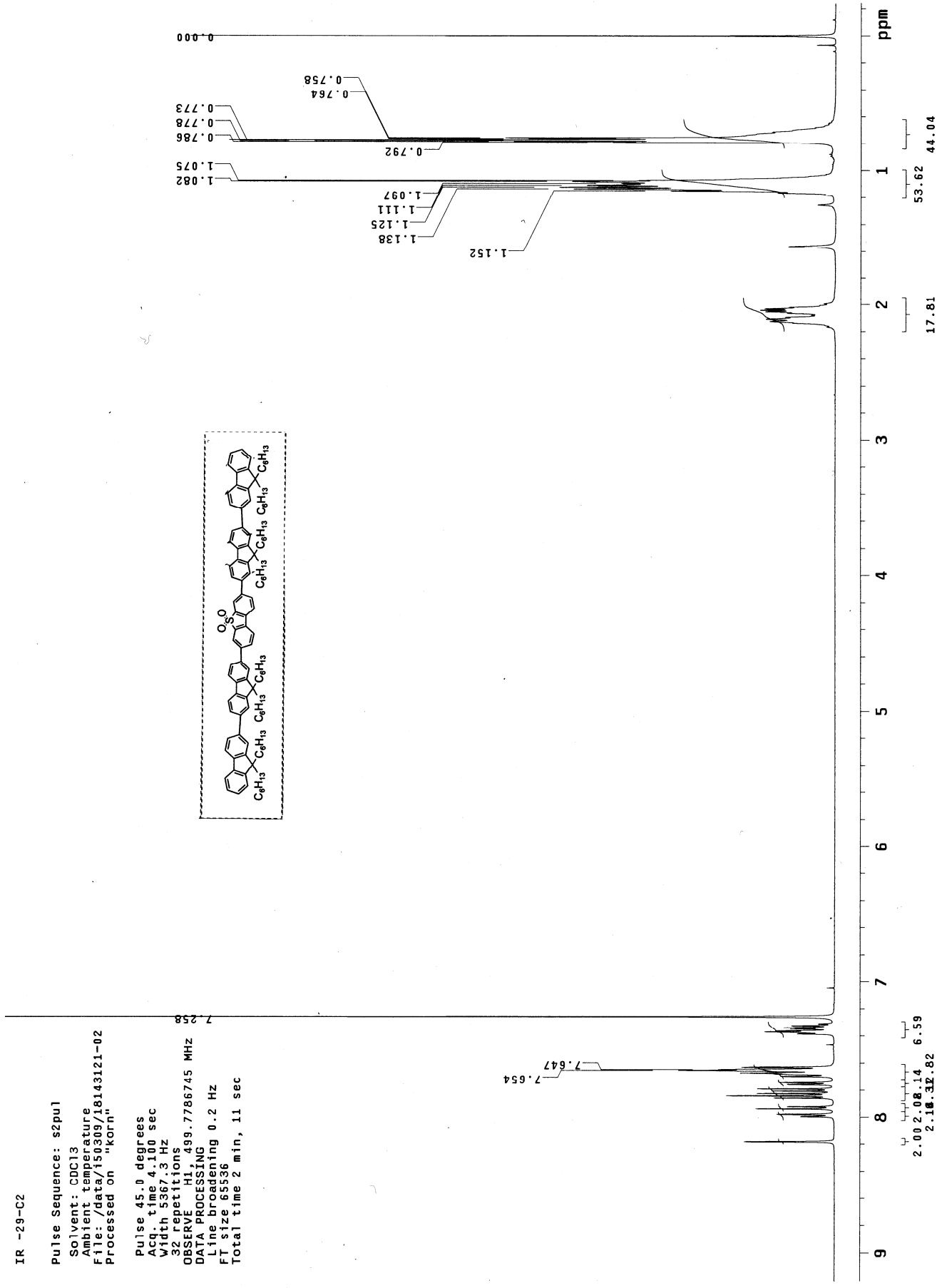

File:IR_25C Ident:169_183-2_9 Mer Def 0.25 Acq:17-SEP-2003 15:41:15 +7:59 Cal:PFKS_18SEP03
AutoSpec EI+ Magnet BpM:1038 BpI:216811 TIC:2755917 Flags:NORM
File Text:Irene Perepichka
100%
1038
1118
1006
960
869
805
713
635
584
519
434
392
350
m/z
Exact mass: 1036.346

