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Supporting Information

For

Structure properties relationship study of electron deficient dihydroindeno[2,1-*b*]fluorene derivatives for n-type Organic Field Effect Transistors

Maxime Romain,^a Michèle Chevrier,^a Sarah Bebiche,^b Tayeb Mohammed-Brahim,^b Joëlle Rault-Berthelot,^a Emmanuel Jacques^{b*} Cyril Poriel^{a*}

Email : cyril.poriel@univ-rennes1.fr and emmanuel.jacques@univ-rennes1.fr

^a UMR CNRS 6226-Institut des Sciences Chimiques de Rennes- Équipe *Ma*tière *C*ondensée et Systèmes Électroactifs, Bat 10C, Campus de Beaulieu - 35042 Rennes Cedex France

^b UMR CNRS 6164-Institut d'Électronique et des Télécommunications de Rennes-Département Microélectronique & Microcapteurs, Bât.11B, Université Rennes 1, Campus de Beaulieu 35042 Rennes Cedex, France

Experimental part:

Synthesis

Commercially available reagents and solvents were used without further purification other than those detailed below. THF was distilled from sodium/benzophenone prior to use. Light petroleum refers to the fraction with bp 40-60°C. DMF and DMSO were purchased from Aldrich ("puriss, absolute over Molecular sieves > 99.5 and 99.8 % respectively). Tert-butyl alcohol (\geq 99 %), methane sulfonic acid (\geq 99.5 %), phenylboronic acid 95 % were purchased from Sigma Aldrich and malonitrile 99 % was purchased from Acros Organics. Reactions were stirred magnetically, unless otherwise indicated. Analytical thin layer chromatography was carried out using aluminum backed plates coated with Merck Kieselgel 60 GF254 and visualized under UV light (at 254 and 360 nm). Chromatography was carried out using Teledvne Isco CombiFlashR Rf 400 (UV detection 200-360 nm), over standard silica cartridges (RedisepR Isco, GraceResolv[™] Grace or PuriflashR columns Interchim). ¹H and ¹³C NMR spectra were recorded using Bruker 300 MHz instruments (¹H frequency, corresponding ¹³C frequency: 75 MHz); chemical shifts were recorded in ppm and J values in Hz. In the ¹³C NMR spectra, signals corresponding to CH, CH₂ or Me groups, assigned from DEPT, are noted; all others are C. The residual signals for the NMR solvents are: CDCl₃; 7.26 ppm for the proton and 77.00 ppm for the carbon, CD_2Cl_2 ; 5.32 ppm for the proton and 53.80 ppm for the carbon. The following abbreviations have been used for the NMR assignment: s for singlet, d for doublet, t for triplet and m for multiplet. High resolution mass spectra were recorded at the Centre Regional de Mesures Physiques de l'Ouest (Rennes) on (i) Bruker MicrO-Tof-Q II (Source: Atmospheric Pressure Chemical Ionization (APCI - direct introduction) (ASAP-Atmospheric Solids Analysis Probe) at a temperature of 30°C - positive mode) or on (ii) Waters Q-Tof II (source: electrospray (ESI)).

Tert-butanol (\geq 99 %), methane sulfonic acid (\geq 99.5 %), phenylboronic acid 95 % were purchased from Sigma Aldrich and malonitrile 99 % was purchased from Acros Organics.

4,6-dibromoisophtalic acid 2. 1,5-dibromo-2,4-dimethylbenzene (10 g, 38 mmol) and sodium hydroxide (2.7 g, 68 mmol) were dissolved in a mixture of *tert*-butanol/water (1 : 1, 500 mL). The reaction mixture was heated to 100°C with stirring, and small portions (*ca* 200 mg) of potassium permanganate (total: 42 g, 0.27 mol) were added to the solution once the purple colour of the previous portion had faded. The excess of potassium permanganate was reduced by addition of sodium thiosulfate pentahydrate (2.5 g) and the hot solution was immediately filtered on Celite®. The resulting MnO₂ was washed with boiling water (1 L). The aqueous filtrate was concentrated to eliminate the *tert*-butanol and acidified to pH=1 using concentrated hydrochloric acid. The colourless precipitate formed was further collected by filtration, washed with cold water and dried in an oven at 80°C to give the *title compound* as a colourless solid (8.6 g, 71 %). ¹H NMR (DMSO-*d*₆): δ 7.96 (s, 1H), 8.14 (s, 1H) ppm. ¹³C NMR (DMSO-*d*₆): δ 123.5 (C), 132.1 (CH), 132.4 (C), 138.2 (CH), 165.5 (C) ppm. m.p:

217°C (degradation). IR (ATR Platinum): 3090 (O-H), 3029 (Ar), 2900 (Ar), 1705 (C=O), 1576, 1537, 1390, 1266 (C-O), 1239, 1058, 910, 861, 754, 574 cm⁻¹.

