

Supporting Information

5,5'-Bis[9-(2-ethylhexyl)-9*H*-carbazol-3-yl]-4,4'-diphenyl-2,2'-bithiazole

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S1. UV-vis Spectrum of Bithiazole 6

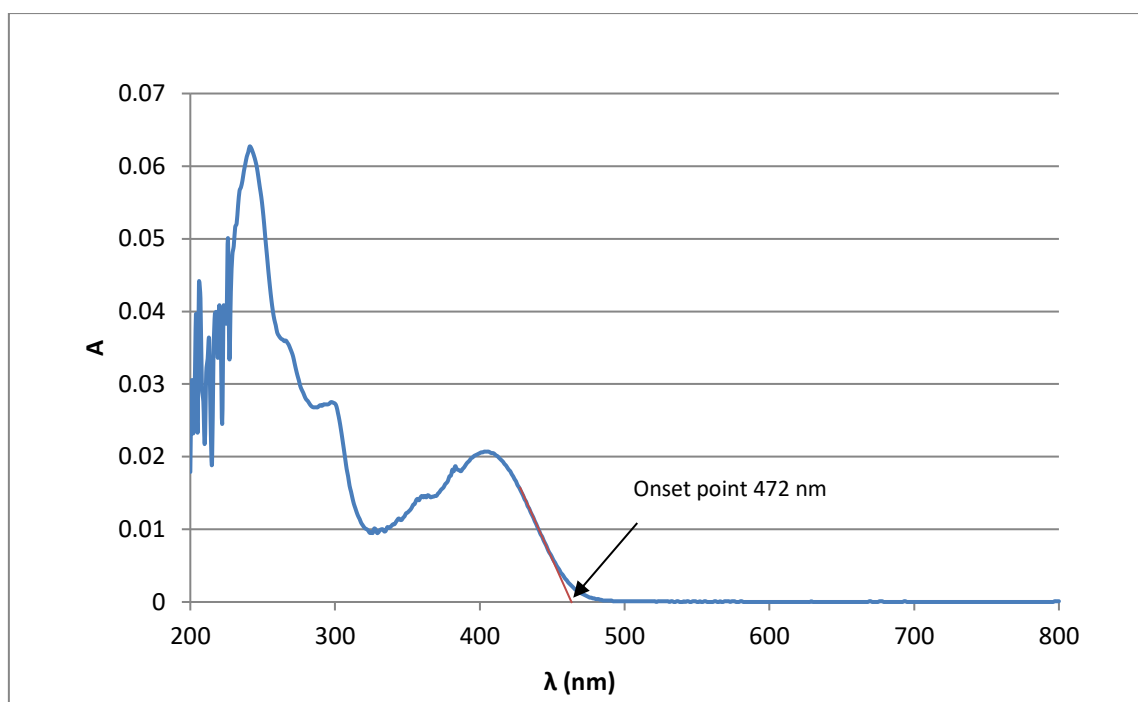


Figure S1. UV-vis absorption spectrum of bithiazole **6** in CH₂Cl₂ at 0.010 mM. Peaks: 241 (log ϵ 3.78), 265 inf (3.54), 298 inf (3.43), 363 inf (3.15), 383 inf (3.25), 405 (3.30).

Calculation of optical band gap

The optical band gap was calculated using the formula (derived from Beer-Lambert Law):

$$E_g^{opt} = \frac{h \times c}{\lambda_{max}^{onset}}$$

Where h is Plank's constant (6.626×10^{-34} J·s), c is the speed of light (3.0×10^8 m·s⁻¹) and λ_{max}^{onset} (m) is onset of the absorption band with the highest wavelength. Conversion factor: 1 eV = 1.6×10^{-19} J.