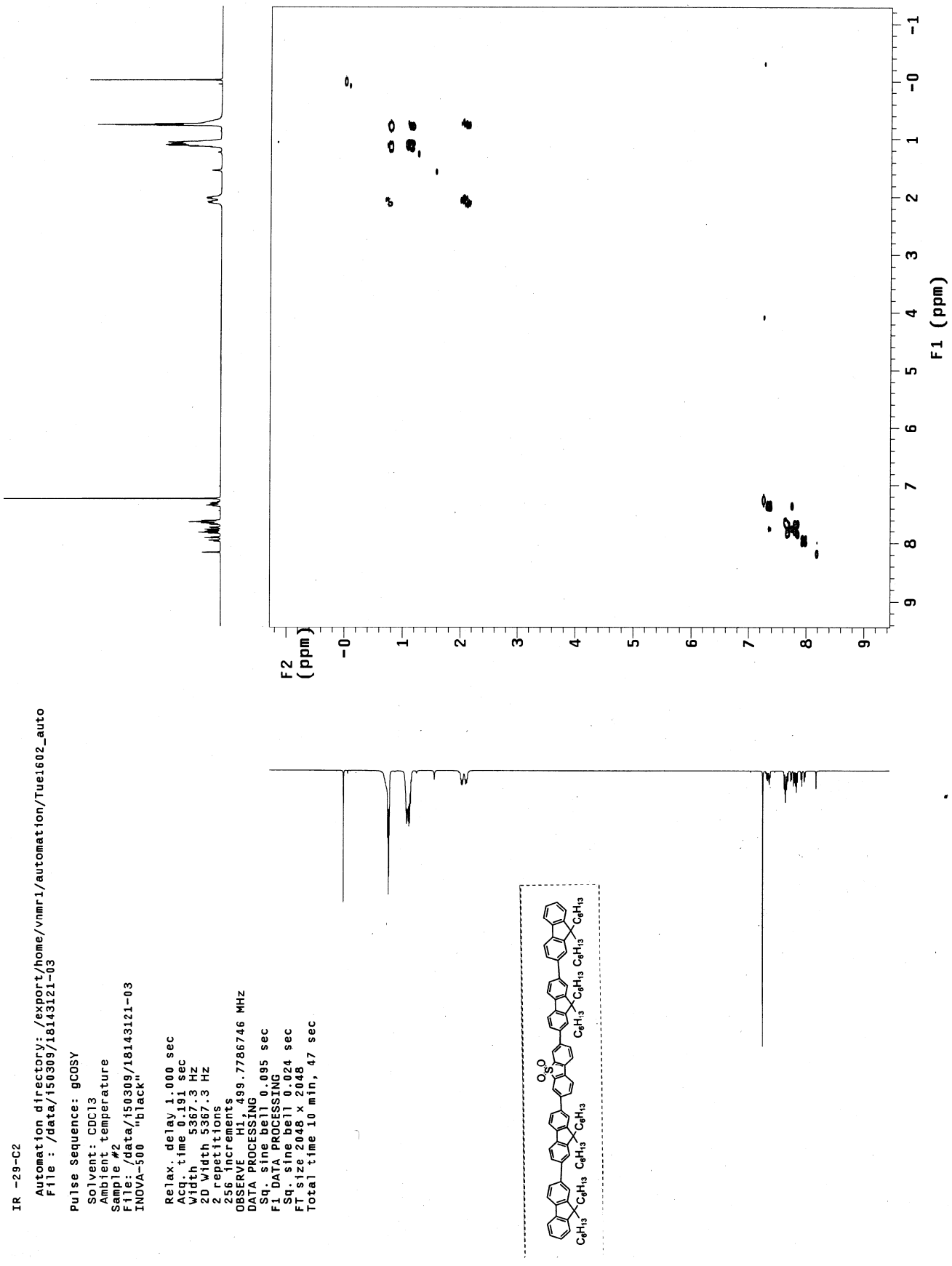

IR -10-B4
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: /data/c50307/09165724-01
Processed on "daneka"
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 7998.4 Hz
32 repetitions
OBSERVE H1, 499.8853740 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 0 sec
0.000
0.753
0.768
0.782
1.055
1.063
1.072
1.086
1.103
1.116
1.130
1.556
7.261
7.358
7.609
7.919
8.155
8.158
ppm
1.97
2.02
2.01
2.03
2.07
6.23
23.87
7.79
11.56
8.00

