Electronic Supporting Information

Electronic Communication Accross N-Linked Unconjugated Polymers: Important Insight into the Charge Transfer Processes of Polyaniline

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Experimental Section

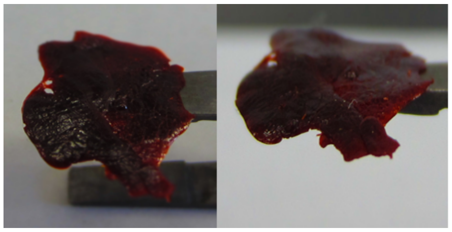
Materials. Compound trans-$Pt(PBu_3)_2Cl_2$, [1] *trans*-$[PtCl(Ph)(PBu_3)_2]$, [2] 4-iodo-N-methylaniline(**3**),[3] **8** [4]were prepared according to literature procedures. All reactions were performed in Schlenk-tube flasks under purified nitrogen. All flasks were dried under a flame to eliminate moisture. All solvents were distilled from appropriate drying agents. All other reagents were used as received.

Synthesis.

Polymer 1.

A 73.2 mg quantity (0.200 mmol) of **6**, 134 mg (0.200 mmol) of *trans*-$Pt(PBu_3)_2Cl_2$, and 1.91 mg of CuI were dissolved in THF (50 mL) and Et_3N (50 mL), and the reaction was stirred at 65 °C for 48h under N_2. The solvent was evaporated, and the residue was purified by column chromatography using CH_2Cl_2/hexane (1:1, v/v) as the eluent to give **P1** (100 mg, 50%) as a black solid. IR (KBr): 2097 ($\nu_{C\equiv C}$), 1633 ($\nu_{C=O}$), 1542 cm^{-1}.^1H NMR (400 MHz, $CDCl_3$): δ 7.26-7.21 (m, 4H, Ar), 6.93-6.91 (m, 4H, Ar), 5.50-5.48 (m, 2H, Ar), 3.39-3.36 (m, 6H, CH_3), 2.10 (b, 12H, $P\underline{CH_2}C_3H_7$), 1.58 (b, 12H, $PCH_2\underline{CH_2}C_2H_5$),1.45-1.43(m, 12H, $PCH_2CH_2\underline{CH_2}CH_3$),0.94-0.90 (m, 18H, $PCH_2CH_2CH_2\underline{CH_3}$).$^{31}P$ NMR (162 MHz, $CDCl_3$): δ 4.23 ($^1J_{P\text{-}Pt}$ = 2358 Hz). Anal. Calc. for $(C_{48}H_{70}N_2O_2P_2Pt)_n$: C, 59.80; H, 7.32; N, 2.91. Found: C, 57.16; H, 7.64; N, 2.70%.

Polymer 2.



A 32.6 mg quantity (0.100 mmol) of **11**, 67.0 mg (0.100 mmol) of *trans*-$Pt(PBu_3)_2Cl_2$, and 1.91 mg of CuI were dissolved in THF (50 mL) and Et_3N (50 mL). The reaction was stirred at 65 °C for 48h under N_2. The solvent was evaporated, and the residue was purified by column chromatography using CH_2Cl_2/hexane (1:1, v/v) as the eluent to give **P2** (60.2 mg, 60.2%) as an orange solid. IR (KBr): 2091 ($\nu_{C\equiv C}$), 2057 ($\nu_{C\equiv C}$), 1742 ($\nu_{C=O}$), 1585 cm^{-1}. ^1H

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[1] G. B. Kauffmann, L. A. Teterm, *Inorg. Synth*., 1963, **7**, 245.

[2] W. D. Miillrr, G. Schmidlbery and H. A. Brune, *Chem. Ber.*, 1985, 4653.

[3] D. V. Kosynkin, J. M. Tour, *Org. Lett.,* 2001, **3**, 991.

[4] M. G. Banwell, M. T. Jones, D. T. J. Loong, D. W. Lupton, D. M. Pinkerton, A. C. Willis, J. K. Ray, *Tetrahedron*, 2010, **66**, 9252.

NMR (400 MHz, $CDCl_3$): δ 7.29-7.25 (m, 4H, Ar), 7.16 (d, J=5.4 Hz, 2H, Ar), 7.08 (d, J=10 Hz, 2H, Ar), 5.09 (s, 1H, Ar), 3.60 (s, 3H, CH_3), 2.09 (b, 12H, $P\underline{CH_2}C_3H_7$), 1.56 (b, 12H, $PCH_2\underline{CH_2}C_2H_5$), 1.42 (b, 12H, $PCH_2CH_2\underline{CH_2}CH_3$), 0.91 (b, 18H, $PCH_2CH_2CH_2\underline{CH_3}$). ^{31}P NMR (162 MHz, $CDCl_3$): δ 4.32 ($^1J_{P\text{-}Pt}$ = 2348 Hz). Anal. Calc. for $(C_{45}H_{66}N_2O_2P_2Pt)_n$: C, 58.5; H, 7.2; N, 3.0. Found: C, 56.8; H, 7.5; N, 3.2 %.

Compound 4. 4-iodo-N-methylaniline **3** (2.33 g, 10.0 mmol), benzoquinone (1.08 g, 10.0 mmol) and $In(OTf)_3$ (280 mg, 0.500 mmol) were stirred in water (100 mL) at room temperature for 24 h. The reaction was monitored by TLC. After **3** was totally consumed, the reaction mixture was extracted with $CHCl_3$. The combined organic layer was dried over Na_2SO_4 and evaporated to remove the solvent. The crude product was purified by chromatography on silica gel using CH_2Cl_2/hexane (1:1, v/v) to give **4** as a brown solid; yield: 1.43 g (50%). IR (KBr): 1643 ($\nu_{C\equiv O}$), 1576, 1226 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, J=12 Hz, 4H, Ar), 6.83 (d, J=8 Hz, 4H, Ar), 5.57 (s, 2H, Ar), 3.27 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$): δ 181.7 (C=O), 151.0, 148.0, 138.8, 127.4, 108.2, 90.8, 43.1. ESI-TOF: m/z calculated: 592.9193 (MNa^+), m/z observed: 592.9197 (MNa^+).

Compound 5. To a solution of **4** (855 mg, 1.50 mmol), $PdCl_2(Ph_3P)_2$ (52.7 mg, 0.0750 mmol) and CuI (14.3 mg, 0.0750 mmol) in Et_3N (75 mL) and THF (75 mL), $Me_3SiC\equiv CH$ (0.60 mL, 4.5 mmol) was added under N_2. After stirring overnight at 65 °C, all volatile components were removed under reduced pressure. The residue was purified by column chromatography using CH_2Cl_2/hexane (1:1, v/v) as the eluent to give **5** (352 mg, 46%) as a brown solid. IR (KBr): 2154 ($\nu_{C\equiv C}$), 1641 ($\nu_{C=O}$), 1573 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 7.43 (d, J=8 Hz, 4H, Ar), 7.00 (d, J=8 Hz, 4H, Ar), 5.61 (s, 2H, Ar), 3.29 (s, 6H, CH_3), 0.24 (s, 18H, $Si(CH_3)_3$). ^{13}C NMR (101 MHz, $CDCl_3$): δ 181.52 (C=O), 150.9, 148.0, 133.1, 124.9, 120.7, 108.5, 104.5, 94.8, 42.8, 0.00. ESI-TOF: m/z calculated: 533.2051 (MNa^+), m/z observed: 533.2052 (MNa^+).

Compound 6. Tetrabutylammonium fluoride solution (3 mL, 1 M in THF) was added to a stirred solution of **5** (510 mg, 1.00 mmol) in $CHCl_3$ (100 mL). After stirring at room temperature for 3h, water (30 mL) was added to quench the reaction. The reaction mixture was extracted with $CHCl_3$. The combined organic layer was dried over Na_2SO_4 and evaporated to remove the solvent. The product was purified by column chromatography using CH_2Cl_2/hexane (1:1, v/v) as the eluent to give **6** (300 mg, 82%) as a brown solid. IR

(KBr): 3298 ($\nu_{\equiv CH}$), 2154 ($\nu_{C\equiv C}$), 1641 ($\nu_{C=O}$), 1554, cm^{-1}.^{1}H NMR (400 MHz, CDCl$_3$): δ 7.47 (d, J=12 Hz, 4H, Ar), 7.03 (d, J=8 Hz, 4H, Ar), 5.63 (s, 2H, Ar), 3.30 (s, 6H, CH$_3$), 3.08 (s, 2H, C≡CH). ^{13}C NMR (101 MHz, CDCl$_3$): δ 181.7, 151.1, 148.6, 133.5, 125.18, 119.9, 108.7, 83.3, 43.0. ESI-TOF: m/z calculated: 389.1260 (MNa$^+$), m/z observed: 389.1264 (MNa$^+$).

Compound 7. To a stirred mixtures of ligand **6** (18.3 mg, 0.0500 mmol) and two molar equivalents of *trans*-PtCl(Ph)(PBu$_3$)$_2$ (71.2 mg, 0.100 mmol) in NEt$_3$ (50 mL) and THF (50 mL), CuI (2.00 mg) was added as the catalyst. The solution was stirred at 65 °C for 16 h under nitrogen, after which all volatile components were removed under vacuum. The crude product was purified by column chromatography using CH$_2$Cl$_2$/hexane (1:1, v/v) as the eluent to give **7** (50 mg, 56%) as a black solid. IR (KBr):1650 ($\nu_{C=O}$), 1554 cm^{-1}.^{1}H NMR (400 MHz, CDCl$_3$): δ 7.29-7.23 (m, 8H, Ar), 6.96-6.91 (m, 8H, Ar), 6.78 (t, J=7.2 Hz, 2H, Ar), 5.49 (s, 2H, Ar), 3.38 (s, 6H, N-CH$_3$), 1.72-1.68 (m, 24H, P$\underline{CH_2}$C$_3$H$_7$),1.48-1.45 (m, 24H, PCH$_2$$\underline{CH_2}C_2H_5$), 1.37-1.31 (m, 24H, PCH$_2$CH$_2$$\underline{CH_2}CH_3$), 0.88 (t, J= 7.2 Hz, H, PCH$_2$CH$_2$CH$_2$$\underline{CH_3}$).^{31}P NMR (162 MHz, CDCl$_3$): δ 3.06 ($^{1}J_{P\text{-}Pt}$ = 2619 Hz). ^{13}C NMR (101 MHz, CDCl$_3$): δ 182.1, 156.6, 151.8, 139.4, 132.0, 125.0, 121.5, 115.2, 109.7, 107.0, 43.3, 26.3, 23.2, 22.83, 14.1. ESI-TOF: m/z calculated: 1740.8600 (MNa$^+$), m/z observed: 1740.8600 (MNa$^+$). Anal. Calc. for C$_{84}$H$_{134}$N$_2$O$_2$P$_4$Pt$_2$: C, 58.72; H, 7.86; N, 1.63. Found: C, 58.39; H, 8.05; N, 2.03%.

Compound 9. 4-iodo-N-methylaniline (2.33 g, 10.0 mmol), 3-bromo-1-iodophenyl-1H-pyrrole-2,5-dione (3.78 g, 10.0 mmol) and Et$_3$N (2 mL) in xylene (10 mL) were under reflux for 2 h after cooling down, The crude product was purified by chromatography on silica gel directly using CH$_2$Cl$_2$/hexane (2:1, v/v) to give **9** as a yellow solid; yield: 1.33 g (25%). IR (KBr): 1708 ($\nu_{C=O}$), 1608 cm^{-1}.^{1}H NMR (400 MHz, CDCl$_3$): δ 7.75 (m, 4H, Ar), 7.11 (d, J=6.8 Hz, 2H, Ar), 7.01 (d, J=6.4 Hz, 2H, Ar), 5.21 (s, 1H, Ar), 3.54 (s, 3H, CH$_3$). ^{13}C NMR (101 MHz, CDCl$_3$): δ 169.19 (C=O), 164.98(C=O), 149.4, 144.9, 139.1, 138.2, 131.7, 127.9, 127.54, 93.2, 92.6, 92.5, 42.0. ESI-TOF: m/z calculated: 552.8880 (MNa$^+$), m/z observed: 552.8885 (MNa$^+$).

Compound 10. To a solution of **9** (530 mg, 1.00 mmol), PdCl$_2$(Ph$_3$P)$_2$ (35.1 mg, 0.0500 mmol) and CuI (9.55 mg, 0.0500 mmol) in Et$_3$N (50 mL) and THF (50 mL), Me$_3$SiC≡CH (0.30 mL, 3.00 mmol) was added under N$_2$. After stirring overnight at rt, all volatile components were removed under reduced pressure. The residue was purified by column chromatography using CH_2Cl_2/hexane (1:1, v/v) as the eluent to give **10** (248 mg, 60%) as a yellow solid. IR (KBr): 2114 ($\nu_{C≡C}$), 2091 ($\nu_{C≡C}$),1708 ($\nu_{C=O}$), 1596 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25 (t, J=7.6 Hz, 4H, Ar), 7.07 (d, J=8.4 Hz, 2H, Ar), 6.92 (d, J=8.4 Hz, 2H, Ar), 4.95 (s, 1H, Ar), 3.28 (s, 3H, CH_3), 0.00 (d, J=3.6 Hz, 18H, $Si(CH_3)_3$). ^{13}C NMR (101 MHz, $CDCl_3$): δ 169.2, 164.9, 149.2, 144.9, 133.3, 132.4, 132.0, 125.5, 125.1, 122.4, 121.9, 104.5, 104.0, 95.7, 94.9, 93.3, 41.6, 0.05 ppm. ESI-TOF: m/z calculated: 493.1738 (MNa^+), m/z observed: 493.1734 (MNa^+).

Compound 11. Tetrabutylammonium fluoride solution (1.50 mL, 1 M in THF) was added to a stirred solution of **10** (282 mg, 0.600 mmol) in $CHCl_3$ (100 mL). After stirring at room temperature for 3 h, water (30 mL) was added to quench the reaction. The reaction mixture was extracted with $CHCl_3$. The combined organic layer was dried over Na_2SO_4 and evaporated to remove the solvent. The product was purified by column chromatography using CH_2Cl_2/hexane (2:1, v/v) as the eluent to give **11** (100 mg, 51%) as a yellow solid. IR (KBr): 3115 ($\nu_{≡CH}$), 2114 ($\nu_{C≡C}$), 2091 ($\nu_{C≡C}$),1708 ($\nu_{C=O}$), 1585 cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (dd, J=8, 2.4 Hz, 4H, Ar), 7.33 (d, J=8.4 Hz, 2H, Ar), 7.20 (d, J=8.4 Hz, 2H, Ar), 5.23 (s, 1H,Ar), 3.55 (s, 3H, CH_3) , 3.12 (s, 1H, C≡CH), 3.08 (s, 1H, C≡CH). ^{13}C NMR (101 MHz, $CDCl_3$): δ 169.0, 164.8, 149.1, 145.1, 133.4, 132.5, 132.1, 125.6, 125.2, 121.3, 120.8, 93.3, 83.0, 82.6, 78.4, 77.8, 41.6. ESI-TOF: m/z calculated: 349.0948 (MNa^+), m/z observed: 349.0968 (MNa^+).

Compound 12. To a stirred mixtures of ligand **11** (16.3 mg, 0.0500 mmol) and two molar equivalents of *trans*-$PtCl(Ph)(PBu_3)_2$ (71.2 mg, 0.100 mmol) in NEt_3 (50 mL) and THF (50 mL), CuI (2.00 mg) was added as the catalyst. The solution was stirred at 65 °C for 16 h under nitrogen, after which all volatile components were removed under vacuum. The crude product was purified by column chromatography using CH_2Cl_2/hexane (1:2, v/v) as the eluent to give **12** (45.1 mg, 52%) as a yellow gel. IR (KBr): 2141 ($\nu_{C≡C}$), 1738 ($\nu_{C=O}$) cm^{-1}.^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.27 (m, 8H, Ar), 7.15 (d, J=6.8 Hz, 2H, Ar), 7.08 (d, J=6.4 Hz, 2H, Ar), 6.97-6.92 (m, 4H, Ar), 6.78 (dd, J=12.8, 6.4 Hz, 4H, Ar), 5.09 (s, 1H, Ar), 3.62 (s, 3H, CH_3), 1.72-1.68 (m, 24H, $P\underline{CH_2}C_3H_7$), 1.48-1.45 (m, 24H, $PCH_2\underline{CH_2}C_2H_5$), 1.37-1.30 (m, 24H, $PCH_2CH_2\underline{CH_2}CH_3$), 0.88 (m, 36H, $PCH_2CH_2CH_2\underline{CH_3}$).^{31}P NMR (162 MHz, $CDCl_3$): δ 4.20 ($1^{J}_{P\text{-}Pt}$ = 2352 Hz). ^{13}C NMR (101

MHz, $CDCl_3$): δ 170.3, 165.9, 156.6, 156.3, 149.9, 141.7, 139.4, 139.3, 132.0, 131.2, 129.2, 129.1, 128.2, 127.5, 127.4, 125.9, 124.8, 121.6, 121.5, 116.5, 115.0, 109.9, 109.5, 91.8, 41.4, 26.3, 24.6, 23.0, 14.0. ESI-TOF: m/z calculated: 1677.8449 (MH^+), m/z observed: 1677.8483 (MH^+). Anal. Calc. for $C_{81}H_{130}N_2O_2P_4Pt_2$: C, 57.98; H, 7.81; N, 1.67. Found: C, 58.23; H, 8.16; N, 1.99%.