S2. Cyclic Voltammetry

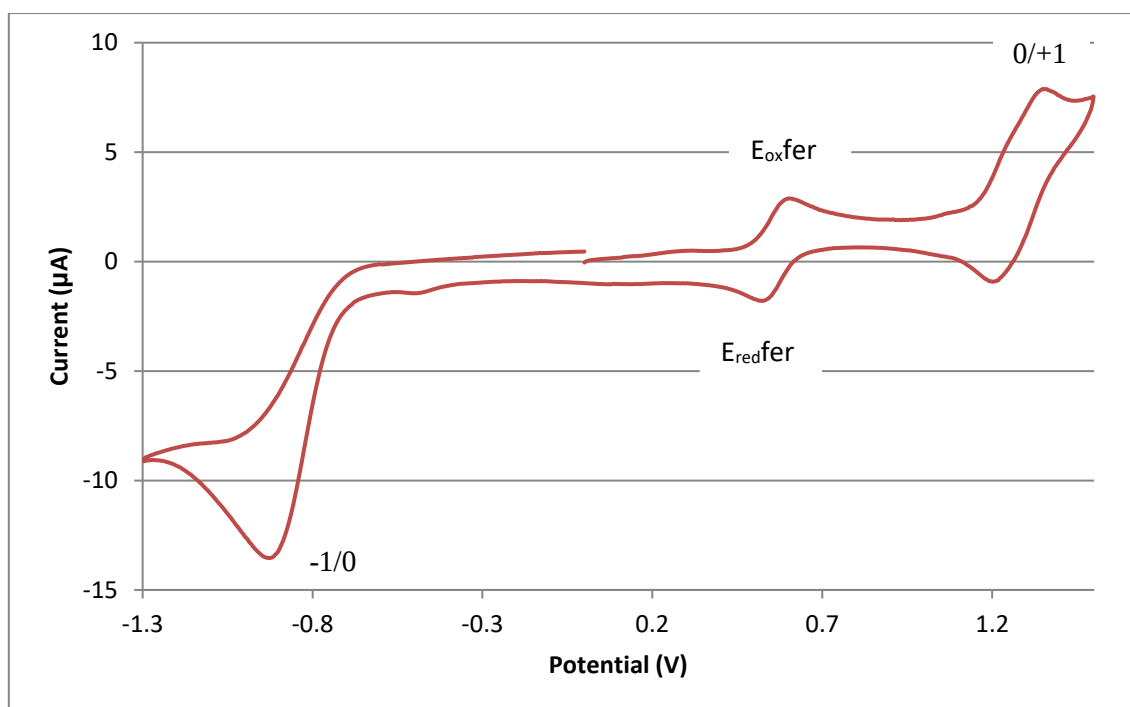


Figure S2. Cyclic voltammogram of bithiazole **6**. The voltammogram was run in a 1.0 mM solution of compound **6** in dry (over CaH_2), HPLC grade DCM containing TBABF_4 (0.1 M) as an electrolyte. A three-electrode electrochemical cell was used with an Au working electrode ($\varnothing$ 3 mm), Pt wire as counter electron and Ag/AgCl (1.0 M KCl) as reference electrode. Scan rate $50 \text{ mV} \cdot \text{s}^{-1}$. Temperature = 20°C . Fc/Fc^+ ($E_{\text{Fc}/\text{Fc}^+} = 0.475 \text{ V vs. SCE}$ [1]) was used as an internal reference.

Calculation of HOMO/LUMO values and electrochemical band gap

$$E_{\text{HOMO}} = -[(E_{1/2}^{+1/0} - E_{\text{Fc}/\text{Fc}^+}) + 5.1] \text{ eV}$$

$$E_{\text{LUMO}} = -[(E_{1/2}^{0/-1} - E_{\text{Fc}/\text{Fc}^+}) + 5.1] \text{ eV}$$

$$E_{\text{g}}^{\text{echem}} = E_{1/2}^{+1/0} - E_{1/2}^{0/-1}$$

S3. References

[1] Aranzaes, J. R.; Daniel, M.-C.; Astruc, D. Metallocenes as references for the determination of redox potentials by cyclic voltammetry - Permethylated iron and cobalt sandwich complexes, inhibition by polyamine dendrimers, and the role of hydroxy-containing ferrocenes. *Can. J. Chem.* **2006**, *84*, 288-299. DOI: 10.1139/v05-262.

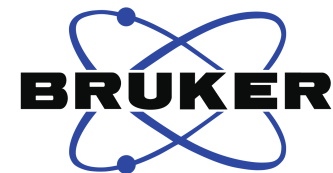
S4. ^1H , ^{13}C NMR and Mass Spectra of Bithiazole 6

AK520

8.195
8.021
7.679
7.478
7.419
7.346
7.299
7.240

4.177

2.080
1.401
1.289
0.948
0.876



Current Data Parameters
NAME Andreas Kalogirou
EXPNO 279
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130710
Time 5.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 90.5
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 500.0361158 MHz
NUC1 1H
P1 11.75 usec
PLW1 15.41699982 W

F2 - Processing parameters
SI 65536
SF 500.0330402 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