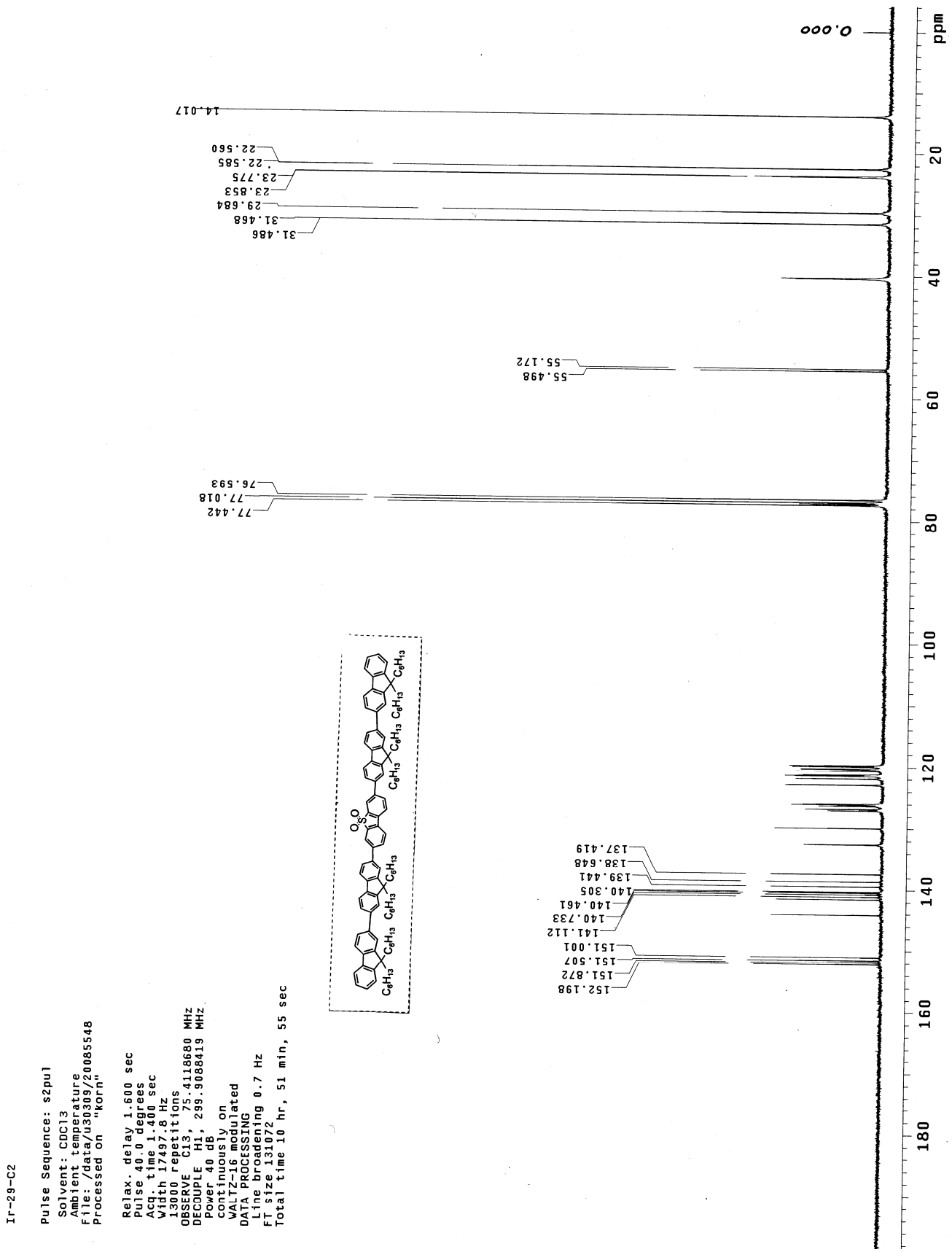

IR -10-B4
Automation directory: /export/home/vnmr1/automation/Wed0903_auto
File : /data/c50307/09165724-03
Pulse Sequence: gCOSY
Solvent: CDCl3
Ambient temperature
Sample #1
File: /data/c50307/09165724-03
INOVA-500 "orr"
Relax. delay 1.000 sec
Acq. time 0.196 sec
Width 5222.6 Hz
2D Width 5222.6 Hz
2 repetitions
256 increments
OBSERVE H1, 499.8853740 MHz
DATA PROCESSING
Sq. sine bell 0.098 sec
F1 DATA PROCESSING
Sq. sine bell 0.025 sec
FT size 2048 x 2048
Total time 10 min, 50 sec
F2 (ppm)
F1 (ppm)
O
S
O
C_6H_{13}
C_6H_{13}
C_6H_{13}
C_6H_{13}