Instruments: The ^{1}H NMR, ^{13}C NMR and ^{31}P NMR spectra were collected on a Bruker DRX400 spectrometer using the solvent as chemical shift standard. High resolution mass measurements (HR-MS) were carried out in the same conditions as previously using PEG ion series as internal calibrant or on a Bruker Micro-QTOF instrument in ESI mode. The spectra were measured from freshly prepared samples. The IR spectra were acquired on a Bomem FT-IR MB series spectrometer equipped with a baseline-diffused reflectance. The UV-vis spectra were recorded on a Hewlett-Packard diode array model 8452A. The emission and excitation spectra were obtained using a double monochromator Fluorolog 2 instrument from Spex. The fluorescence lifetimes were measured on a Timemaster Model TM-3/2003 apparatus from PTI. The source was a nitrogen laser with a high-resolution dye laser (fwhm ~ 1.5 ns), and the fluorescence lifetimes were obtained from high-quality decays and deconvolution or distribution lifetime analysis. The thermogravimetric analysis (TGA) measurements were performed on thermal gravimetric analyzer (model Perkin-Elmer TGA-6) under a nitrogen flow at a heating rate of 10 °C/min.

SAXS: The Small-Angle X-ray Scattering, SAXS, patterns were collected with a Bruker AXS Nanostar system equipped with a Microfocus Copper Anode at 45 kV/0.65 mA, MONTAL OPTICS and a VANTEC 2000 2D detector at 106.40 cm distance from the samples calibrated with a Silver Behenate standard. The solutions were prepared saturated in distilled 2-MeTHF, and placed in quartz cells for measurements. The blanks were measured first and subtracted to the measured data. The diffracted intensities were integrated from 0.10 to 3.40 deg. 2-theta and treated with Primus GNOM 3.0 program from ATSAS 2.3 softwares, to determine the particle sizes by pair distance distribution. (see detail in .C. D. Putnam, M. Hammel, G. L. Hura, and J. A. Taner. *Quart. Rev. Biophys*. 2007, **40**, 191). The collection exposure times were 1000 seconds / sample. From Braggs law 2d sinθ = nλ and q = 2π/d, we can calculate the pair distance distribution function eq 1.

$$p(r) = \frac{r^2}{(2\pi)^3}\int_0^\infty \mathrm{d}q\ 4\pi q^2 \frac{\sin qr}{qr} I(q) \qquad (1)$$

The pair distance distribution function *p*(*r*) represents the probability of finding two points in the particle separated by a distance *r*. The largest diameter of the particle can be obtained from the *p*(*r*) function where the *p*(*r*) tends to zero. The shape of the function is related to the shape of the particles; a Gaussian represents a globular shape. From the definition, polymers **1** and **2** adopt a globular shape with a maximal size close to 98 nm (Figures S4 and S5).

Electrochemistry: Electrochemical measurements were carried out using a three-electrode configuration (Pt working electrode, a Pt counter electrode and a Ag/Ag^+ (0.1M $AgNO_3$, 0.1M Bu_4NPF_6 in MeCN) reference electrode) and a PARC 273A potentiostat interfaced to a personal computer at room temperature under a flow of nitrogen gas. The solvent in all measurements was deoxygenated THF, and the supporting electrolyte was 0.1 M Bu_4NPF_6.

Computations: Calculations were performed with Gaussian 09[5] at the Université de Sherbrooke with Mammouth super computer supported by le Réseau Québécois de Calculs de Haute Performances.The hybrid B3LYP exchange-correlation function has been considered because of the high accuracy of the ensued results.[6] LANL2DZ pseudopotentials were used on platinum and phosphorus atoms, with LANL2DZ basis set for platinum and 3-

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[5] M. J. Frisch, G. W.Trucks, H. B., Schlegel, G. E., M. A. Scuseria, J. R. Robb, V. G. Cheeseman, J. A., Jr. Zakrzewski, R. E. Montgomery, J. C. Stratmann, S. Burant, J. M. Dapprich, A. D. Millam, K. N. Daniels, M. C. Kudin, O. Strain, J. Farkas, V. Tomasi, M. Barone, R, Cossi, B. Cammi, C. Mennucci, C. Pomelli, S. Adamo, J. Clifford, G. A. Ochterski, P. Y. Petersson, Q. Ayala, K. Cui, D. K. Morokuma, A. D. Malick, K. Rabuck, J. B. Raghavachari, J. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I., Komaromi, R., Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. C. Nanayakkara, M. Gonzalez, P. M. Challacombe, W. Gill, B. G. Johnson, W. Chen, M. W. Wong, J. L. Andres, M. Head-Gordon, E. S. Replogle, and J. A. Pople. *Gaussian, Inc.* Pittsburgh P.A., 1998.

[6] (a) A. D. Becke, *J. Chem. Phys*., 1993, **98**, 5648. (b) C. Lee, W. Yang, R. G. Parr, *Phys. ReV. B: Condens. Matter Mater. Phys.,* 1988, 785. (c) B. Miehlich, A. Savin, H. Stoll, H. Preuss, *Chem. Phys. Lett*., 1989,**157**, 200.

21G* for all other atoms.[7] The model compound for **polymer 1** and **2** were optimized before the time-dependent density-functional theory (TDDFT) calculations. Only the relevant (stronger oscillator strength and wave function coefficients) molecular orbitals are shown. All computations were performed without symmetry constraints. Note that the DFT methods are not ideal for properly predicting the positions of the CT transitions. In a qualitative sense, the difference between the calculated (H-1→L (transition with sufficient intensity): 615 and 431 nm) and estimated experimental positions (long tail at ~600 and shoulder at 420 nm) for **1** and **2**, respectively, is adequate for a description of the phenomenon.

X-ray analysis. Diffraction data frames for **5** and **9** were collected at 100 K on a Bruker Apex Duo and integrated with the Bruker SAINT software package using a narrow-frame algorithm. Data were corrected for absorption effects using the multi-scan method (SADABS),The structure was solved by direct methods (SIR 92) [8] and refined with SHELXL97. [9] All non–hydrogen atoms were refined with anisotropic thermal parameters. The hydrogen atoms were placed in calculated positions and included in final refinement in a riding model with isotropic temperature parameters set to $U_{\mathrm{iso}}(\mathrm{H}) = 1.5U_{\mathrm{eq}}(\mathrm{C})$.

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[7] (a) K. D. Dobbs, W. J. Hehre, *J. Comput. Chem.,* 1986, **7**, 359. (b) K. D. Dobbs, W. J. Hehre, *J. Comput. Chem.,* 1987, **8**, 861. (c) K. D. Dobbs, W. J. Hehre, *J. Comput. Chem*., 1987, **8**, 880.

[8] A. Altomare, G. Cascarano, C. Giacovazzo, A.Guagliardi, *J. Appl. Crystallogr.,*1993, **32**, 115.

[9] G. M. Sheldrick. *Acta Cryst*., 2008, **A64**, 112.

Table S1. X-ray data for 5

Identification code	Harvey_wxr_2_14	
Chemical formula	$C_{30}H_{34}N_2O_2Si_2$	
Formula weight	510.77	
Temperature	173(2) K	
Wavelength	1.54186 Å	
Crystal size	0.100 x 0.170 x 0.550 mm	
Crystal habit	clear dark purple Needle	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 12.4957(5) Å	α = 90°
	b = 22.4434(8) Å	β = 113.2100(10)°
	c = 11.2136(4) Å	γ = 90°
Volume	2890.29(19) $Å^3$	
Z	4	
Density (calculated)	1.174 g/cm^3	
Absorption coefficient	1.330 mm^{-1}	
F(000)	1088	

Table S2. X-ray data for 9

Identification code	Harvey_wrx_2_8b	
Chemical formula	$C_{17}H_{12}I_2N_2O_2$	
Formula weight	530.09	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal size	0.035 x 0.100 x 0.647 mm	
Crystal habit	clear light yellow Needle	
Crystal system	monoclinic	
Space group	C 1 2 1	
Unit cell dimensions	a = 25.385(4) Å	α = 90°
	b = 4.1207(6) Å	β = 98.230(4)°
	c = 15.706(2) Å	γ = 90°
Volume	1626.0(4) $Å^3$	
Z	4	
Density (calculated)	2.165 g/cm^3	
Absorption coefficient	3.879 mm^{-1}	
F(000)	1000	

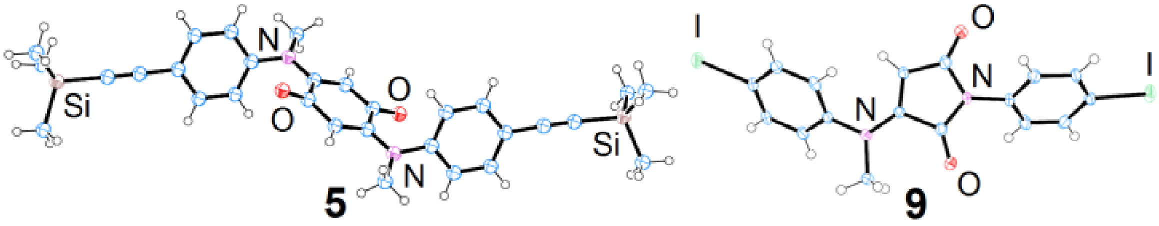
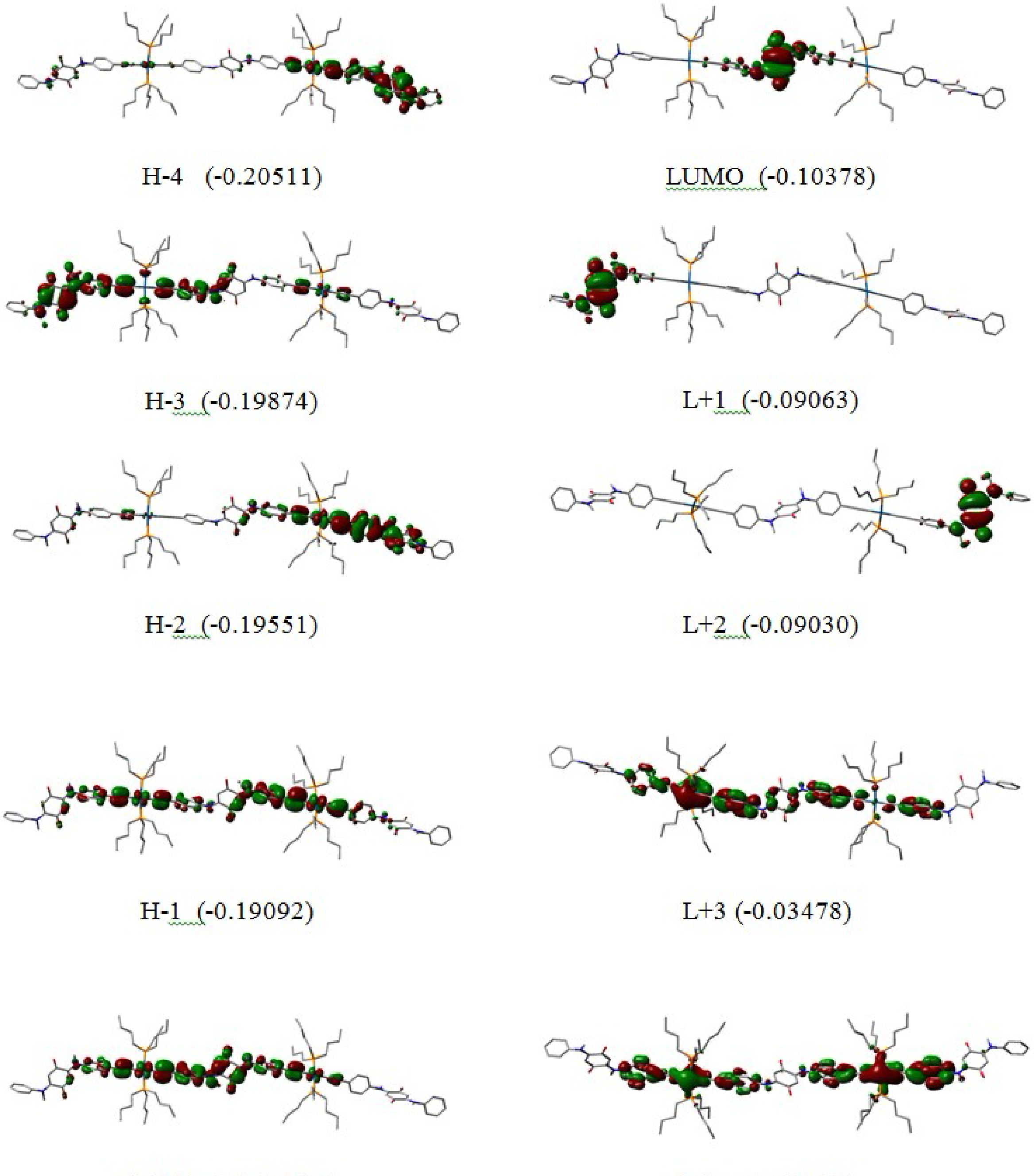


Fig. S1. ORTEP drawings of **5** and **9** (the thermal ellipsoids are at 50% probability). Full detail is provided in the ESI.



H-4 (-0.20511)

LUMO (-0.10378)

H-3 (-0.19874)

L+1 (-0.09063)

H-2 (-0.19551)

L+2 (-0.09030)

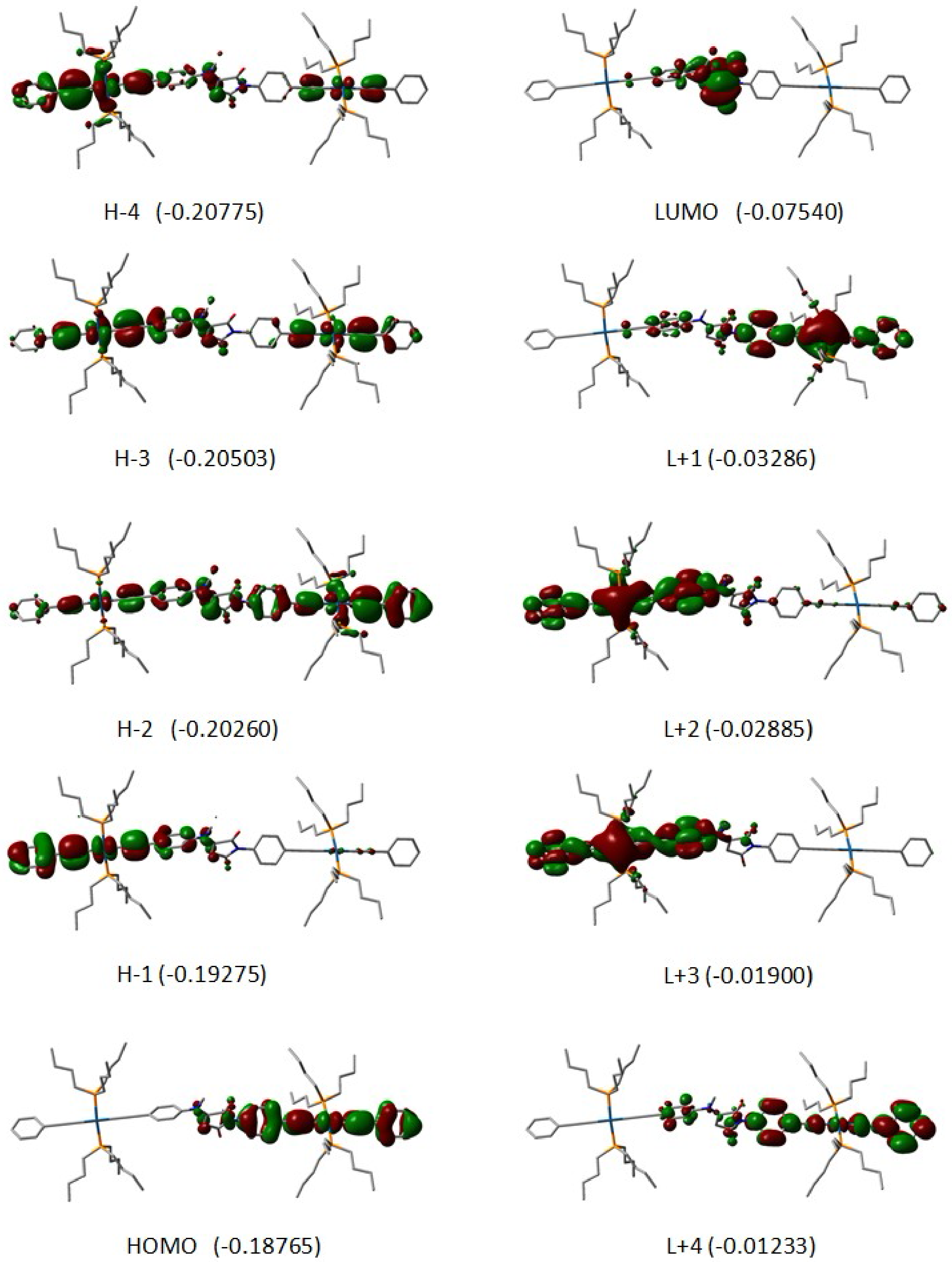
H-1 (-0.19092)

L+3 (-0.03478)

HOMO (-0.18783)

L+4 (-0.03163)

Fig. S2. Representation of the frontier MOs of **1**. The MO energies are in Hartree. H = HOMO; L = LUMO.



H-4 (-0.20775)

LUMO (-0.07540)

H-3 (-0.20503)

L+1 (-0.03286)

H-2 (-0.20260)

L+2 (-0.02885)

H-1 (-0.19275)

L+3 (-0.01900)

HOMO (-0.18765)

L+4 (-0.01233)

Fig. S3. Representation of the frontier MOs of **2**. The MO energies are in Hartree. H = HOMO; L = LUMO

Table S3. Calculated positions, oscillator strength (f), and major contributions of the first 100 electronic transitions for **1**.