Diethyl-4,6-dibromoisophtalate 3. Methanesulfonic acid (4.0 mL, 62 mmol) was added to a suspension of 4,6-dibromoisophtalic acid **2** (5.0 g, 15 mmol) in ethanol absolute (135 mL). The mixture was stirred under reflux for 3 days. The resulting solution was concentrated by evaporation to a volume of about 25 mL (80 %), whereupon water (200 mL) was added. The coulourless precipitate formed was collected by filtration and the residue was purified by column chromatography on silica gel using gradient light petroleum/ethyl acetate (100:0 to 95:5) as eluent to give the *title compound* as a colourless solid (4.2 g, 78 %). [column conditions: Silica cartridge 80 g (Serlabo) ; solid deposit on Celite®; $\lambda_{detection}$: (254 nm, 280 nm); ethyl acetate in light petroleum at 30 mL/min (2 min / 0% ; 15 min / 0% -> 5%); collected fraction: 9-11 min]. ¹H NMR (CDCl₃): δ 1.41 (t, 6H, J = 7.1 Hz), 4.41 (q, 4H, J = 7.1 Hz), 8.01 (s, 1H), 8.24 (s, 1H) ppm. ¹³C NMR (CDCl₃): δ 14.3 (CH₃), 62.3 (CH₂), 125.6 (C), 131.4 (C), 133.9 (CH), 139.8 (CH), 164.8 (C) ppm. m.p: 58°C. MS (ESI) m/z [M+H]⁺: calcd for C₁₂H₁₃O₄⁷⁹Br₂, 378.9181; found 378.9183. IR (ATR Platinum): 3442, 3104, 2977, 2932, 2908, 1729 (C=O), 1280, 1228, 1109, 1047 (C-O), 1012, 866, 764, 618 cm⁻¹.

Diethyl [1,1':3',1''-terphenyl]-4',6'-dicarboxylate 4. Diethyl 4,6-dibromoisophthalate 3 (1.5 g, 4.0 mmol), phenylboronic acid (1.2 g, 10 mmol), tetrakis(triphenylphosphine) palladium⁰ (458 mg, 0.40 mmol) and potassium carbonate (2.7 g, 20 mmol) were dissolved in a mixture THF/water (2.5:1, 35 mL) under an argon atmosphere. The resulting mixture was degassed and stirred overnight at 70°C. The resulting mixture wad quenched with a saturated solution of ammonium chloride and extracted with ethyl acetate. The combined extracts were dried over MgSO₄, filtered, evaporated in vacuo and purified by column chromatography on silica gel eluting with a gradient of light petroleum – ethyl acetate (100:0 to 95:5) to give the *title* compound as a colourless solid (1.4 g, 95 %) [column conditions: Silica cartridge 24 g (Serlabo) ; solid deposit on Celite®; $\lambda_{detection}$: (254 nm, 280 nm); ethyl acetate in light petroleum at 30 mL/min (5 min / 0%; 20 min / 0% -> 5%); collected fraction: 10-13 min]. 1 H NMR (CDCl₃): δ 1.03 (t, 6H, J = 7.1 Hz) ; 4.13 (q, 4H, J = 7.1 Hz) ; 7.37 (m, 11H) ; 8.32 (s, 1H) ppm. ¹³C NMR (CDCl₃): δ 13.8 (CH₃), 61.4 (CH₂), 127.8 (CH), 128.2 (CH), 128.4 (CH), 130.1 (C), 131.8 (CH), 133.3 (CH), 140.5 (C), 145.2 (C), 167.9 (C) ppm. m.p: 73°C. MS (ESI) m/z $[M+H]^+$: calcd for C₂₄H₂₃O₄, 375.1518; found 375.1523. IR (ATR Platinum): 1711 (C=O), 1288, 1241, 1109, 1037 (C-O), 764, 696, 598 cm⁻¹.