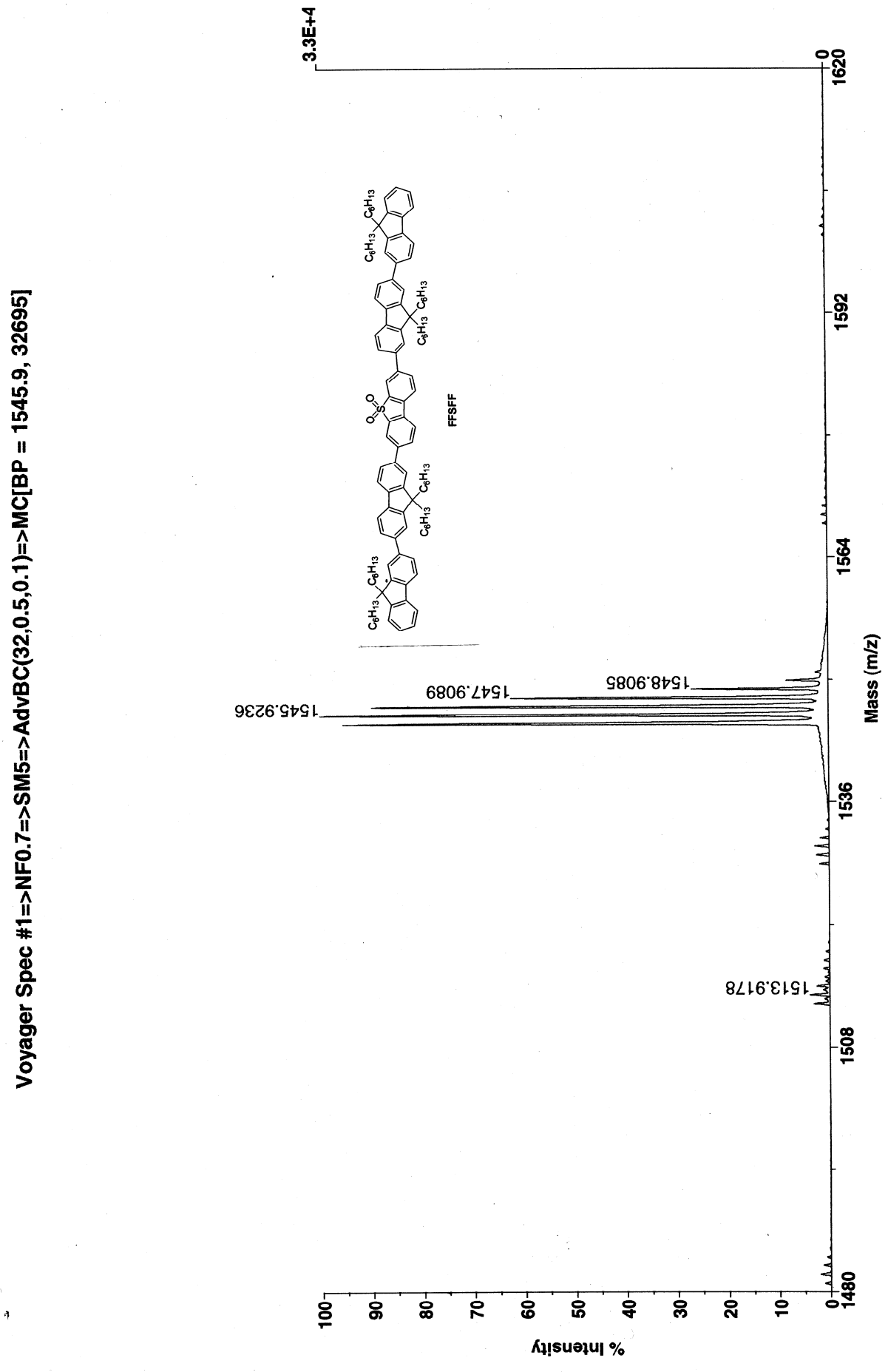

IR-10-B4
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: /data/u30308/05080206
Processed on "korn"
Relax. delay 1.600 sec
Pulse 40.0 degrees
Acq. time 1.400 sec
Width 17497.8 Hz
9200 repetitions
OBSERVE C13, 75.4118678 MHz
DECOUPLE H1, 299.9088419 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.7 Hz
FT size 131072
Total time 7 hr, 41 min, 21 sec
-0.000
14.006
22.359
22.592
23.792
29.702
31.507
40.465
55.339
76.600
77.021
77.226
77.446
120.018
120.297
120.637
121.236
121.912
122.963
125.867
126.918
127.555
129.952
132.569
137.437
138.609
140.284
141.817
144.164
151.089
151.886
ppm
20
40
60
80
100
120
140
160
C6H13
C6H13
C6H13
C6H13
S
O
O