Wavelength (nm)	Osc. Strength	Major contribs
656.2	0.0022	HOMO→LUMO (88%)
615.2	0.5013	H-1→LUMO (89%)
546.2	0.0011	H-2→LUMO (85%)
536.5	0.0393	H-3→L+1 (31%), H-1→L+1 (20%), HOMO→L+1 (41%)
531.8	0.0526	H-5→LUMO (10%), H-3→LUMO (72%)
527.7	0.0266	H-4→L+2 (14%), H-2→L+2 (65%), H-1→L+2 (15%)
499.1	0.0176	H-5→L+1 (17%), H-3→L+1 (31%), HOMO→L+1 (41%)
497.5	0.0046	H-1→L+2 (24%), HOMO→L+2 (60%)
493.3	0.0005	H-6→LUMO (17%), H-5→LUMO (50%), H-4→LUMO (11%), H-3→LUMO (12%)
483.0	0.0120	H-7→LUMO (27%), H-6→LUMO (28%), H-4→LUMO (27%)
479.8	0.0210	H-4→L+2 (22%), H-1→L+2 (41%), HOMO→L+2 (34%)
476.3	0.0115	H-1→L+1 (71%), HOMO→L+1 (16%)
475.4	0.0000	H-6→LUMO (18%), H-5→LUMO (12%), H-4→LUMO (50%)
471.6	0.0435	H-4→L+2 (46%), H-2→L+2 (24%), H-1→L+2 (19%)
463.3	0.0182	H-7→LUMO (30%), H-6→LUMO (36%), H-5→LUMO (17%)
450.1	0.0320	H-6→L+1 (12%), H-5→L+1 (16%), H-2→L+1 (54%)
443.8	0.0263	H-6→L+1 (15%), H-5→L+1 (13%), H-3→L+1 (26%), H-2→L+1 (42%)
439.2	0.0125	H-31→LUMO (10%), H-21→LUMO (11%), H-20→LUMO (23%), H-13→LUMO (13%), H-10→LUMO (19%)
434.0	0.0002	H-3→L+2 (94%)
430.4	0.0049	H-31→LUMO (14%), H-21→LUMO (17%), H-20→LUMO (18%), H-13→LUMO (15%), H-7→LUMO (13%)
429.8	0.0001	H-6→L+1 (60%), H-5→L+1 (35%)
421.8	0.0003	H-20→LUMO (43%), H-10→LUMO (30%), H-8→LUMO (19%)
415.4	0.0012	H-17→L+1 (30%), H-16→L+1 (67%)
415.1	0.0004	H-15→L+2 (97%)
408.4	0.0144	H-19→L+1 (89%)
407.5	0.0109	H-18→L+2 (91%)
407.3	0.0010	H-9→LUMO (15%), H-8→LUMO (11%), H-4→L+1 (65%)
407.2	0.0043	H-9→LUMO (36%), H-8→LUMO (27%), H-4→L+1 (27%)
405.8	0.0003	H-10→LUMO (21%), H-9→LUMO (44%), H-8→LUMO (33%)
405.8	0.0004	H-5→L+2 (84%)
396.6	0.0004	H-7→L+2 (10%), H-6→L+2 (89%)
392.6	0.0034	H-7→L+2 (76%), H-6→L+2 (11%)
391.9	0.0000	H-11→LUMO (100%)
390.4	0.0004	H-12→LUMO (100%)
383.7	0.1560	H-21→LUMO (13%), H-13→LUMO (66%)
380.1	0.0379	H-7→L+1 (94%)
373.3	0.4672	H-8→L+2 (79%)
372.8	0.3653	H-9→L+1 (73%)

359.0	0.0088	H-10→L+2 (54%), H-9→L+2 (32%)
358.5	0.0010	H-8→L+1 (85%)
356.7	0.0392	H-14→LUMO (82%)
353.9	0.0019	H-10→L+2 (38%), H-9→L+2 (57%)
352.0	0.0019	H-10→L+1 (87%)
351.6	0.0001	H-11→L+1 (99%)
349.4	0.0001	H-12→L+2 (100%)
346.6	0.0083	H-21→LUMO (12%), H-17→LUMO (56%), H-16→LUMO (27%)
341.3	0.1090	H-26→LUMO (17%), H-24→LUMO (27%), H-23→LUMO (34%)
340.7	1.1526	H-1→L+4 (14%), HOMO→L+3 (35%)
338.7	0.5826	H-31→LUMO (23%), H-21→LUMO (15%), HOMO→L+3 (21%)
336.2	0.0393	H-13→L+2 (83%)
335.1	0.0005	H-13→L+1 (77%)
334.7	0.0234	H-13→L+1 (15%), H-1→L+3 (35%), HOMO→L+4 (32%)
333.6	0.0000	H-11→L+2 (100%)
333.2	0.0000	H-12→L+1 (97%)
332.5	0.0000	H-15→LUMO (99%)
332.1	0.0000	H-17→LUMO (33%), H-16→LUMO (67%)
325.1	0.0949	H-2→L+3 (49%), H-2→L+4 (23%)
324.4	0.0007	H-18→LUMO (99%)
324.1	0.0000	H-19→LUMO (99%)
319.2	0.0033	H-14→L+2 (85%)
317.4	0.0016	H-26→LUMO (35%), H-22→LUMO (45%)
316.4	0.0004	H-23→LUMO (10%), H-17→L+1 (22%), H-6→L+4 (10%)
316.1	0.0041	H-26→LUMO (11%), H-23→LUMO (19%), H-17→L+1 (17%)
315.3	0.0153	H-1→L+4 (21%), HOMO→L+5 (19%)
313.3	0.0092	H-17→L+1 (19%), H-6→L+3 (15%), H-6→L+4 (19%), H-5→L+4 (10%)
312.3	0.0007	H-30→LUMO (11%), H-29→LUMO (80%)
312.2	0.0002	H-30→LUMO (87%)
311.9	0.0034	H-24→L+1 (52%), H-23→L+1 (23%)
311.4	0.0016	H-25→L+2 (56%), H-22→L+2 (29%)
309.1	0.0124	H-28→L+1 (90%)
309.1	0.0112	H-27→L+2 (87%)
308.8	0.0001	H-25→LUMO (61%), H-24→LUMO (11%), H-22→LUMO (18%)
308.7	0.0003	H-26→LUMO (11%), H-25→LUMO (10%), H-24→LUMO (53%), H-23→LUMO (18%)
308.6	0.0047	H-1→L+3 (30%), HOMO→L+4 (35%)
307.4	0.0666	H-3→L+3 (21%), H-3→L+4 (27%), H-1→L+5 (19%)
307.1	0.0014	H-14→L+1 (87%)
305.3	0.0075	H-33→L+1 (91%)
305.1	0.0061	H-32→L+2 (88%)
302.9	0.2450	H-4→L+3 (15%), H-2→L+5 (41%)
301.4	0.0000	H-27→LUMO (98%)

301.3	0.0000	H-28→LUMO (98%)
300.5	0.0505	H-1→L+4 (27%), H-1→L+5 (10%)
299.2	0.0001	H-17→L+2 (56%), H-16→L+2 (42%)
298.4	0.0000	H-15→L+1 (99%)
297.5	0.0000	H-17→L+2 (43%), H-16→L+2 (57%)
297.2	0.0000	H-32→LUMO (99%)
297.0	0.0211	HOMO→L+5 (21%), HOMO→L+6 (28%)
296.7	0.0000	H-33→LUMO (99%)
295.4	0.1339	H-5→L+3 (12%), H-1→L+4 (13%)
292.9	0.0025	H-25→L+2 (18%), H-22→L+2 (45%)
291.9	0.0433	H-7→L+3 (13%), H-4→L+5 (12%)
291.9	0.0001	H-18→L+1 (100%)
291.0	0.0000	H-19→L+2 (100%)
290.9	0.0002	H-26→L+1 (36%), H-23→L+1 (39%)
289.1	0.0098	H-1→L+17 (21%), HOMO→L+17 (20%), HOMO→L+18 (11%)
289.0	0.0258	H-3→L+3 (11%), H-2→L+3 (15%), H-2→L+4 (25%)
288.8	0.0056	H-1→L+16 (12%), H-1→L+18 (34%), HOMO→L+17 (23%)
287.8	0.0016	
287.1	0.0001	H-20→L+1 (89%)
286.8	0.0646	HOMO→L+11 (22%), HOMO→L+14 (17%)

Table S4. Calculated positions, oscillator strength (f), and major contributions of the first 100 electronic transitions for **2**.

Wavelength (nm)	Osc. Strength	Major contribs
470.6	0.0012	HOMO→LUMO (88%)
431.1	0.2559	H-1→LUMO (89%)
398.8	0.0765	H-3→LUMO (20%), H-2→LUMO (63%)
386.2	0.0326	H-3→LUMO (69%), H-2→LUMO (14%)
377.1	0.0084	H-5→LUMO (20%), H-4→LUMO (63%), H-2→LUMO (10%)
371.5	0.0577	H-5→LUMO (66%), H-4→LUMO (27%)
344.4	0.3989	H-6→LUMO (76%), HOMO→L+1 (11%)
340.9	0.9396	H-6→LUMO (11%), HOMO→L+1 (77%)
323.7	0.1295	H-20→LUMO (70%), H-1→L+2 (14%)
322.5	0.4369	H-20→LUMO (15%), H-1→L+2 (54%)
320.0	0.0001	H-7→LUMO (100%)
318.7	0.0046	H-5→L+1 (19%), H-3→L+1 (25%), H-2→L+1 (33%)
316.6	0.0001	H-8→LUMO (99%)
310.5	0.0118	H-4→L+2 (35%), H-3→L+2 (32%)
303.9	0.0255	H-9→LUMO (17%), HOMO→L+2 (51%)
302.3	0.007	H-13→LUMO (22%), H-9→LUMO (47%)
301.0	0.0021	H-13→LUMO (64%), H-9→LUMO (16%)

300.1	0.0224	H-1→L+1 (32%), H-1→L+3 (12%), HOMO→L+2 (19%)
297.7	0.0654	H-5→L+1 (15%), H-2→L+1 (15%), H-1→L+3 (24%)
294.7	0.0014	H-5→L+1 (14%), H-1→L+1 (39%)
292.4	0.0009	HOMO→L+9 (43%), HOMO→L+10 (36%), HOMO→L+12 (12%)
291.0	0.1891	H-10→LUMO (11%), H-4→L+2 (10%), H-2→L+2 (13%)
287.9	0.0495	HOMO→L+4 (50%)
287.5	0.0154	H-10→LUMO (50%), H-4→L+2 (10%)
287.0	0.0022	H-1→L+8 (81%)
285.4	0.0018	H-18→LUMO (36%), H-1→L+5 (29%)
284.0	0.1541	H-10→LUMO (26%), H-3→L+3 (19%), H-2→L+3 (10%), HOMO→L+3 (14%)
280.7	0.0465	H-4→L+3 (10%), HOMO→L+3 (52%)
278.9	0.0001	H-3→L+1 (25%), H-2→L+1 (16%)
277.3	0.0128	H-3→L+1 (14%), H-3→L+4 (10%), HOMO→L+9 (11%), HOMO→L+10 (13%)
276.8	0.0025	HOMO→L+7 (54%)
276.0	0.0137	H-18→LUMO (39%), H-1→L+5 (14%), HOMO→L+7 (21%)
275.4	0	H-11→LUMO (100%)
274.9	0.0557	H-4→L+3 (12%), H-2→L+2 (14%), HOMO→L+3 (16%)
274.5	0	H-12→LUMO (99%)
273.3	0.0017	H-4→L+8 (38%), H-3→L+8 (38%)
272.4	0.1359	HOMO→L+9 (29%), HOMO→L+10 (30%)
271.6	0.0024	H-23→LUMO (63%)
270.4	0.0722	H-4→L+1 (35%), H-3→L+2 (14%), H-2→L+2 (10%)
270.2	0.0084	H-14→LUMO (10%), H-1→L+5 (16%), HOMO→L+5 (40%)
270.2	0.0013	H-2→L+9 (10%), H-2→L+10 (10%), HOMO→L+12 (23%)
269.8	0.0324	H-14→LUMO (21%), H-2→L+2 (14%), HOMO→L+5 (16%)
269.4	0.0118	H-2→L+12 (12%), HOMO→L+12 (38%)
269.1	0.0107	H-14→LUMO (30%), H-1→L+6 (34%)
268.5	0.0727	H-4→L+1 (24%), H-4→L+2 (12%), H-4→L+3 (10%), H-1→L+6 (13%)
268.4	0.0323	H-7→L+1 (90%)
267.1	0.0079	H-1→L+11 (74%)
266.0	0.0115	H-15→LUMO (81%)
265.1	0.0009	H-16→LUMO (97%)
264.0	0.0034	H-3→L+5 (43%), H-2→L+5 (19%)
263.4	0.1149	H-5→L+2 (47%)
262.9	0.0045	H-17→LUMO (97%)
262.5	0.3572	H-19→LUMO (10%), H-4→L+6 (36%), H-3→L+6 (17%)
261.7	0.0144	H-19→LUMO (22%), H-5→L+2 (11%), H-1→L+4 (23%)
260.7	0.1051	H-19→LUMO (27%), H-1→L+4 (48%)
259.8	0.0352	H-8→L+2 (82%)
257.9	0.5834	H-6→L+1 (10%), H-6→L+2 (13%), H-5→L+4 (13%), H-2→L+4 (21%)
256.8	0.0743	H-6→L+1 (26%), H-6→L+2 (10%), H-5→L+2 (11%)
255.8	0.0775	H-3→L+3 (14%), H-2→L+3 (23%)

254.8	0.0047	H-7→L+9 (38%), H-7→L+10 (33%), H-7→L+12 (12%)
254.5	0.0036	H-8→L+8 (90%)
253.9	0.0082	H-9→L+1 (10%), H-6→L+2 (21%), H-2→L+3 (27%)
253.7	0.0006	HOMO→L+6 (32%)
253.6	0.0148	HOMO→L+6 (55%)
253.1	0.0009	H-4→L+5 (55%), H-2→L+5 (10%)
250.0	0.0276	HOMO→L+8 (80%)
248.8	0.0001	H-1→L+7 (75%)
248.8	0.001	H-3→L+12 (21%), H-2→L+12 (36%), HOMO→L+12 (10%)
247.9	0.001	H-5→L+3 (53%), H-4→L+3 (13%)
246.7	0.0674	H-5→L+9 (20%), H-5→L+10 (11%), H-2→L+9 (14%), H-2→L+10 (11%)
246.6	0.0803	H-9→L+1 (12%), H-4→L+8 (10%)
246.4	0.0214	H-9→L+1 (25%)
246.3	0.0008	H-5→L+7 (50%), H-4→L+7 (11%), H-3→L+7 (12%)
246.2	0.0122	H-6→L+5 (10%), H-5→L+5 (11%), H-2→L+5 (25%)
245.9	0.0424	H-8→L+3 (67%)
245.2	0.0016	H-5→L+4 (10%), H-3→L+4 (37%), H-2→L+4 (13%)
245.1	0.0004	H-4→L+11 (56%), H-3→L+11 (28%)
244.8	0.0633	H-5→L+3 (16%), H-4→L+6 (13%), H-3→L+6 (17%), H-2→L+6 (18%)
244.4	0.0006	HOMO→L+11 (97%)
243.9	0	H-3→L+7 (10%), H-2→L+7 (61%), HOMO→L+7 (13%)
242.1	0.0089	H-21→LUMO (80%)
241.4	0.0005	H-6→L+5 (11%), H-5→L+5 (16%), H-1→L+9 (14%)
241.3	0.0024	H-6→L+5 (13%), H-5→L+5 (12%), H-1→L+9 (14%)
240.0	0.0009	H-4→L+4 (35%), H-1→L+9 (35%)
239.8	0.0017	H-4→L+4 (24%), H-1→L+9 (19%), H-1→L+10 (40%)
239.3	0.0047	H-7→L+2 (18%), H-7→L+4 (69%)
238.7	0.0002	H-4→L+4 (12%), H-1→L+9 (10%), H-1→L+10 (34%)
237.6	0.0001	H-10→L+2 (54%), H-6→L+3 (17%)
237.5	0.0003	H-8→L+1 (79%), H-8→L+2 (13%)
237.1	0	H-1→L+12 (88%)
236.9	0.0127	H-10→L+2 (14%), H-6→L+3 (53%)
236.0	0.0002	H-5→L+7 (13%), H-3→L+7 (54%), H-2→L+7 (14%)
235.7	0.0001	H-7→L+2 (74%), H-7→L+4 (21%)
235.1	0.0041	H-6→L+5 (40%), H-5→L+5 (40%)
234.4	0.0341	H-22→LUMO (83%)
234.3	0.0726	H-16→L+1 (72%)
233.6	0.0006	H-4→L+11 (13%), H-3→L+11 (23%), H-2→L+11 (29%), H-1→L+11 (16%)
232.9	0.0023	H-11→L+1 (11%), H-5→L+12 (37%)
232.6	0.0008	H-3→L+6 (32%), H-2→L+6 (60%)
229.4	0.0012	H-3→L+8 (20%), H-2→L+8 (63%)

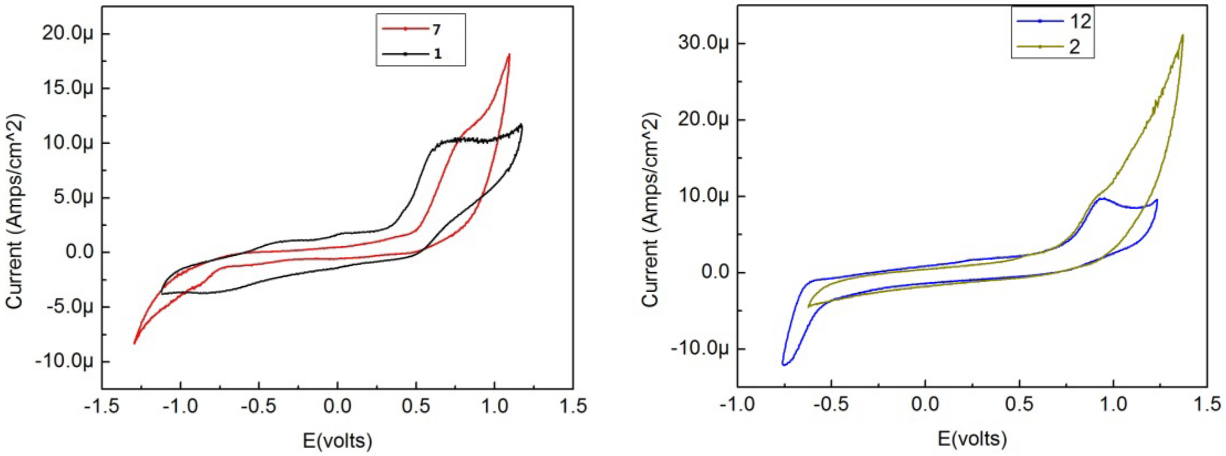


Fig. S4. Cyclic voltammograms of compounds **1**, **2**, **7**, and **12**

Cyclic voltamogramms of **1**, **2**, **7**, and **12**. The cyclic voltammograms were recorded to determine the HOMO and LUMO energies (not possible in this work) of compounds **1**, **2**, 7, 12. The values of the HOMO and LUMO energies can be calculated according to HOMO = -e (φ_{ox}+4.71) and LUMO = -e (φ_{red}+4.71) in eV,[10] where the unit of potential is V vs Ag/Ag$^+$.