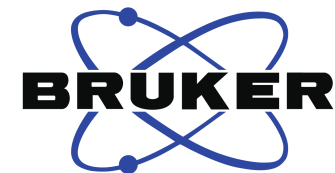
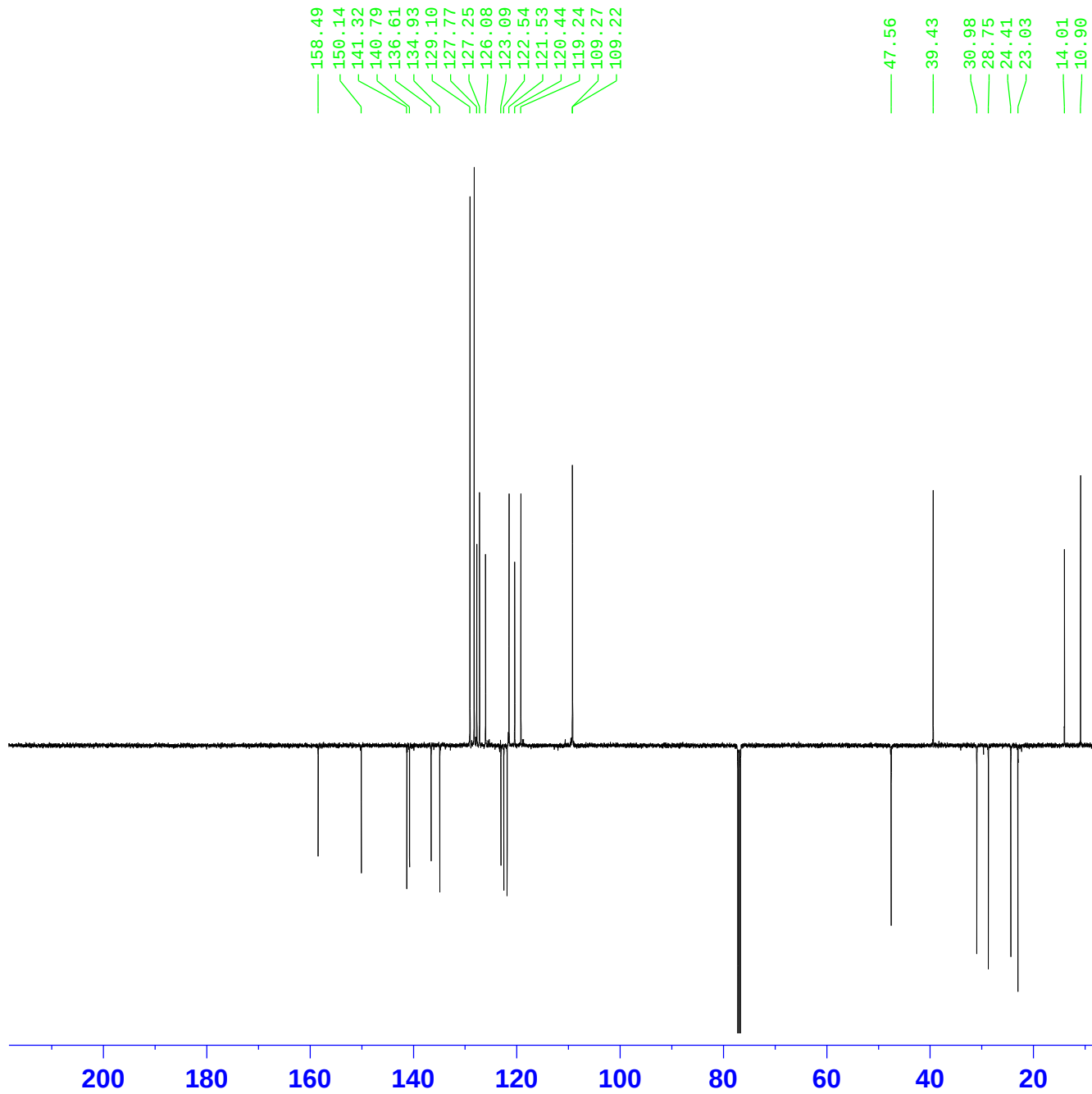
11 10 9 8 7 6 5 4 3 2 1 ppm