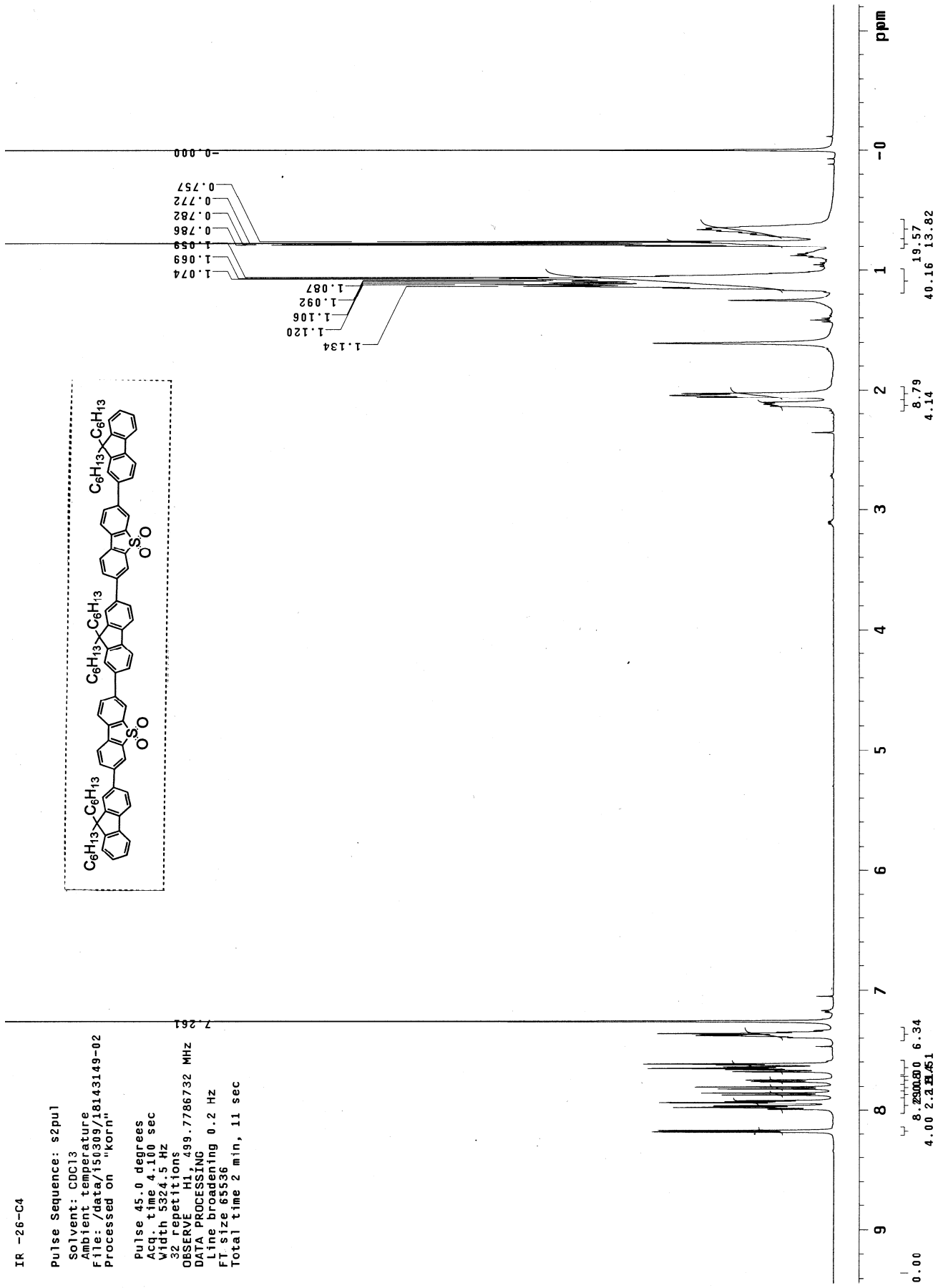

File:IR_10_B4 Ident:2_22 Mer Def 0.25 Acq:15-JUL-2003 10:13:49 +0:24 Cal:PFK_8JUL03
AutoSpec EI+ Magnet BpM:880 BpI:7605 TIC:52230 Flags:HALL
File Text:I. Perepichka
Exact Mass: 880.5253
880.19
848.21
725.06
554.93
504.99
271.09
88.05
m/z

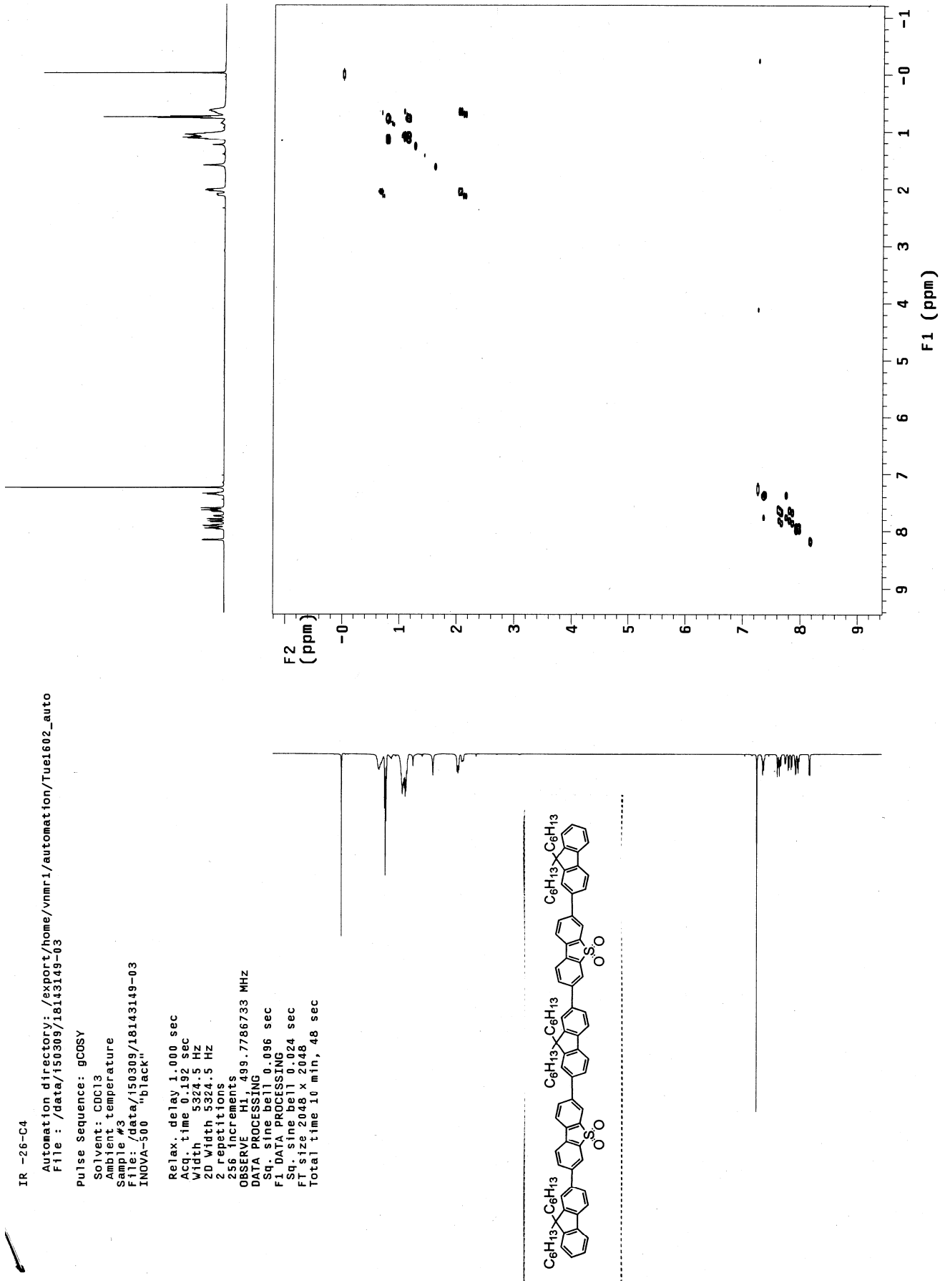

IR -29-C2
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: /data/i50309/18143121-02
Processed on "korn"
Pulse 45.0 degrees
Acq. time 4.100 sec
Width 5367.3 Hz
32 repetitions
OBSERVE H1, 499.7786745 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 2 min, 11 sec
7.258
7.654
7.647
1.152
1.138
1.125
1.111
1.097
1.082
1.075
0.792
0.786
0.778
0.773
0.764
0.758
0.000
ppm
44.04
53.62
17.81
6.59
8.14
2.08
2.00
2.12
1.82