Table S5. Comparison of the computed and experimental E_{HOMO} (scan rate of 50 mV s^{-1}).

compounds	Electrochemical properties		
	V_{ox} (V)	E_{HOMO} (eV; exp.)	E_{HOMO} (eV; DFT)
12	0.90	-5.61	–
2	0.90	-5.61	-5.11
7	0.77	-5.48	–
1	0.74	-5.45	-5.11

Table S6. Spectrocopic data of the CT band and emission lifetimes.

	λ_{abs} (nm) (ε ($M^{-1}cm^{-1}$)) CT band, THF, 298K	λ_{em} (nm) 2MeTHF, 77K	τ_e (µs) 2MeTHF, 77K
12	400 (11700)	445	108 ± 2
1	400 (12100)	445	73 ± 2
7	400 (11000)	530	145 ± 6
2	400 (14500)	567	171 ± 2

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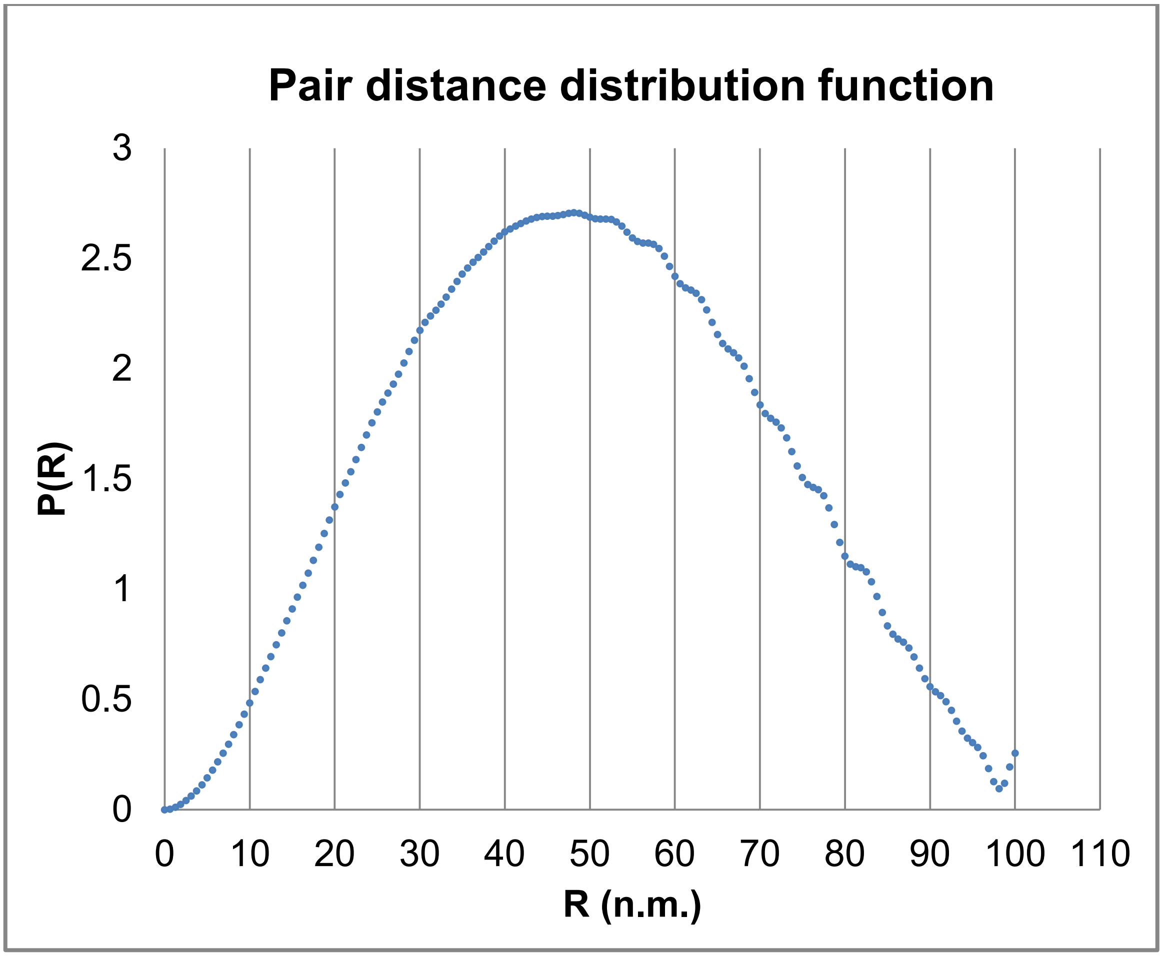
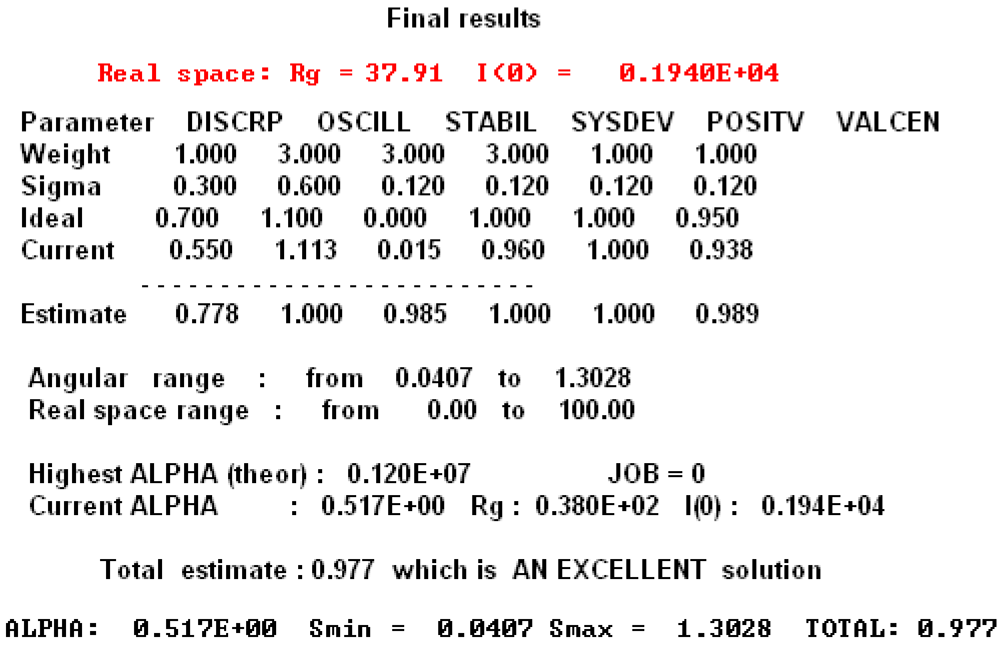
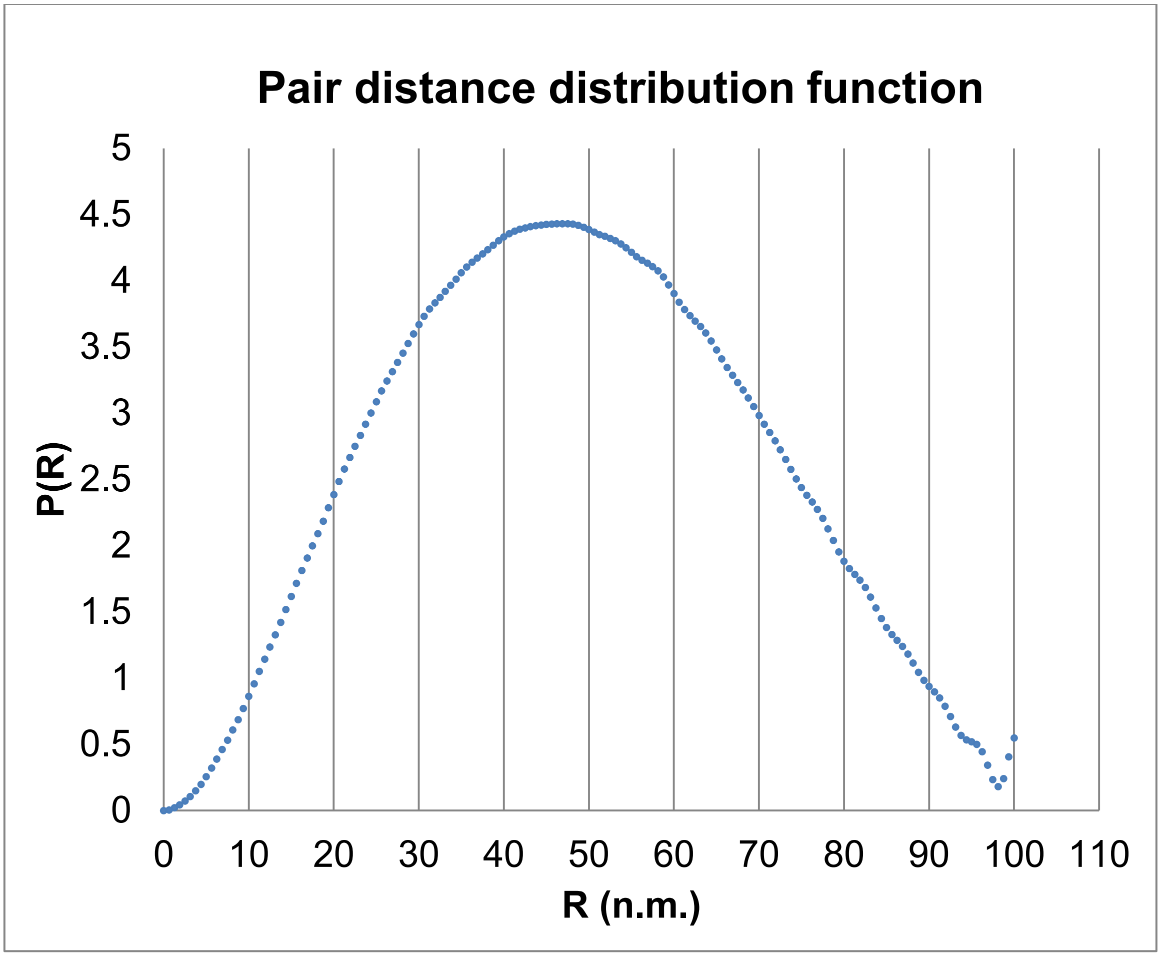
[10] J. Hou, Z. Tan, Y. Yan, Y. He, C. Yang, Y. Li, *J. Am. Chem. Soc.,* 2006, **128**, 4911.

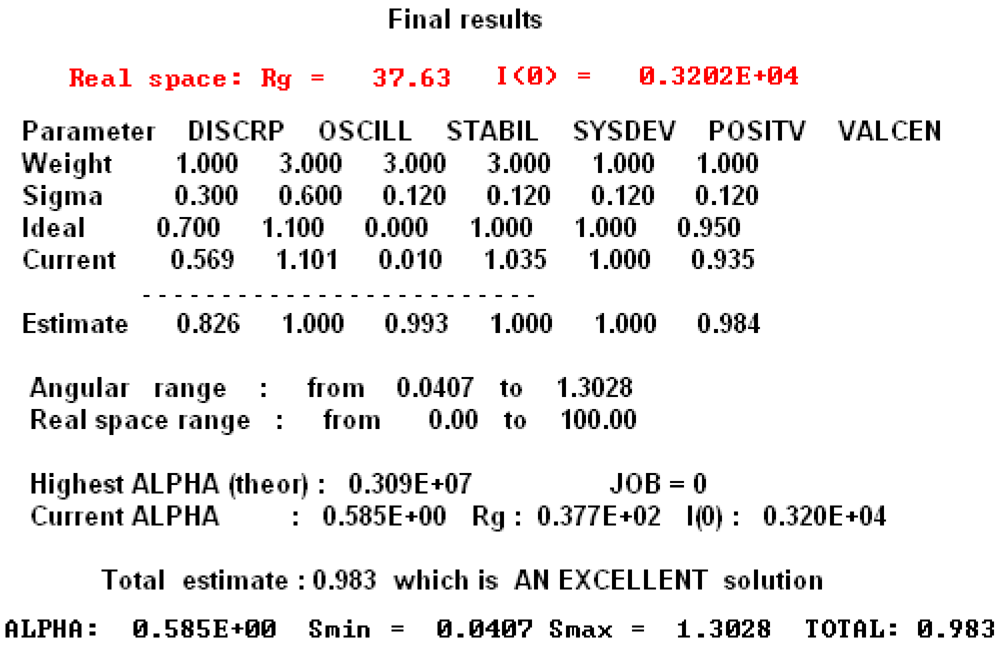




```
                              Final results

        Real space: Rg = 37.91   I(0) =    0.1940E+04

 Parameter   DISCRP   OSCILL   STABIL   SYSDEV   POSITV   VALCEN
 Weight       1.000    3.000    3.000    3.000    1.000    1.000
 Sigma        0.300    0.600    0.120    0.120    0.120    0.120
 Ideal       0.700    1.100    0.000    1.000    1.000    0.950
 Current      0.550    1.113    0.015    0.960    1.000    0.938
           - - - - - - - - - - - - - - - - - - - - - - - - - -
 Estimate     0.778    1.000    0.985    1.000    1.000    0.989

  Angular  range   :    from   0.0407   to    1.3028
  Real space range  :    from     0.00   to   100.00

  Highest ALPHA (theor) :  0.120E+07             JOB = 0
  Current ALPHA       :  0.517E+00   Rg :  0.380E+02   I(0) :  0.194E+04

         Total  estimate : 0.977  which is  AN EXCELLENT  solution

ALPHA:  0.517E+00  Smin =  0.0407 Smax =  1.3028  TOTAL: 0.977
```

Fig. S5. SAXS data of **1.**





```
                    Final results

   Real space: Rg =   37.63   I(0) =   0.3202E+04

 Parameter   DISCRP   OSCILL   STABIL   SYSDEV   POSITV   VALCEN
 Weight       1.000    3.000    3.000    3.000    1.000    1.000
 Sigma        0.300    0.600    0.120    0.120    0.120    0.120
 Ideal      0.700    1.100    0.000    1.000    1.000    0.950
 Current      0.569    1.101    0.010    1.035    1.000    0.935
            -------------------------
 Estimate     0.826    1.000    0.993    1.000    1.000    0.984

  Angular  range   :   from   0.0407   to    1.3028
  Real space range  :   from    0.00   to    100.00

  Highest ALPHA (theor) :  0.309E+07              JOB = 0
  Current ALPHA       :  0.585E+00  Rg :  0.377E+02  I(0) :  0.320E+04

          Total  estimate : 0.983  which is  AN EXCELLENT  solution

ALPHA:   0.585E+00   Smin  =   0.0407 Smax  =   1.3028   TOTAL: 0.983
```