0.92
0.92
1.94
2.00
0.97
1.04
2.92
1.04

1.98

1.00
8.71
3.01
3.45

AK520



Current Data Parameters
NAME Andreas Kalogirou
EXPNO 280
PROCNO 1

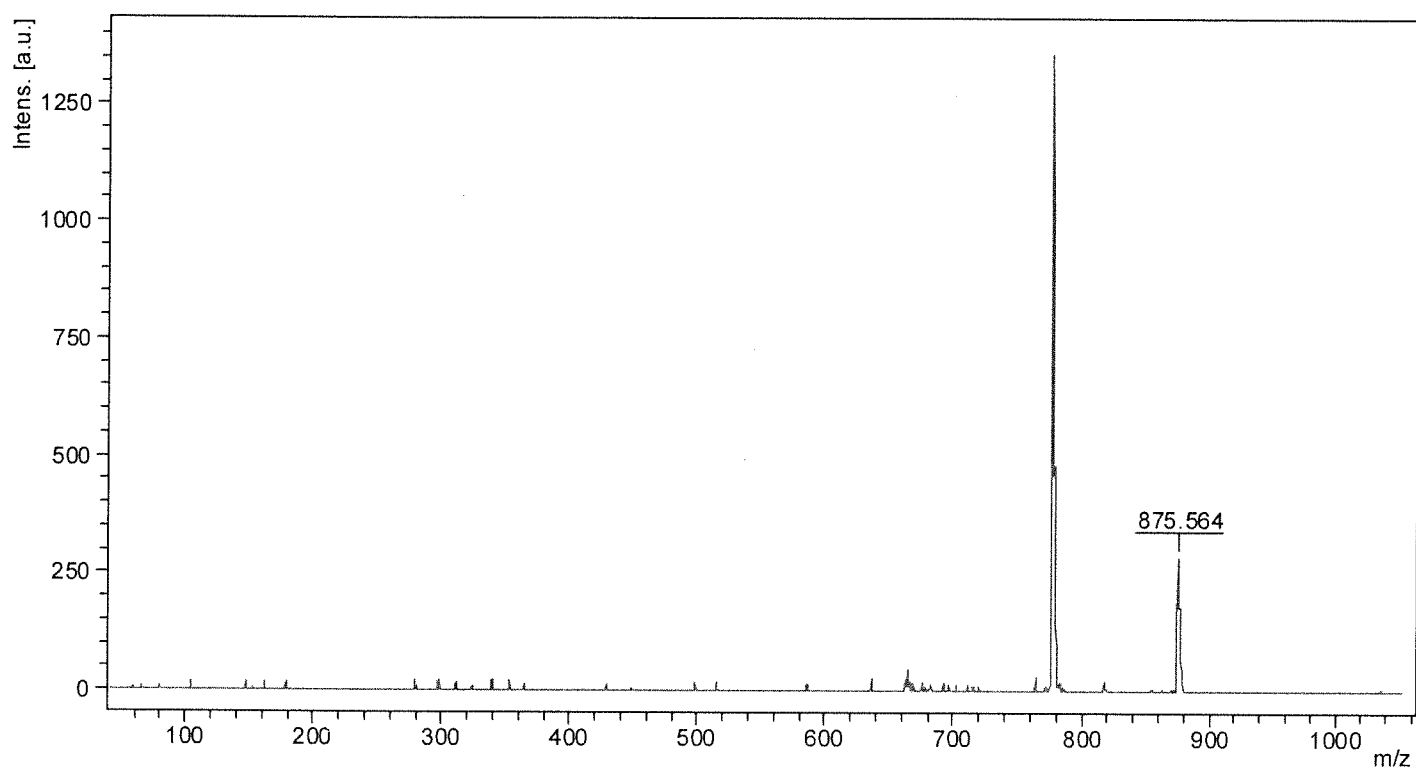
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PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 4904
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.7 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

===== CHANNEL f1 =====
SF01 125.7459782 MHz
NUC1 13C
P1 8.70 usec
P2 17.40 usec
PLW1 138.00000000 W

===== CHANNEL f2 =====
SF02 500.0350280 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.41699982 W
PLW12 0.33258000 W

F2 - Processing parameters
SI 32768
SF 125.7334101 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

AK517



	m/z	Rel. Intens.
M^+ -heptane	776.540	100
	777.573	62
	778.607	35
	779.608	10
	780.595	5
M^+	875.564	21
	876.635	13
	877.700	6
	878.725	3
	879.752	1

Acquisition Parameter

Acquisition operation mode
Voltage polarity

Reflector
POS