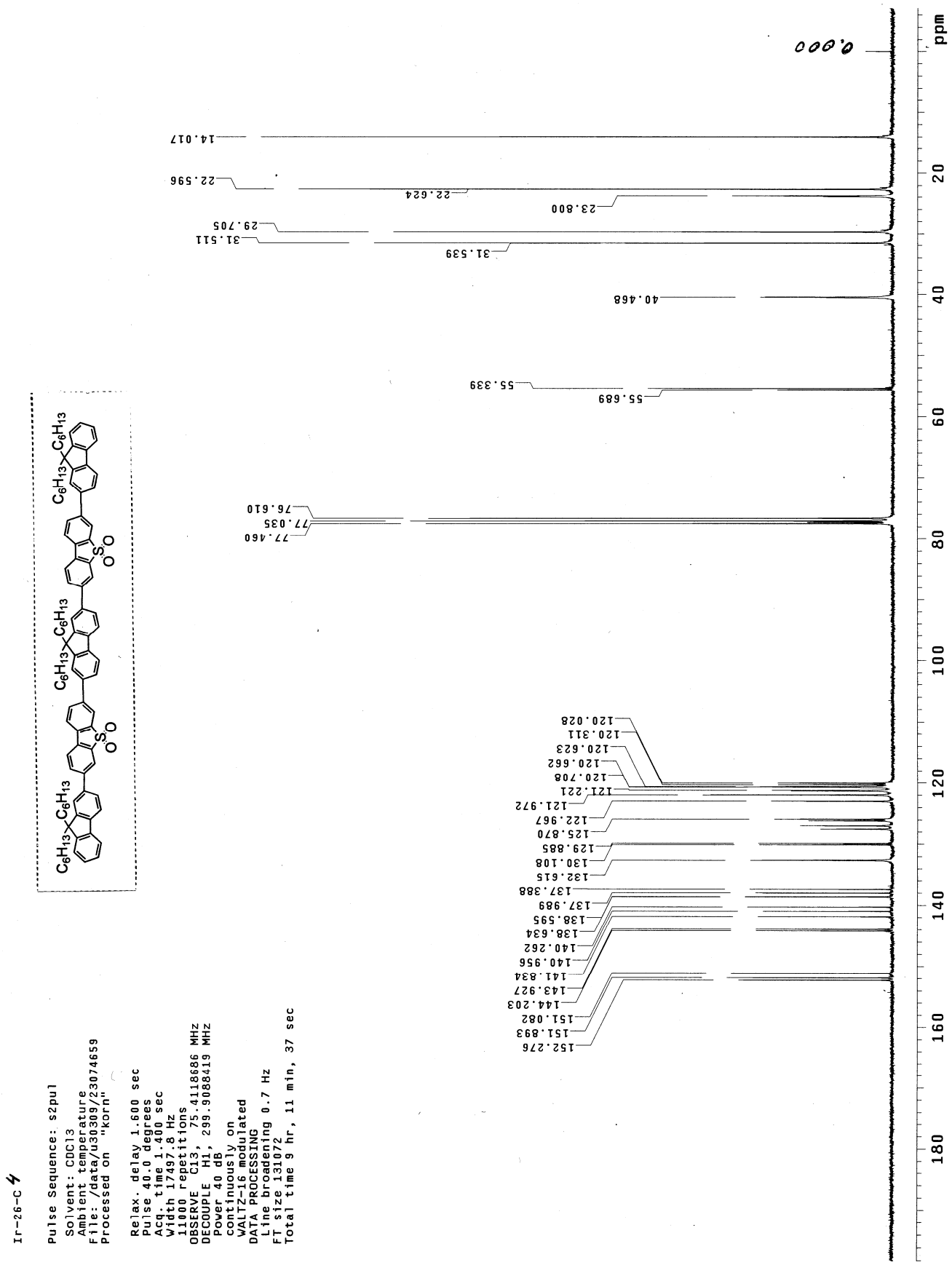

IR -29-C2
Automation directory: /export/home/vnmr1/automation/Tue1602_auto
File : /data/150309/18143121-03
Pulse Sequence: gCOSY
Solvent: CDCl3
Ambient temperature
Sample #2
File: /data/i50309/18143121-03
INOVA-500 "black"
Relax. delay 1.000 sec
Acq. time 0.191 sec
Width 5367.3 Hz
2D Width 5367.3 Hz
2 repetitions
256 increments
OBSERVE H1, 499.7786746 MHz
DATA PROCESSING
Sq. sine bell 0.095 sec
FT DATA PROCESSING
Sq. sine bell 0.024 sec
FT size 2048 x 2048
Total time 10 min, 47 sec
F2 (ppm)
F1 (ppm)