Fig. S6. SAXS data of **2**

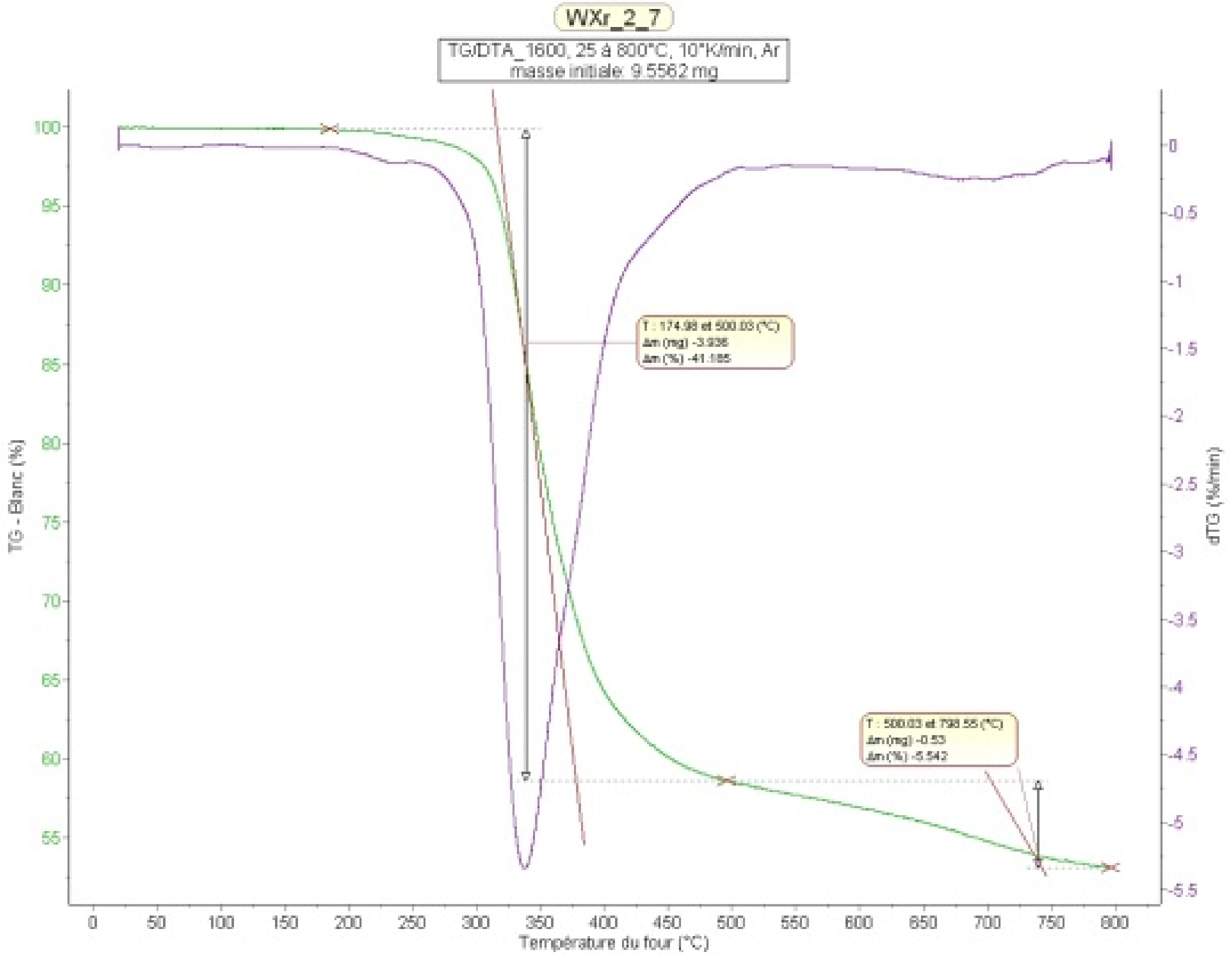


Fig. S7. TGA/DTA of **1**

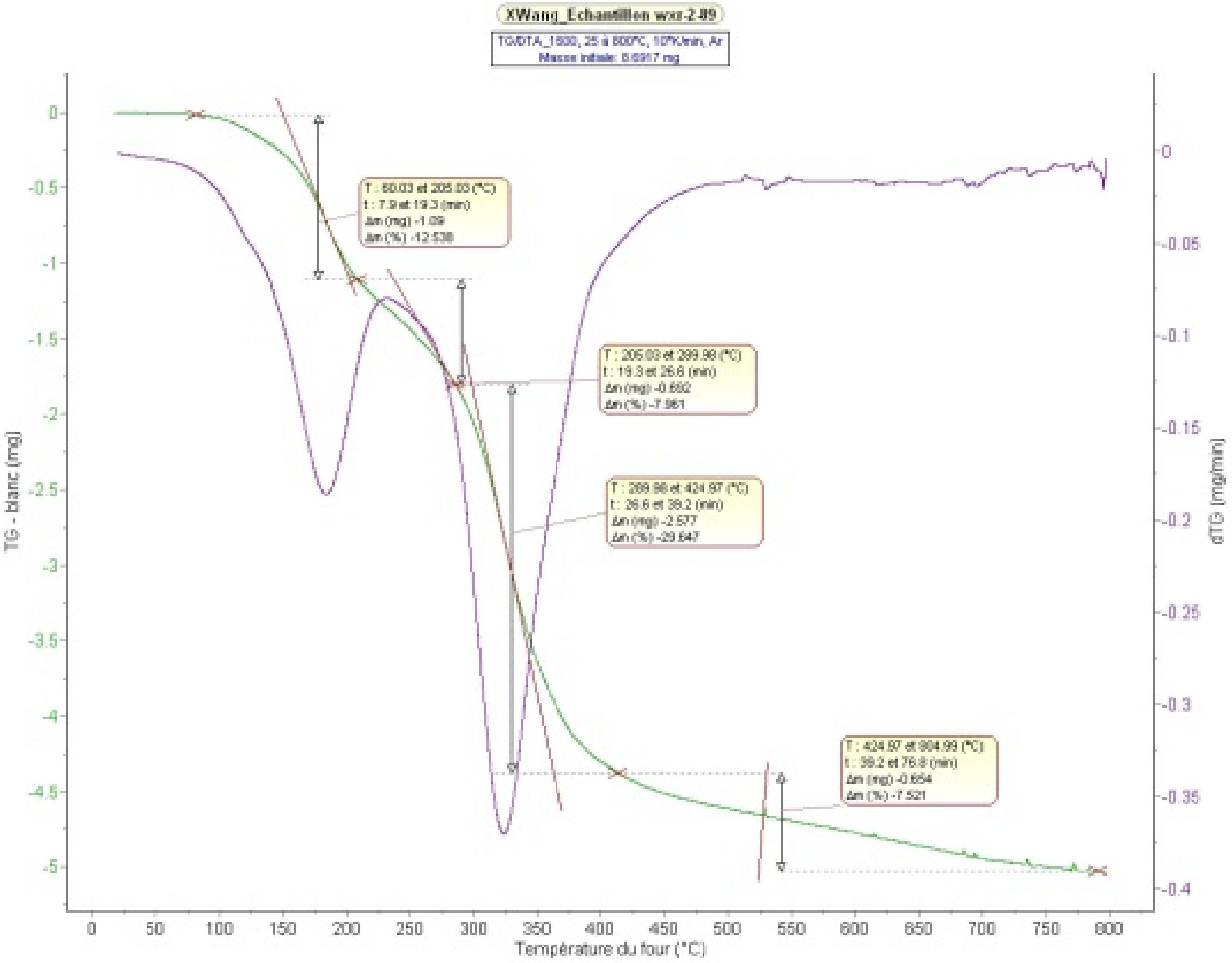


Fig. S8. TGA/DTA of **2**

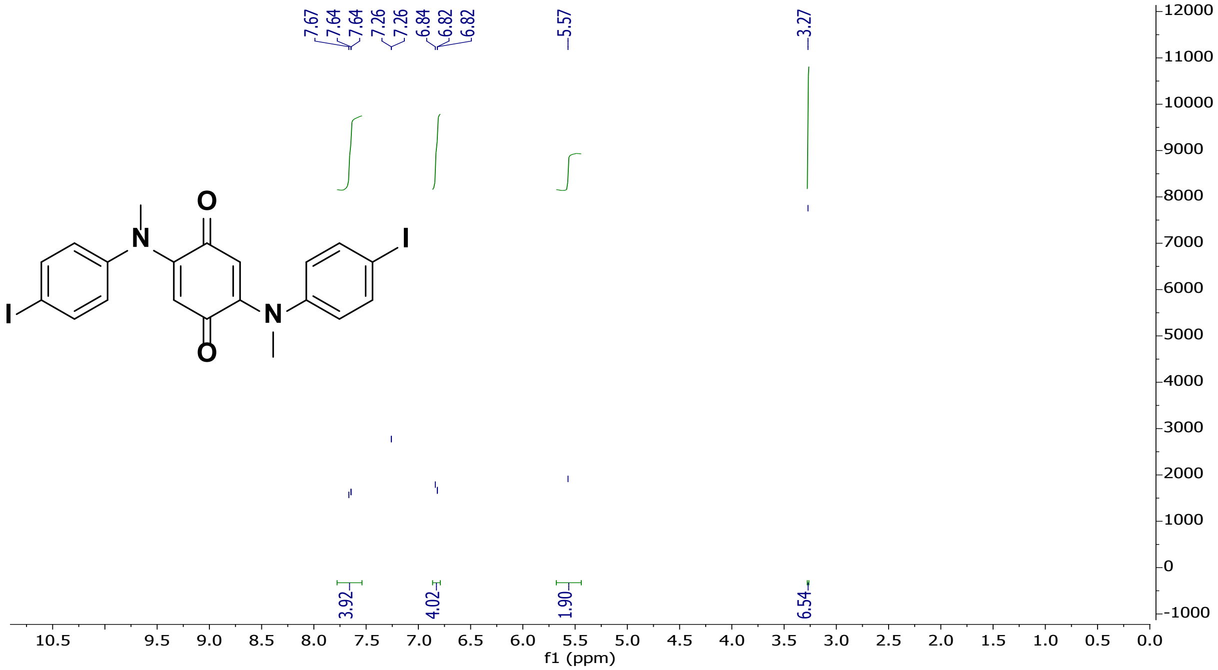


Fig. S9. ^{1}H NMR spectrum of the compound **4** in $CDCl_3$.

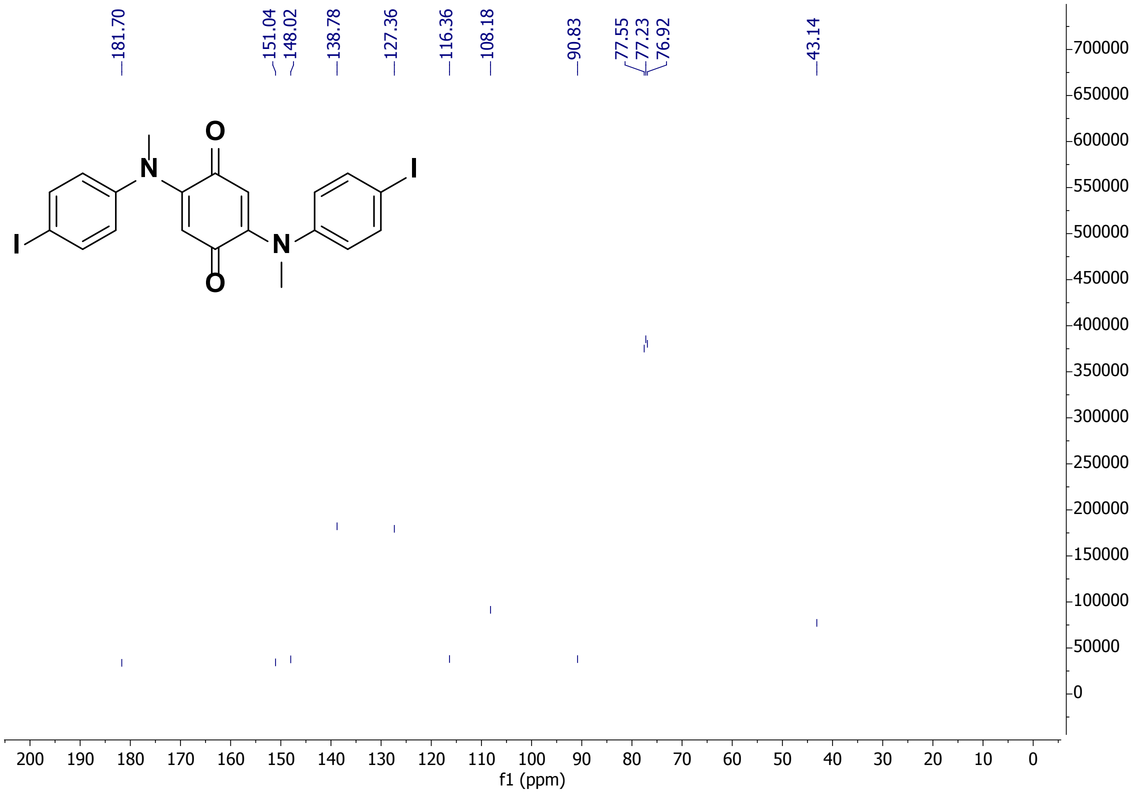


Fig. S10 .^{13}C NMR spectrum of the compound **4** in $CDCl_3$.

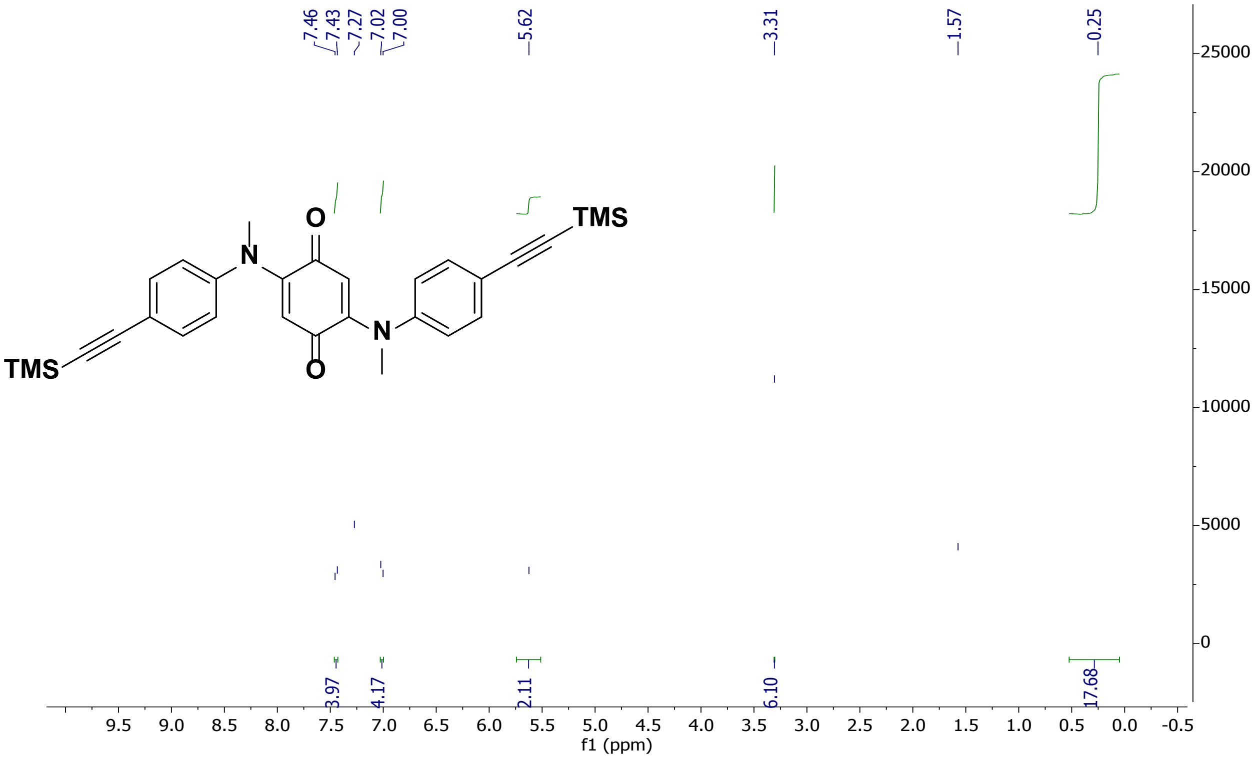


Fig. S11. ^{1}H NMR spectrum of the compound **5** in CDCl$_3$.

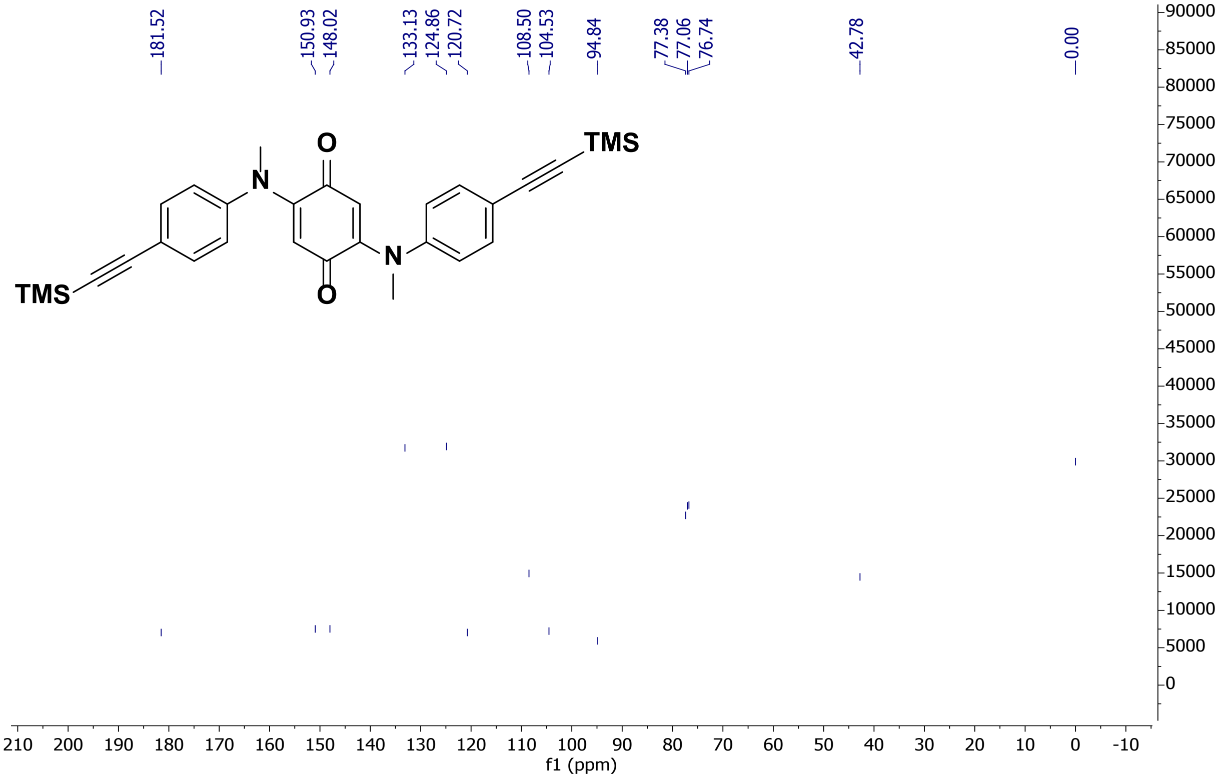


Fig. S12. ^{13}C NMR spectrum of the compound **5** in CDCl$_3$.