Indeno[2,1-*b***]fluorene-5,7-dione** ((**2,1-***b***)-IF**(=**O**)₂). Diethyl [1,1':3',1"-terphenyl]-4',6'dicarboxylate **4** (1.5 g, 4.0 mmol) was dissolved in methane sulfonic acid (40 mL) and stirred 20 minutes at 120 °C. The solution was then poured into 10 % aqueous sodium hydroxide to pH=14. The green precipitate formed was collected by filtration and washed several times with water. The green precipitate was then dissolved in dichloromethane, re-filtered and the solvent was removed *in vacuo* to afford the *title compound* was as a green-brown solid (1.1 g, 98 %). ¹H NMR (CD₂Cl₂): δ 7.43 (td, 2H, J = 7.5, 1.1 Hz), 7.61 (td, 2H, J = 7.5, 1.1 Hz), 7.70 (m, 4H), 7.80 (d, 1H, J = 0.7 Hz), 7.86 (d, 1H, J = 0.7 Hz) ppm. ¹³C NMR (CD₂Cl₂): δ 112.5 (CH), 120.4 (CH), 121.2 (CH), 124.7 (CH), 130.6 (CH), 134.7 (CH), 134.9 (C), 135.1 (C), 142.9 (C), 150.1 (C), 151.7 (C) ppm. m.p: 330°C. MS(ESI) m/z [M+H]⁺: calcd for C₂₀H₁₁O₂, 283.0759; found 283.0753. IR (ATR Platinum): 3019, 3045, 3066, 1703 (C=O), 1603, 1441, 1278, 1183, 1154, 1093, 1067, 732, 661 cm⁻¹. UV-visible (THF) : λ_{abs} [nm] (ϵ [L.mol⁻¹.cm⁻¹]) = 278 (25500), 300 (19740), 315 (18830), 328 (13100).

(7-oxoindeno[2,1-b]fluoren-5(7H)-ylidene)propanedinitrile (2,1-b)-IF(=O)(=C(CN)₂).

Indeno[2,1-*b*]fluorene-10,12-dione (**2,1-***b*)-**IF**(=**O**)₂ (0.10 g, 0.35 mmol) and malononitrile (0.23 g, 4.9 mmol) were dissolved in dry acetonitrile (10 mL) under an argon atmosphere. Pyridine (0.57 mL, 7.0 mmol) and acetic acid (0.49 mL, 3.9 mmol, 11 eq) were then added via syringe. The resulting mixture was stirred 16 hours at room temperature until the colour of the solution became red. Upon cooling, water (10 mL) was added and the red precipitate formed was filtered off and washed several times with water (2 x 10 mL) to afford the *title compound* as a red solid (70 mg, 60 %). ¹H NMR (CD₂Cl₂): δ 7.46 (t, 2H, J = 7.5 Hz), 7.62 (t, 2H, J = 7.5 Hz), 7.74 (m, 3H), 7.82 (s, 1H) ; 8.43 (d, 1H, J = 8.4 Hz), 8.55 (s, 1H) ppm. m.p: 325°C (degradation). MS (ESI) m/z [M+H]⁺: calcd for C₂₃H₁₁N₂O, 331.0870; found 331.0871. IR (ATR Platinum): 2921, 2849, 2221 (CN), 1711 (C=O), 1601, 1558, 1448, 1426, 1291, 1265, 1176, 1121, 900, 781, 735, 659 cm⁻¹. UV-visible (THF) : λ_{abs} [nm] (ϵ [L.mol⁻¹.cm⁻¹]) = 285 (11100), 342 (7020), 363 (7700), 400 (2385), 427 (2100).

2,2'-indeno[2,1-b]fluorene-5,7-diylidenedipropanedinitrile (2,1-b)-IF(=C(CN)₂)₂.

Indeno[2,1-*b*]fluorene-10,12-dione (**2,1-***b*)-**IF**(=**O**)₂ (0.10 g, 0.35 mmol) and malononitrile (0.23 g, 4.9 mmol) were dissolved in dry acetonitrile (10 mL) under argon atmosphere. Pyridine (0.57 mL, 7.0 mmol) and acetic acid (0.49 mL, 3.9 mmol) were added via syringe. The resulting mixture was refluxed 72 hours. The red mixture was quenched by addition of water (10 mL) and the red precipitate formed was filtered off, washed several times with water and dichloromethane and dried in an oven at 80°C to give the *title compound* (49 mg, 37 %). m.p: 325°C (degradation). MS(ESI) m/z [M+Na]⁺: calcd for C₂₆H₁₀N₄Na, 401.0803; found 401.0804. Elemental analysis calculated (%) for C₂₆H₁₀N₄: C 82.53, H 2.66, N: 14.81 found: C 82.48, H 2.42, N: 14.09. IR (ATR Platinum): 2964, 2222 (CN), 1604, 1569, 1449, 1433, 1262 cm⁻¹. UV-visible: λ_{abs} [nm] (ε [L.mol⁻¹.cm⁻¹]) = 295 (34750), 344 (34950), 378 (24 850), 400 (23 480).