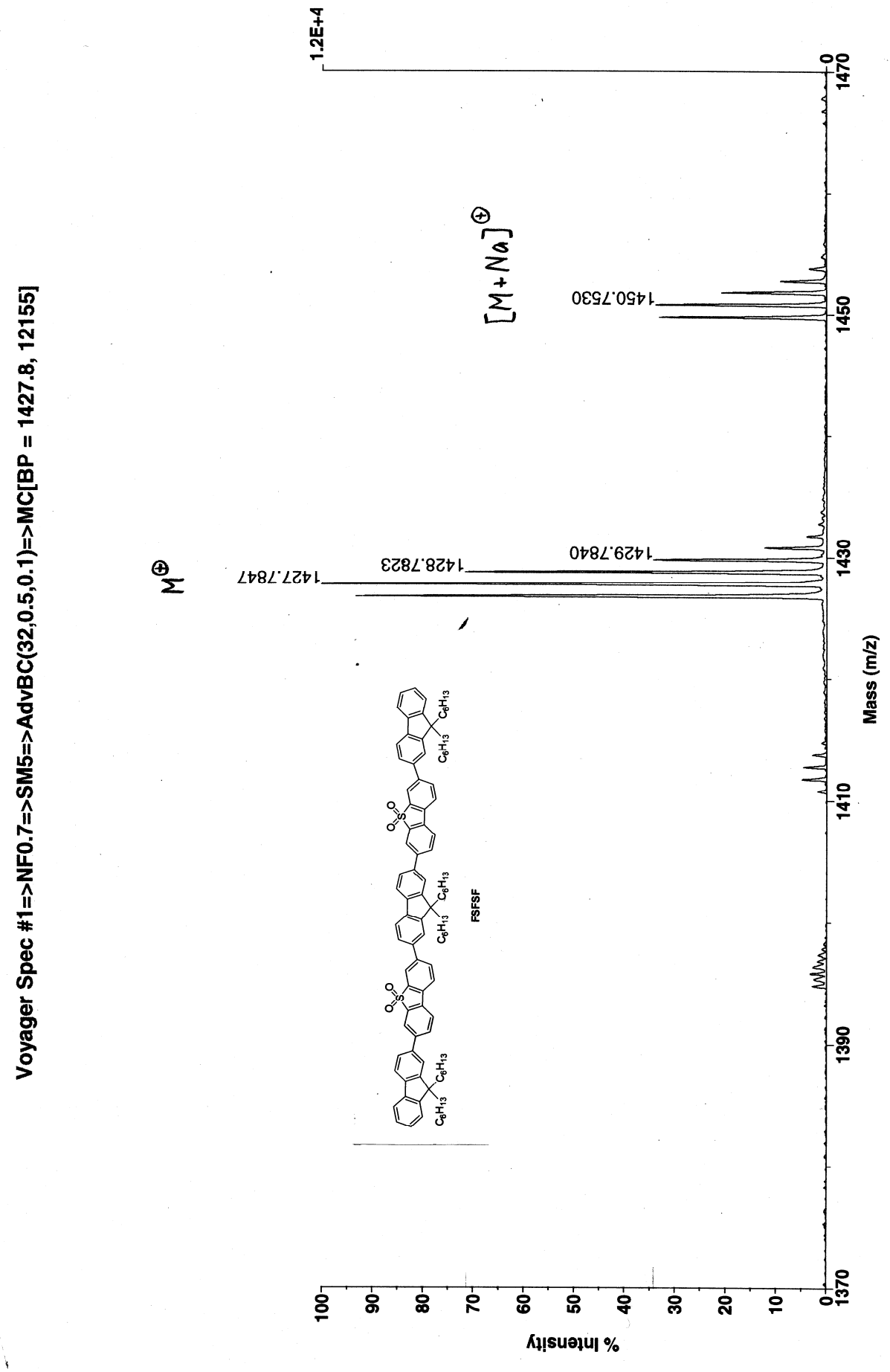

Ir-29-C2
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: /data/u30309/20085548
Processed on "korn"
Relax. delay 1.600 sec
Pulse 40.0 degrees
Acq. time 1.400 sec
Width 17497.8 Hz
13000 repetitions
OBSERVE C13, 75.4118680 MHz
DECOUPLE H1, 299.9088419 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.7 Hz
FT size 131072
Total time 10 hr, 51 min, 55 sec
14.017
22.560
22.585
23.775
23.853
29.684
31.468
31.486
55.172
55.498
76.593
77.018
77.442
137.419
138.648
139.441
140.305
140.461
140.733
141.112
151.001
151.507
151.872
152.198
0.000
ppm
20
40
60
80
100
120
140
160
180