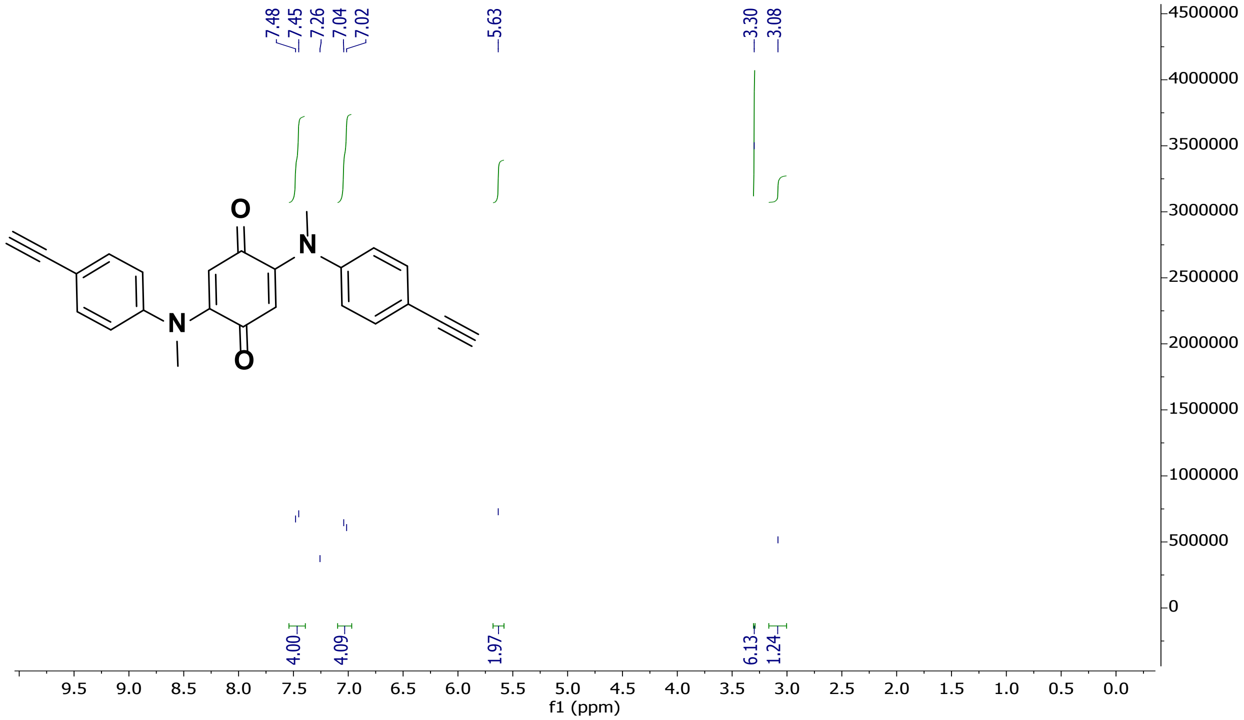


Fig. S13. ^{1}H NMR spectrum of the compound **6** in $CDCl_3$.

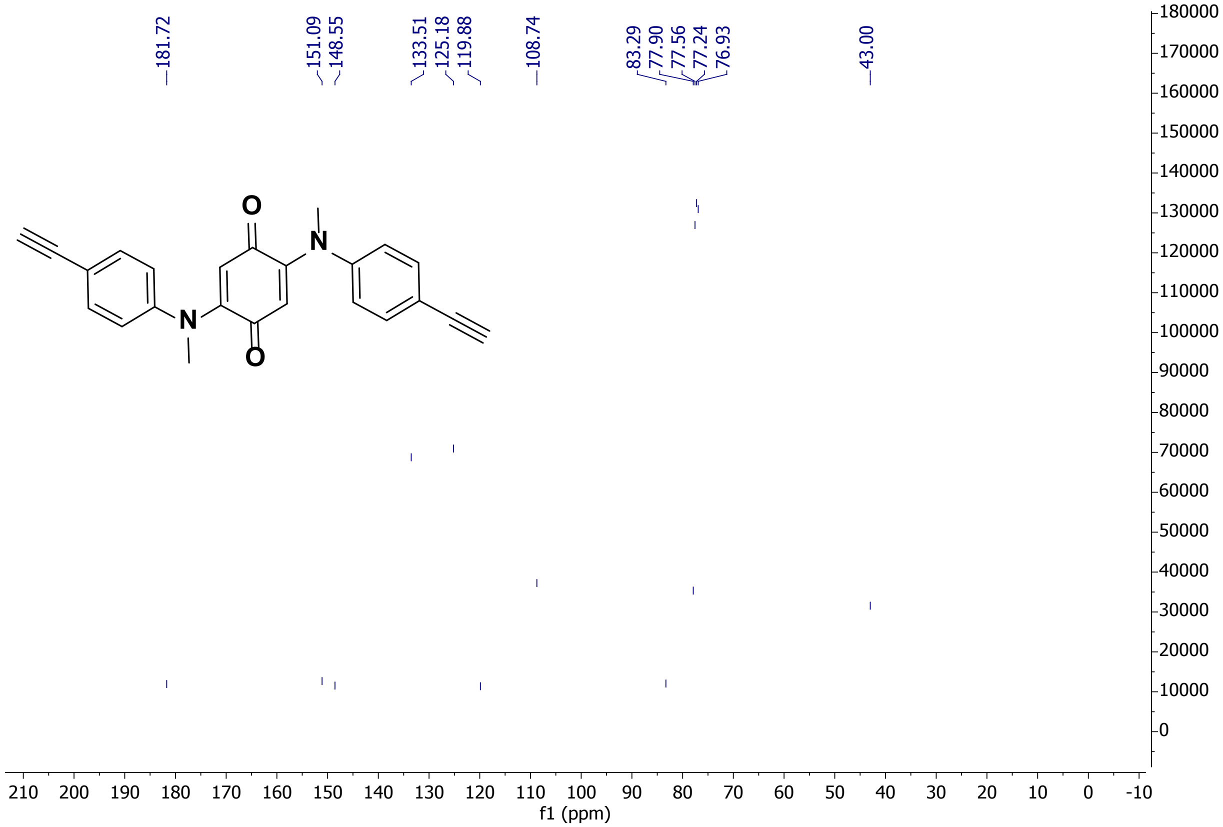


Fig. S14. ^{13}C NMR spectrum of the compound **6** in $CDCl_3$.

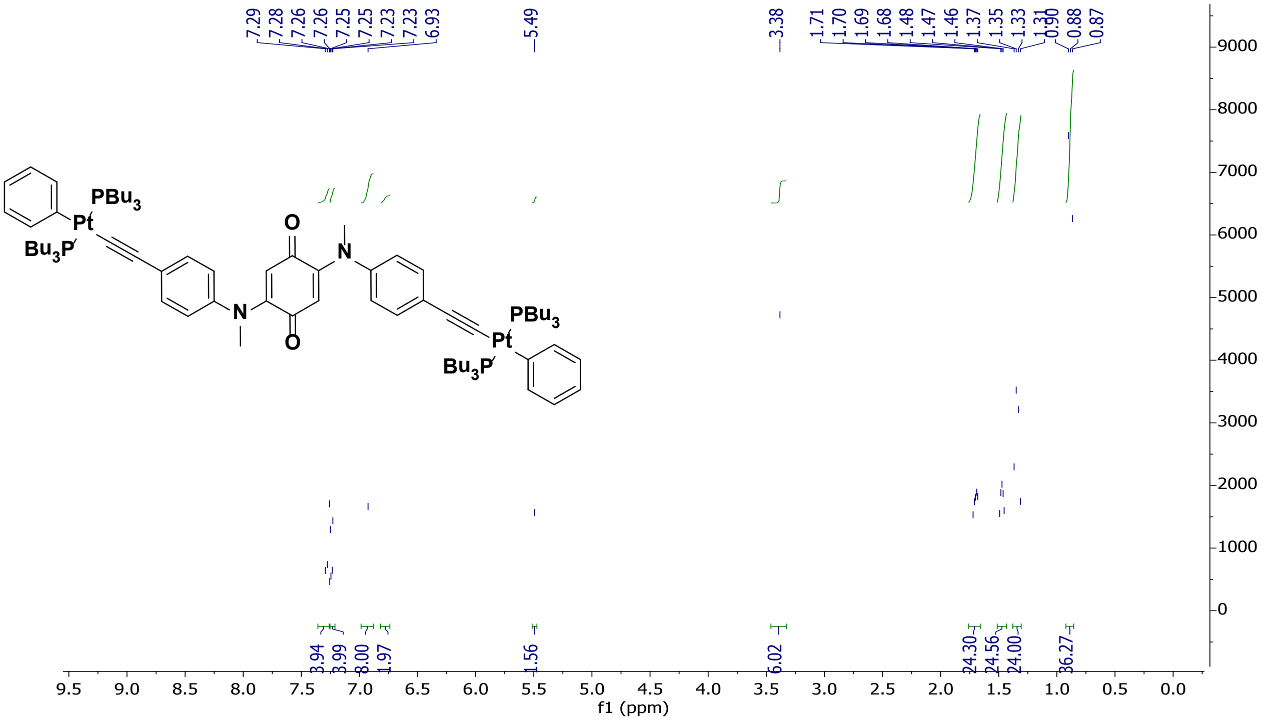


Fig. S15. ^{1}H NMR spectrum of the compound **7** in $CDCl_3$.

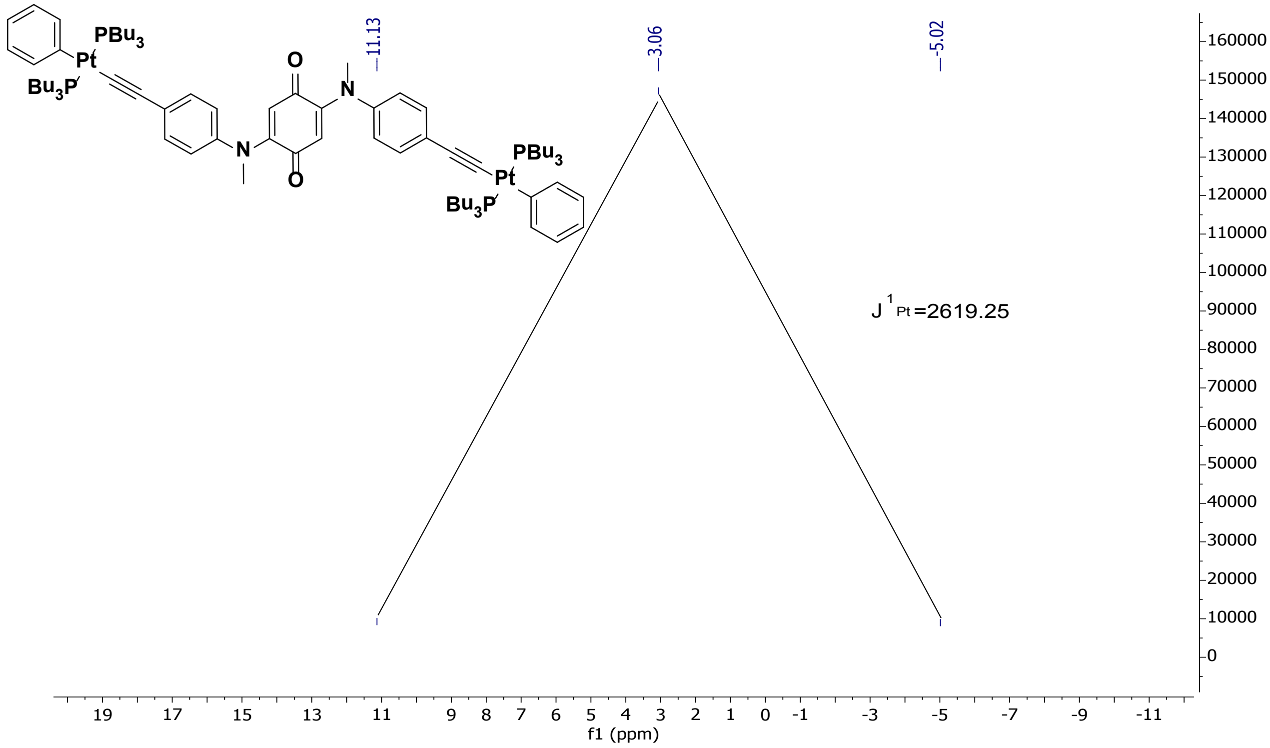


Fig. S16. ^{31}P NMR spectrum of the compound **7** in $CDCl_3$.

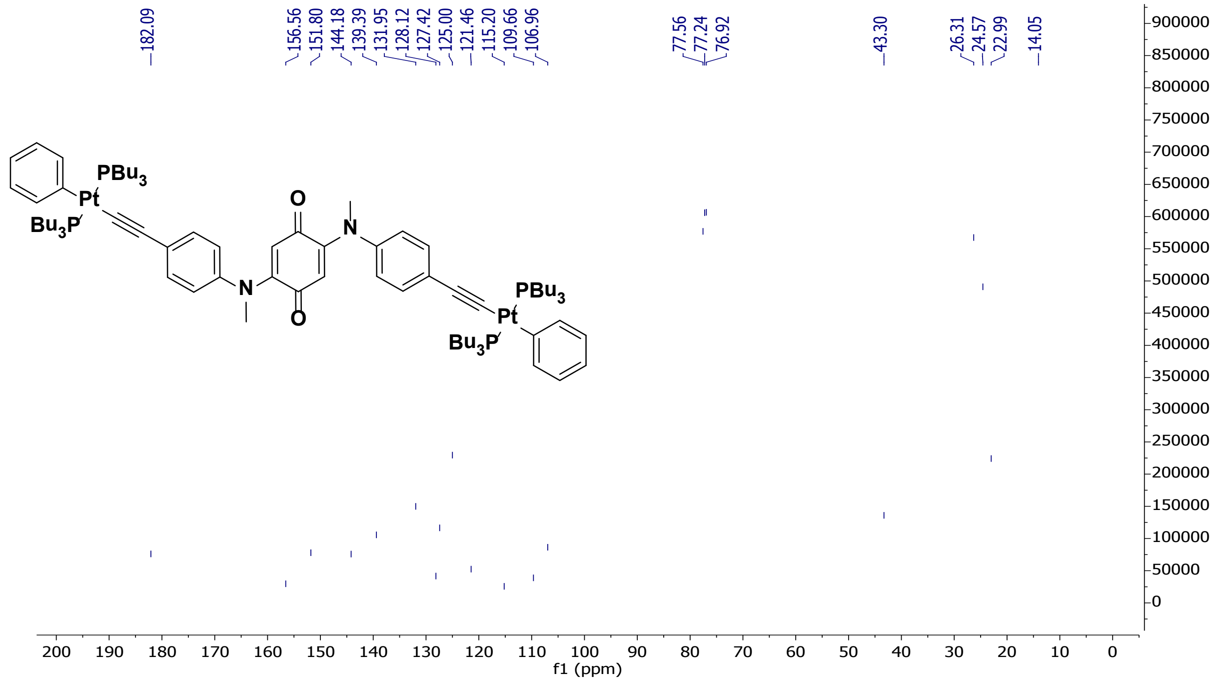


Fig. S17. ^{13}C NMR spectrum of the compound **7** in CDCl$_3$.