Synthesis of 5,7-dihydroindeno[2,1-b]fluorene (2,1-b)-IF.

Indeno[2,1-*b*]fluorene-10,12-dione (**2,1-***b*)-**IF**(=**O**)₂ (50 mg, 0.18 mmol), hydrazine hydrate (330 mL, 5.4 mmol) and potassium hydroxide (240 mg, 4.37 mmol) were dissolved in diethylene glycol (6 mL) and the solution was stirred at 180°C for 24 h. After cooling to room temperature, the mixture was poured into a solution of concentrated HCl at 0°C. A colourless precipitate was obtained, which was filtered off and washed several times with water to afford the *title compound* (30 mg, 65 %). ¹H NMR (CD₂Cl₂) δ 8.20 (s, 1H), 7.90 (d, J = 7.5 Hz, 2H), 7.71 (s, 1H), 7.57 (d, J = 7.4 Hz, 2H), 7.42 (t, J = 7.5 Hz, 2H), 7.32 (t, J = 7.4 Hz, 2H), 3.95

(s, 4H). ¹³C NMR (CD₂Cl₂) δ 144.2 (C), 143.2 (C), 142.3 (C), 141.2 (C), 127.3 (CH), 127.0 (CH), 125.6 (CH), 122.3 (CH), 120.2 (CH), 111.4 (CH), 37.3 (CH₂). m.p: 210°C (degradation). MS(ESI) m/z [M+H]⁺: calcd for C₂₀H₁₅, 255.1159; found 255.1163. Elemental analysis calculated (%) for C₂₀H₁₄: C 94.45, H 5.55, found: C 94.29, H 5.73; IR (ATR Platinum): 3043, 3018, 2922, 1464, 1443, 1404, 1394, 1337, 1306, 1254, 1184, 1151, 1101, 1020, 1005, 953, 868, 762, 733, 694, 658, 575 cm⁻¹. UV-visible (THF) : λ_{abs} [nm] (ϵ [L.mol⁻¹]) = 305 (6139), 311 (7920), 318 (12580), 325 (11170), 333 (17640).

Photophysical studies

Cyclohexane (ACS grade), dichloromethane (analytical grade, VWR), and absolute ethanol was used without further purification. THF was distilled from sodium/benzophenone prior to use. UV/Vis spectra were recorded by using a UV/Vis SHIMADZU UV-1605 spectrophotometer. The optical gap was calculated from the absorption edge of the UV/Vis absorption spectra by using the formula Δ Eopt [eV]=hc/ λ , λ being the absorption edge (in meter), with h = 6.62606×10⁻³⁴ J.s (1eV=1.60217× 10⁻¹⁹ J) and c =2.99792×10⁸ m.s⁻¹, Eg^{opt} (eV) = 1239.84 / λ (in nm). Photoluminescence spectra were recorded with a PTI spectrofluorimeter (PTI-814PDS, MD 5020, LPS 220B) by using a xenon lamp.

Electrochemical studies

All the molecules investigate din this work have been studied using cyclic and differential pulse voltammetry (CV and DPV). All electrochemical experiments were performed under an argon atmosphere, using a Pt disk electrode (\emptyset : 1 mm), the counter electrode was a vitreous carbon rod and the reference electrode was a silver wire in a 0.1M AgNO₃ solution in CH₃CN. Ferrocene was added to the electrolytic solution at the end of a series of experiments. The ferrocene/ferrocenium (Fc/Fc⁺) couple served as the internal standard. All potentials are referred to the SCE electrode that was calibrated at -0.405 V *vs*. Fc/Fc⁺ system. Activated Al₂O₃ was added to the electrolytic solution to remove excess moisture. The three electrode cell was connected to a PAR Model 273 potentiostat/galvanostat (PAR, EG&G, USA) monitored with the ECHEM Software. Following the work of Jenekhe, we estimated the electron affinity (EA) or lowest unoccupied molecular orbital (LUMO) and the ionization potential (IP) or highest occupied molecular orbital (HOMO) from the redox data. The LUMO level was calculated from: LUMO (eV)= -[E_{onset}^{red} (*vs* SCE) + 4.4] and the HOMO level from: HOMO (eV) = -[E_{onset}^{ox} (*vs* SCE) + 4.4], based on an SCE energy level of 4.4 eV relative to the vacuum. The electrochemical gap was calculated from : ΔE^{el} =|HOMO-LUMO| (in eV).^{1,2}