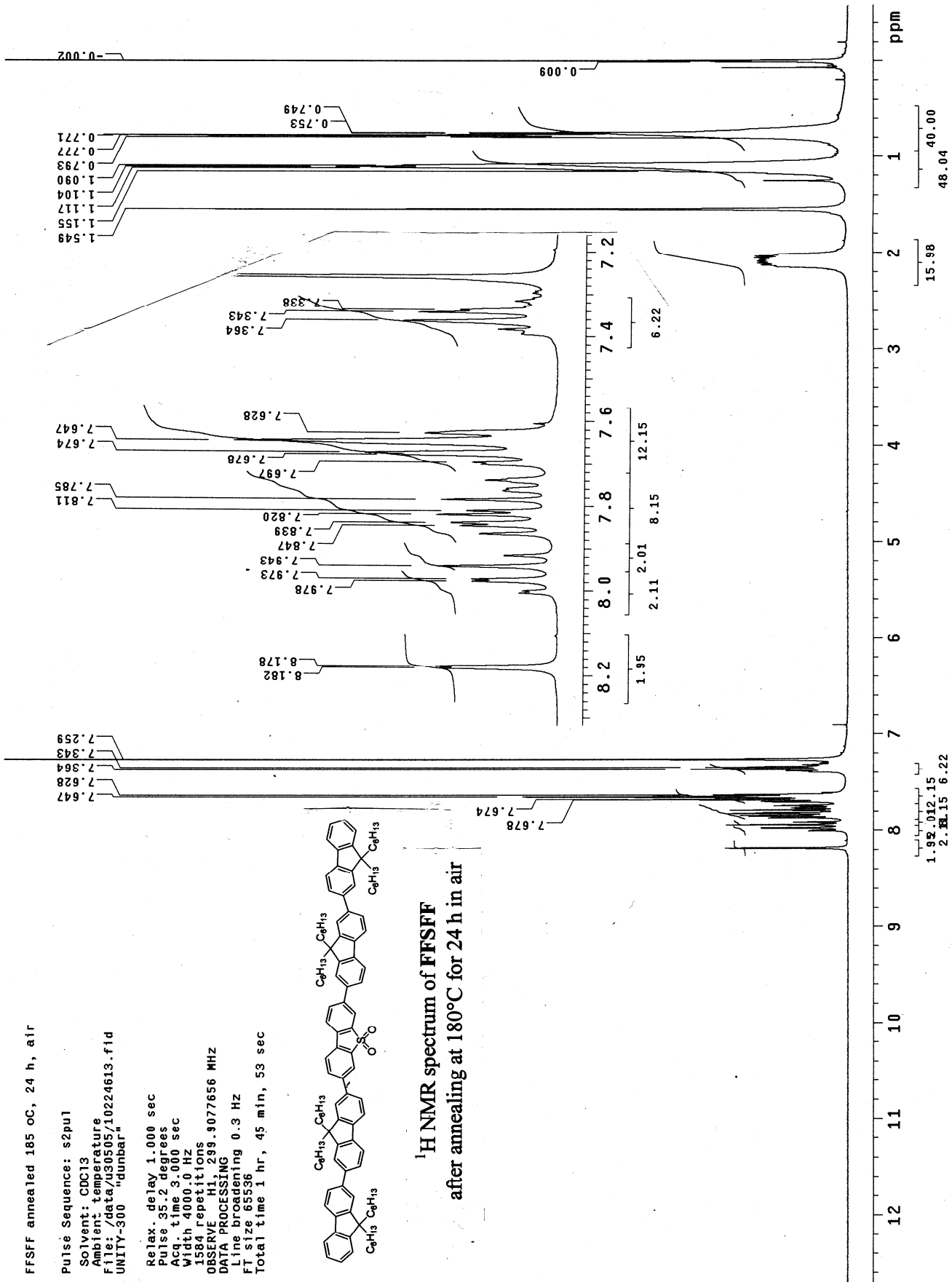

Voyager Spec #1=>NF0.7=>SM5=>AdvBC(32,0.5,0.1)=>MC[BP = 1545.9, 32695]
3.3E+4
0
1620
1592
1564
1536
1508
1480
100
90
80
70
60
50
40
30
20
10
0
% Intensity
Mass (m/z)
1513.9178
1545.9236
1547.9089
1548.9085
FFSFF
IR_29_C3,4 (THF), dithranol matrix (THF), layered, reflector mode
C:\...\IR_29_C3,4_0001.dat
Acquired: 15:20:00, October 01, 2003


IR -26-C4
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: /data/i50309/18143149-02
Processed on "korn"
Pulse 45.0 degrees
Acq. time 4.100 sec
Width 5324.5 Hz
32 repetitions
OBSERVE H1, 499.7786732 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 2 min, 11 sec
ppm
7.261
1.134
1.120
1.106
1.092
1.087
1.074
1.069
1.059
0.786
0.782
0.772
0.757
0.000
C6H13
S
O


IR -26-C4
Automation directory: /export/home/vnmr1/automation/Tue1602_auto
File : /data/i50309/18143149-03
Pulse Sequence: gCOSY
Solvent: CDCl3
Ambient temperature
Sample #3
File: /data/i50309/18143149-03
INOVA-500 "black"
Relax. delay 1.000 sec
Acq. time 0.192 sec
Width 5324.5 Hz
2D Width 5324.5 Hz
2 repetitions
256 increments
OBSERVE H1, 499.7786733 MHz
DATA PROCESSING
Sq. sine bell 0.096 sec
F1 DATA PROCESSING
Sq. sine bell 0.024 sec
FT size 2048 x 2048
Total time 10 min, 48 sec
F2 (ppm)
F1 (ppm)
C6H13
C6H13
S
O
O


Ir-26-C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: /data/u30309/23074659
Processed on "korn"
Relax. delay 1.600 sec
Pulse 40.0 degrees
Acq. time 1.400 sec
Width 17497.8 Hz
11000 repetitions
OBSERVE C13, 75.4118686 MHz
DECOUPLE H1, 299.9088419 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.7 Hz
FT size 131072
Total time 9 hr, 11 min, 37 sec
14.017
22.596
22.624
23.800
29.705
31.511
31.539
40.468
55.339
55.689
76.610
77.035
77.460
120.028
120.311
120.623
120.662
120.708
121.221
121.972
122.967
125.870
129.885
130.108
132.615
137.388
137.989
138.595
138.634
140.262
140.956
141.834
143.927
144.203
151.082
151.893
152.276
ppm


Voyager Spec #1=>NF0.7=>SM5=>AdvBC(32,0.5,0.1)=>MC[BP = 1427.8, 12155]
M⊕
1427.7847
1428.7823
1429.7840
1450.7530
[M+Na]⊕
FSFSF
% Intensity
Mass (m/z)
IR_26_C4 (THF), dithranol matrix (THF), layered, reflector mode
C:\...\IR_26_C4_0001.dat
Acquired: 15:15:00, October 01, 2003



^{1}H NMR spectrum of **FFSFF**
after annealing at 180°C for 24 h in air