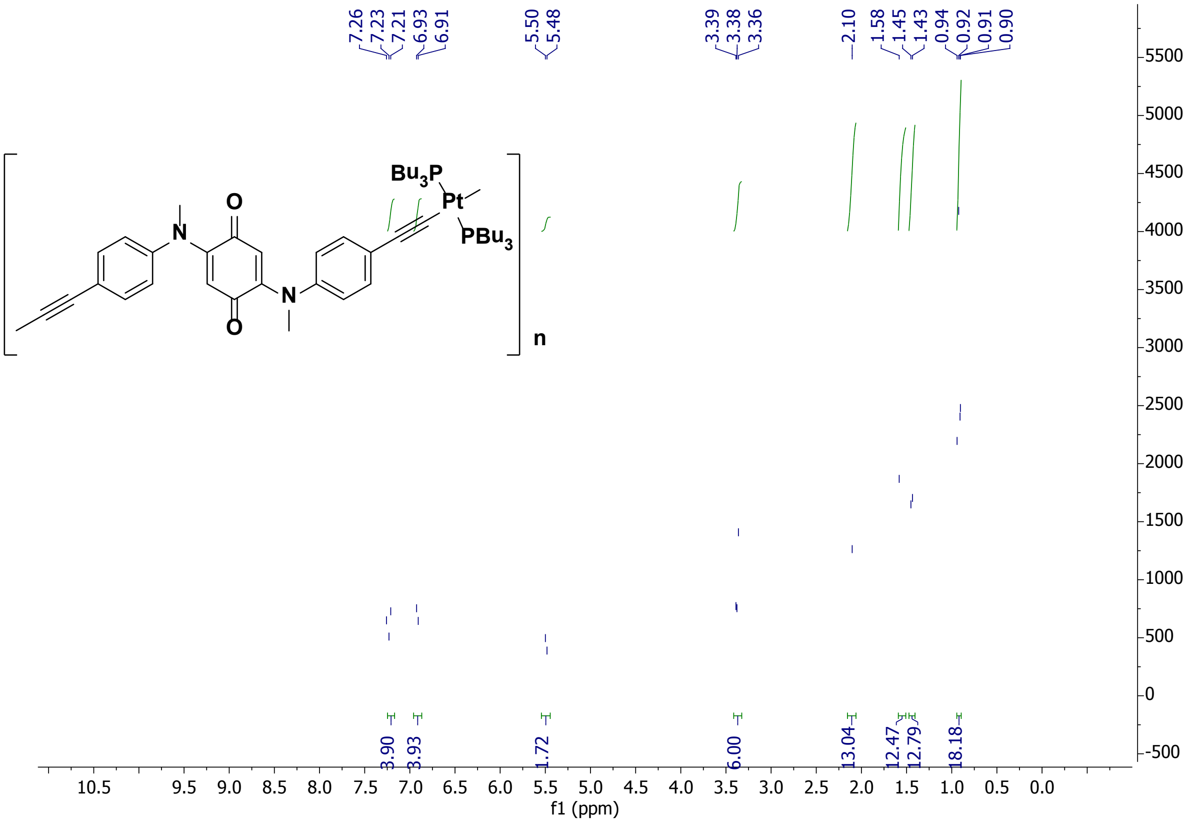


Fig. S18. ^{1}H NMR spectrum of the compound **1** in CDCl$_3$.

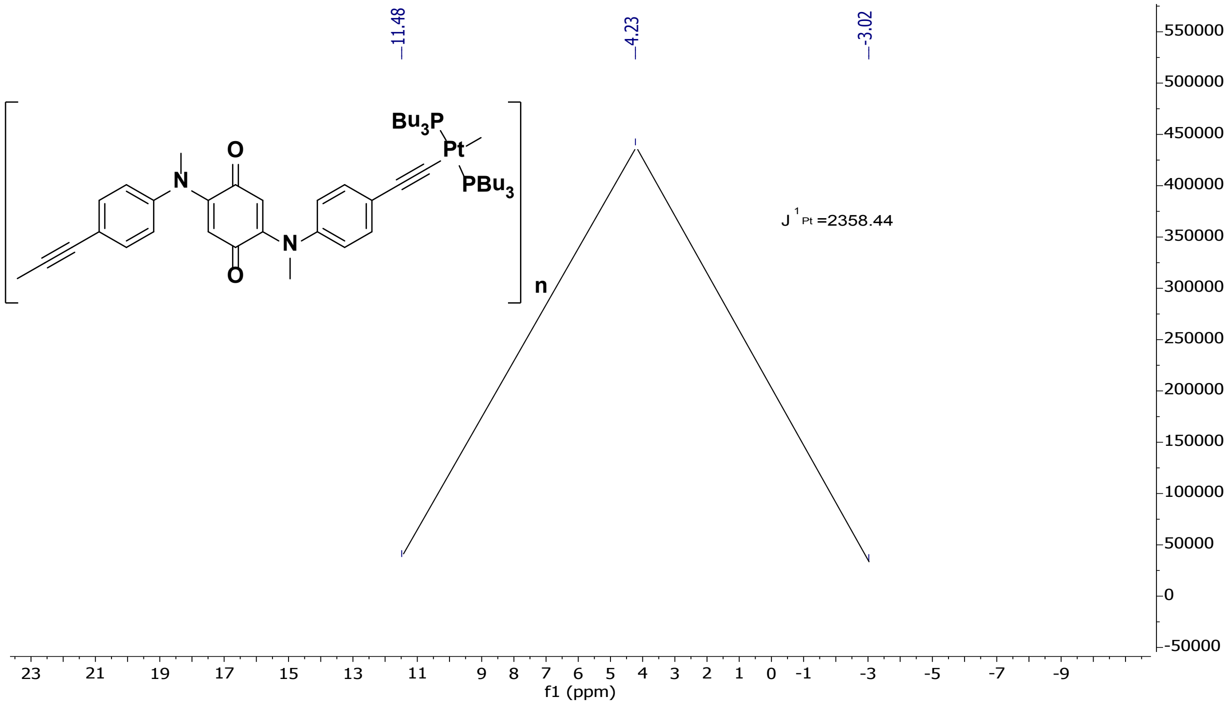


Fig. S19. ^{31}P NMR spectrum of the compound **1** in CDCl$_3$.

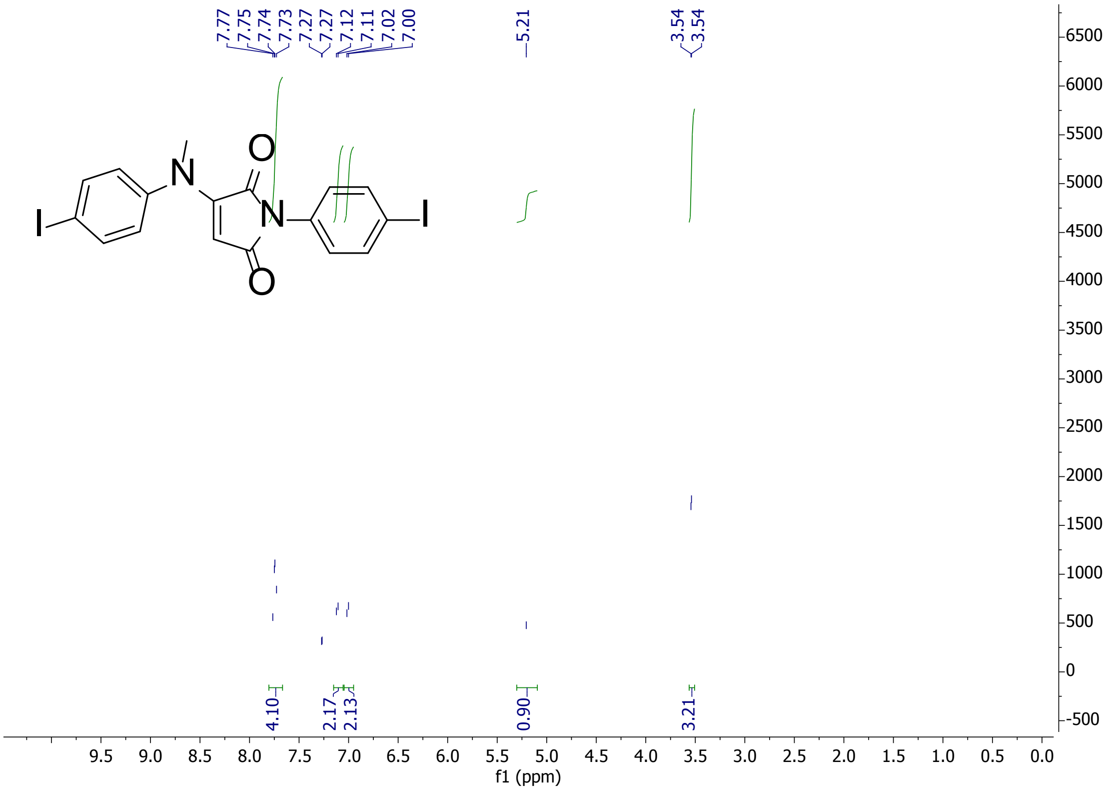


Fig. S20. ^{1}H NMR spectrum of the compound **9** in CDCl$_3$.

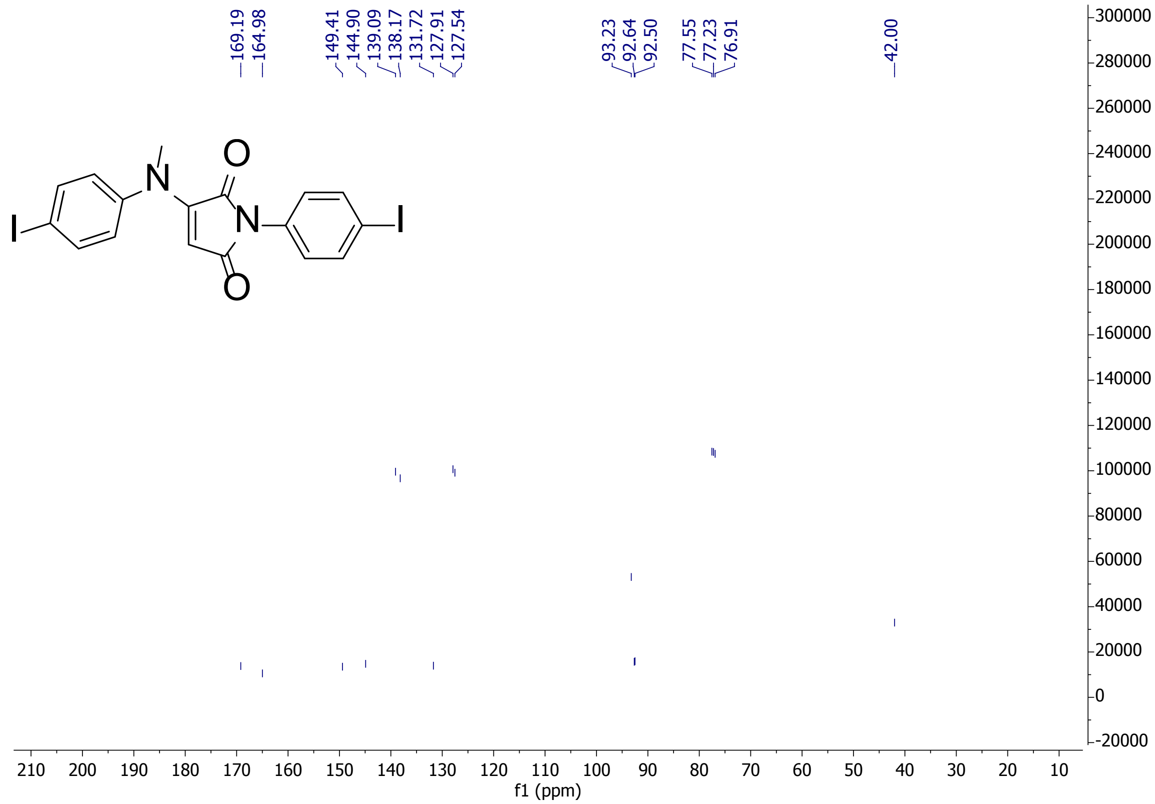


Fig. S21. ^{13}C NMR spectrum of the compound **9** in CDCl$_3$.

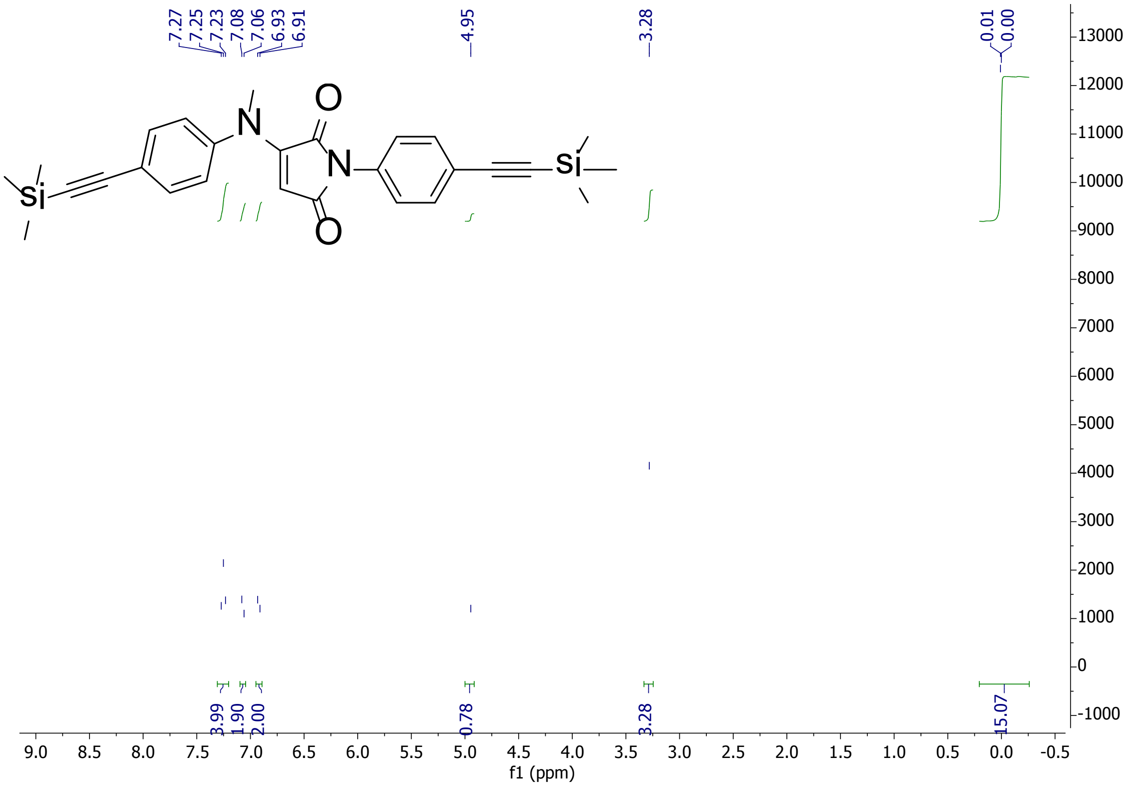


Fig. S22. ^{1}H NMR spectrum of the compound **10** in CDCl$_3$.

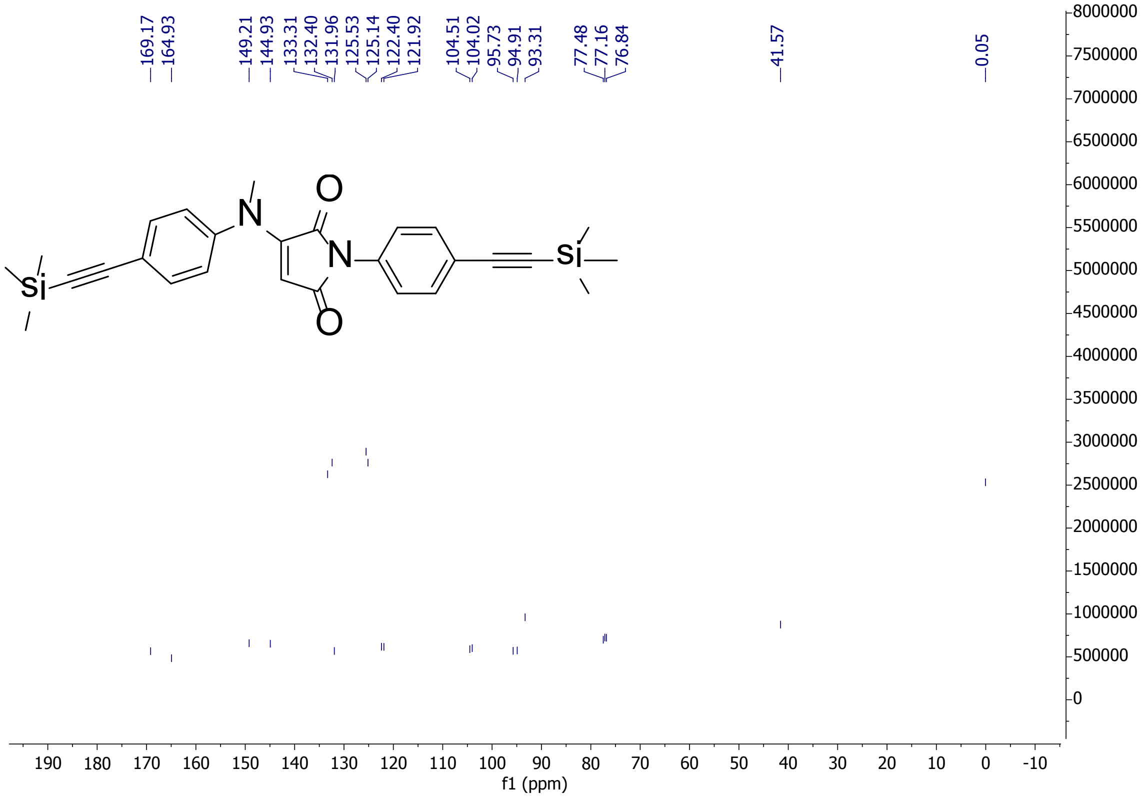


Fig. S23. ^{13}C NMR spectrum of the compound **10** in $CDCl_3$.