Theoretical modeling

Full geometry optimization with Density functional theory $(DFT)^{3-5}$ and Time-Dependent Density Functional Theory (TD-DFT) calculation were performed with the hybrid Becke-3 parameter exchange⁶⁻⁸ functional and the Lee-Yang-Parr non-local correlation functional⁹ (B3LYP) implemented in the Gaussian 09 (Revision B.01) program suite¹⁰ using the 6-311G+(d,p) basis set and the default convergence criterion implemented in the program. The figures were generated with GaussView 5.0.

OFET fabrication

A 100 nm thick aluminum layer is thermally evaporated on previously cleaned glass substrate. This layer was wet etched to define the gate contact. The insulator (SU-8 photoresist 2000.5 from Microchem) was spin-coated and annealed. The final thickness of this SU-8 layer is about 300 nm. Evaporation of 50 nm thick gold layer follows. This layer was wet etched to form the source and drain contacts. Gold was chosen due to its stability and its work function, -5 eV, which is compatible with the LUMO level of the investigated materials. The last step is the evaporation under vacuum $(10^{-6}-10^{-7} \text{ mbar})$ of a layer of the investigated material (20 nm) with a deposition rate about 0.2 nm/s. All the patterning steps have been made with classical photolithography tools.

Quantitatively, the different OFET parameters can be calculated using the known relation (1) between the drain-source current and the drain-source and gate-source voltages in the linear regime.

$$I_{DS} = \frac{W \,\mu C_{INS}}{L} \left(V_{GS} - V_{TH} \right) V_{DS} \tag{1}$$

In this equation, L is the channel length (in μ m), W the channel width (in μ m), C_{INS} (in F/cm²) is the capacitance of the gate insulator per area unit, and μ (in cm²/V.s) is the field effect mobility, V_{GS} (in V) is the gate source voltage, V_{TH} (in V) is the threshold voltage and V_{DS} (in V) is the drain source voltage.

The threshold voltage V_{TH} can be determined by a linear extrapolation on the gate voltage axis of the transfer characteristic I_{DS} - V_{GS} at constant V_{DS} . The field effect mobility can be calculated from the slope $W\mu C_{INS}V_{DS}/L$ of this linear extrapolation.

The switch from the off to the on state is quantified by the subthreshold swing S that is the inverse of the maximum slope of the transfer characteristics plotted in semi-logarithmic plot.



6,12-dihydroindeno[1,2-*b*]fluorene (1,2-*b*)-IF



11,12-dihydroindeno[2,1-*a*]fluorene (2,1-*a*)-IF



7,12-dihydroindeno[1,2-a]fluorene

(1,2-*a*)-IF

5,7-dihydroindeno[2,1-b]fluorene

(2,1-*b*)-IF



5,8-dihydroindeno[2,1-c]fluorene

(2,1-c)-IF

Figure S1. Molecular structures of the 5 positional isomers of dihydroindenofluorene isomers.

The synthesis of (2,1-b)-**IF**(=**O**)₂ has been first envisaged through the intramolecular electrophilic bicyclization of terphenyldiethanoate **A** (see below),^{*} easily obtained through Suzuki Miayura cross coupling between 1,2-bromoethylbenzoate and phenyl 1,3-diboronic acid (Pd(PPh₃)₄, K₂CO₃, THF/H₂O). Similar intramolecular cyclizations have been widely studied by our group for the last years, providing a library of organic semiconductors with different geometric profiles.¹¹⁻¹⁴ However, the present electrophilic bicyclization of **A**, in acidic media appears to be poorly regioselective and leads to a mixture of (1,2-a)-**IF**(=**O**)₂ and (2,1-b)-**IF**(=**O**)₂, appearing very difficult to separate on column chromatography and inseparable by crystallization. This synthetic approach was hence clearly not efficient enough to provide (2,1-b)-**IF**(=**O**)₂ and has been given up. In addition, we unfortunately did not manage to direct the synthesis preferentially towards one positional isomer over the other by altering the nature of the acid used (Bronsted and Lewis), the solvent and the temperature of the reaction ¹¹



Figure S2 Synthesis of (2,1-*b*)-IF(=O)₂ and (1,2-*a*)-IF(=O)₂

^{*} RMN¹H (CDCl₃, 300 MHz, ppm) δ 7.68 (2H, d) 7.39-7.11 (10H, m), 3.51 (6H, s)



Figure S3. Left: Cyclic voltammetry recorded in a solution of (2,1-b)-IF in CH₂Cl₂ (Bu₄NPF₆ 0.2 M): 10 recurrent sweeps between -140 to 1760 mV, working electrode: platinum disk diameter 0.25 mm, sweep-rate: 100 mV/s. Right: Cyclic voltammetry recorded in CH₂Cl₂ (Bu₄NPF₆ 0.2 M): 3 recurrent sweeps between -90 to 1300 mV, working electrode: platinum disk diameter 0.25 mm previously covered in A by a poly((2,1-*b*)IF) deposit, sweep-rate: 100 mV/s.



Figure S4. IR spectra of (2,1-*b*)-IF (black line) (2,1-*b*)-IF(=O)₂ (red line), (2,1-*b*)-IF(=O)(=C(CN)₂) (blue line) and (2,1-*b*)-IF(=C(CN)₂)₂ (green line)



Figure S5. Normalized UV-Vis spectra of (2,1-b)-IF(=O)₂ (red line), (2,1-b)-IF(=O)(=C(CN)₂) (blue line) and (2,1-b)-IF(=C(CN)₂)₂ (green line), in thermally evaporated thin film. Normalization was performed at λ_{max} in the 210 nm to 800 nm range.



Figure S6: Absorption vs Integrated Fluorescence intensity of (2,1-*b*)-IF and quinine sulphate

		Solution 1	Solution 2	Solution 3	Solution 4	slope	<i>n</i> _D	φ
(2,1-b)- IF	А	0.05	0.063	0.087	0.102		1.407	51%
	Integrated fluorescence intensity (a.u.)	9502	12417	17323	19976	196463		
Quinine Sulfate	А	0.047	0.055	0.091	0.096		1.3355	55%
	Integrated fluorescence intensity (a.u.)	11054	13244	21223	22580	235231		

Quantum y	vield ca	lculation	of (2	,1- <i>b</i>)-IF
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Figure S7. TGA curves of (2,1-*b*)-IF(=C(CN)₂)₂

The *Td* is defined as the temperature at which the sample has lost the first 5 % of mass during heating. 5% decomposition (Td) of (2,1-b)-IF $(=C(CN)_2)_2$ occurs at 311°C.



Figure S8 . Cyclic voltammetries of (2,1-b)-IF $(=O)_2$ (top), (2,1-b)-IF $(=O)(=C(CN)_2)$ (middle) and (2,1-b)-IF $(=C(CN)_2)_2$ (bottom) recorded in CH₂Cl₂ (Bu₄NPF₆ 0.2 M), working electrode: platinum disk diameter 0.25 mm, sweep-rate: 100 mV/s).

Copy of NMR spectra







DEPT (DMSO-d6) 4,6-dibromoisophtalic acid 2



¹H (CDCl₃) Diethyl-4,6-dibromoisophtalate 3



¹³C (CDCl₃) Diethyl-4,6-dibromoisophtalate





¹**H** (**CDCl**₃) Diethyl [1,1':3',1"-terphenyl]-4',6'-dicarboxylate



¹³C (CDCl₃) Diethyl [1,1':3',1"-terphenyl]-4',6'-dicarboxylate



DEPT (CDCl₃) Diethyl [1,1':3',1''-terphenyl]-4',6'-dicarboxylate

¹H (CD₂Cl₂) Indeno[2,1-*b*]fluorene-5,7-dione





¹³C (CDCl₃): Indeno[2,1-*b*]fluorene-5,7-dione

DEPT (**CDCl**₃) Indeno[2,1-*b*]fluorene-5,7-dione





¹H (CD₂Cl₂) 7-oxoindeno[2,1-b]fluoren-5(7H)-ylidene)propanedinitrile



¹H (CD₂Cl₂) 5,7-dihydroindeno[2,1-*b*]fluorene (2,1-*b*)-IF.



¹³C (CD₂Cl₂): 5,7-dihydroindeno[2,1-*b*]fluorene (2,1-*b*)-IF.

MF-MR-IFcis - 1E+05 -1E+05 -90000 -80000 - 70000 -60000 - 50000 40000 - 30000 - 20000 10000 -0 -10000 -20000 -30000 -40000 -50000 -60000 -70000 -80000 -90000 --1E+05 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

DEPT (CD₂Cl₂): 5,7-dihydroindeno[2,1-*b*]fluorene (2,1-*b*)-IF.

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