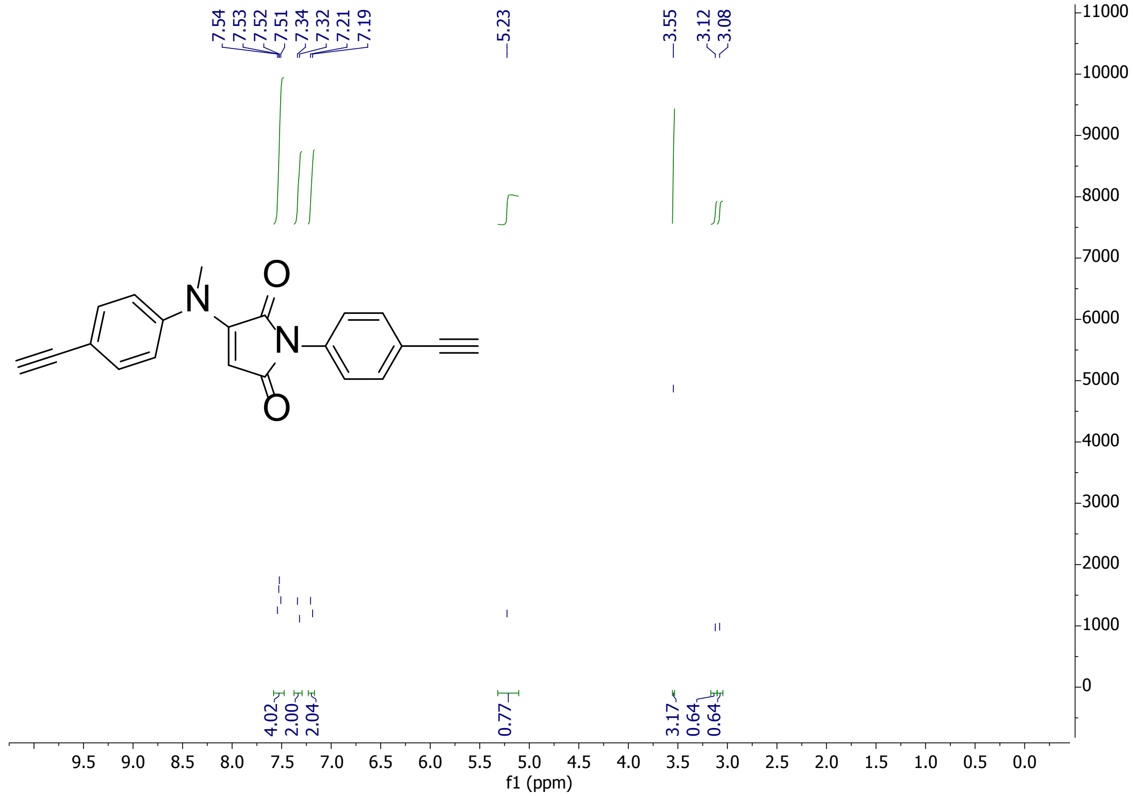


Fig. S24. ^{1}H NMR spectrum of the compound **11** in $CDCl_3$.

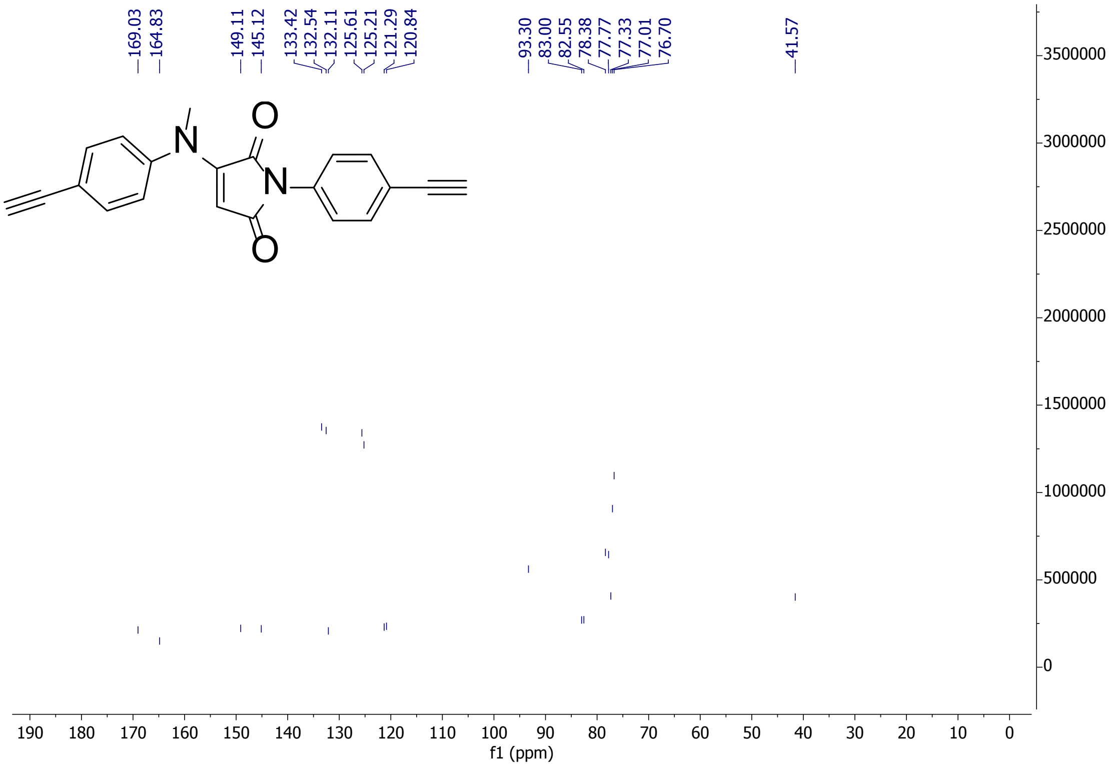


Fig. S25. ^{13}C NMR spectrum of the compound **11** in $CDCl_3$.

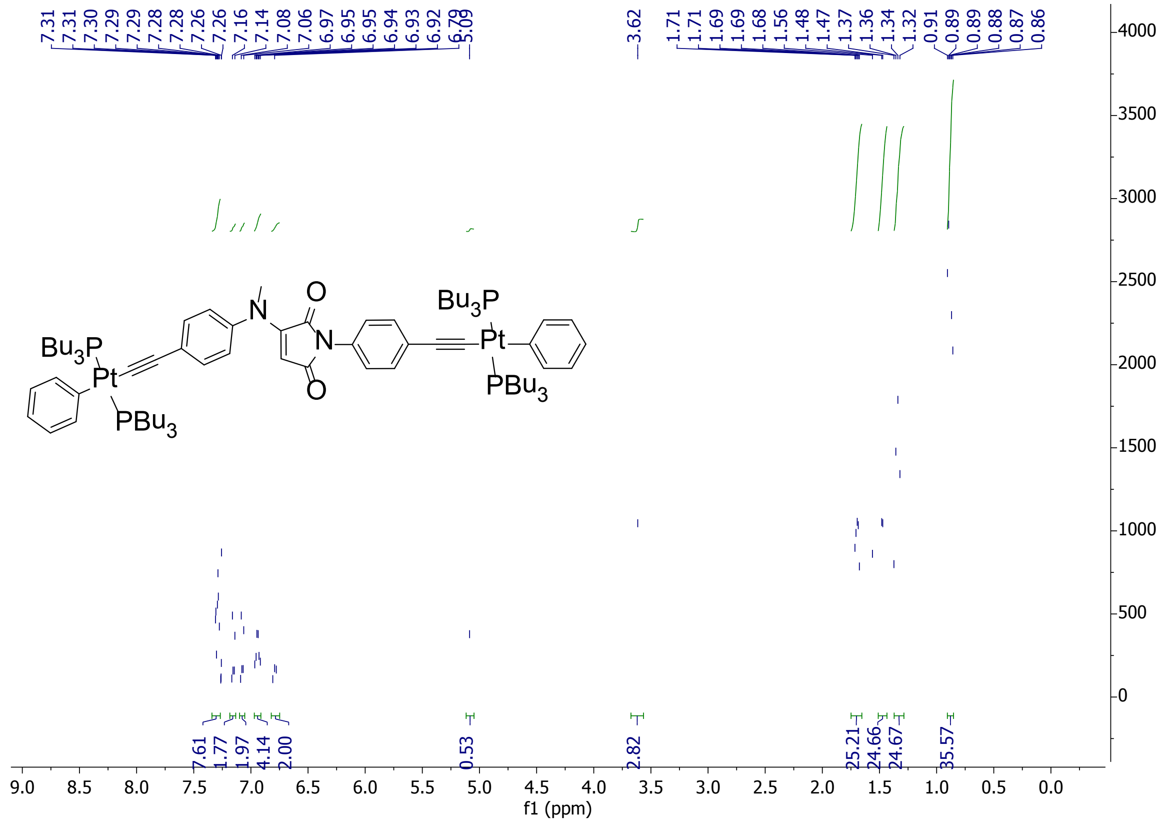


Fig. S26. ^{1}H NMR spectrum of the compound **12** in $CDCl_3$.

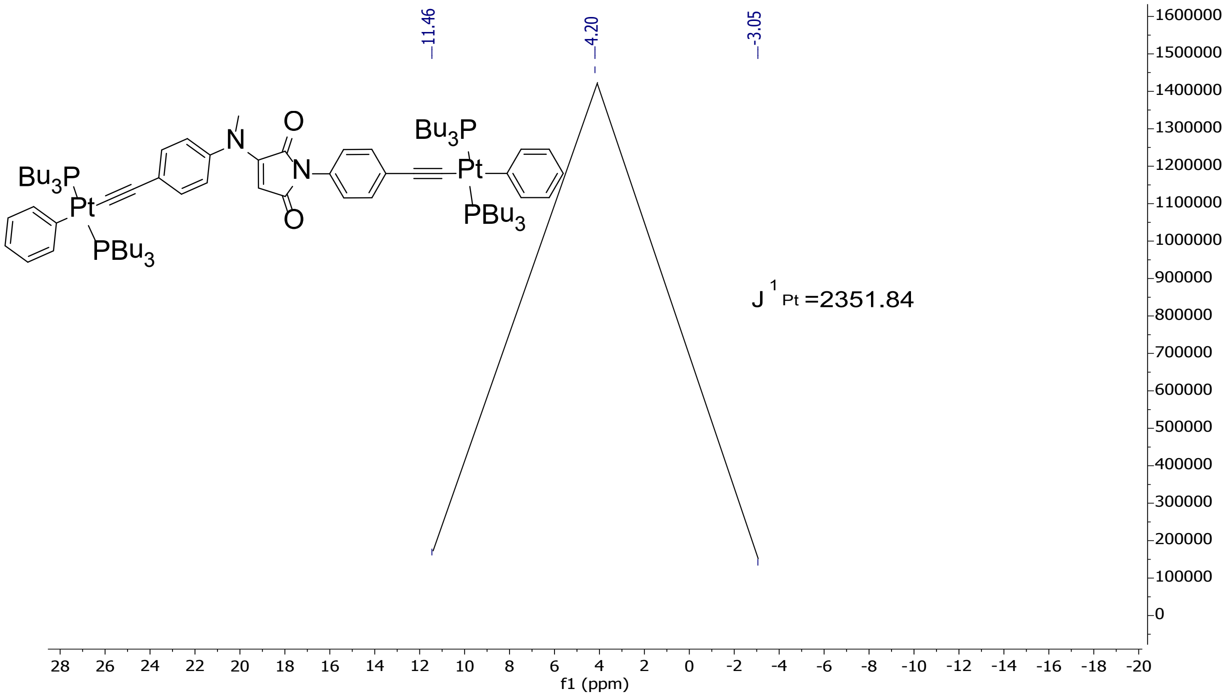


Fig. S27. ^{31}P NMR spectrum of the compound **12** in $CDCl_3$.

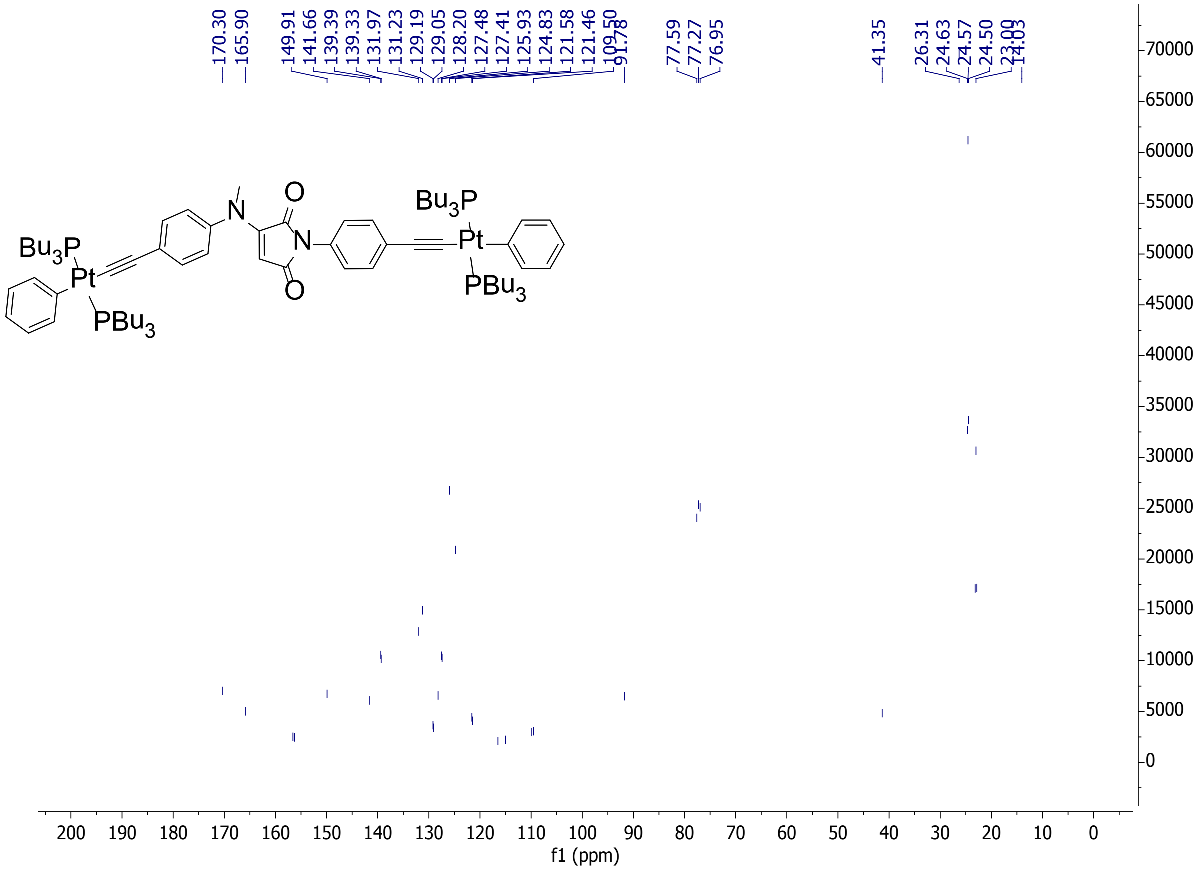


Fig. S28. ^{13}C NMR spectrum of the compound **12** in $CDCl_3$.

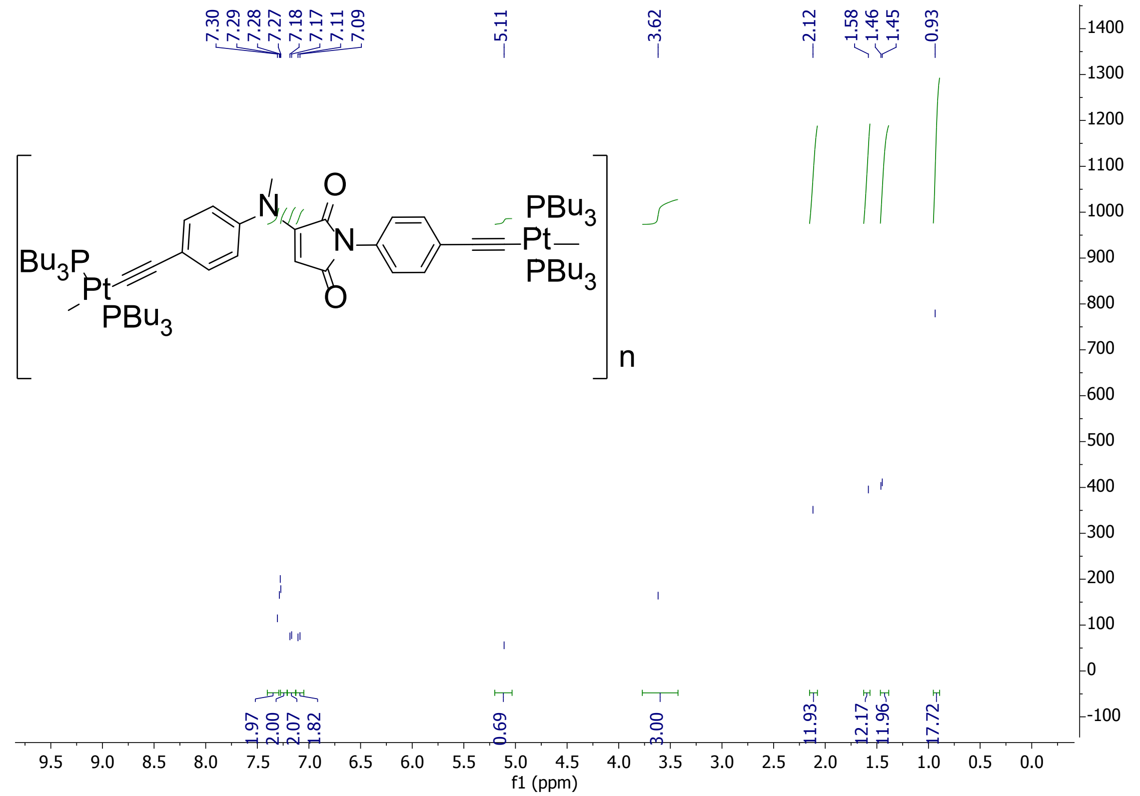


Fig. S29. ^{1}H NMR spectrum of the compound **2** in $CDCl_3$.

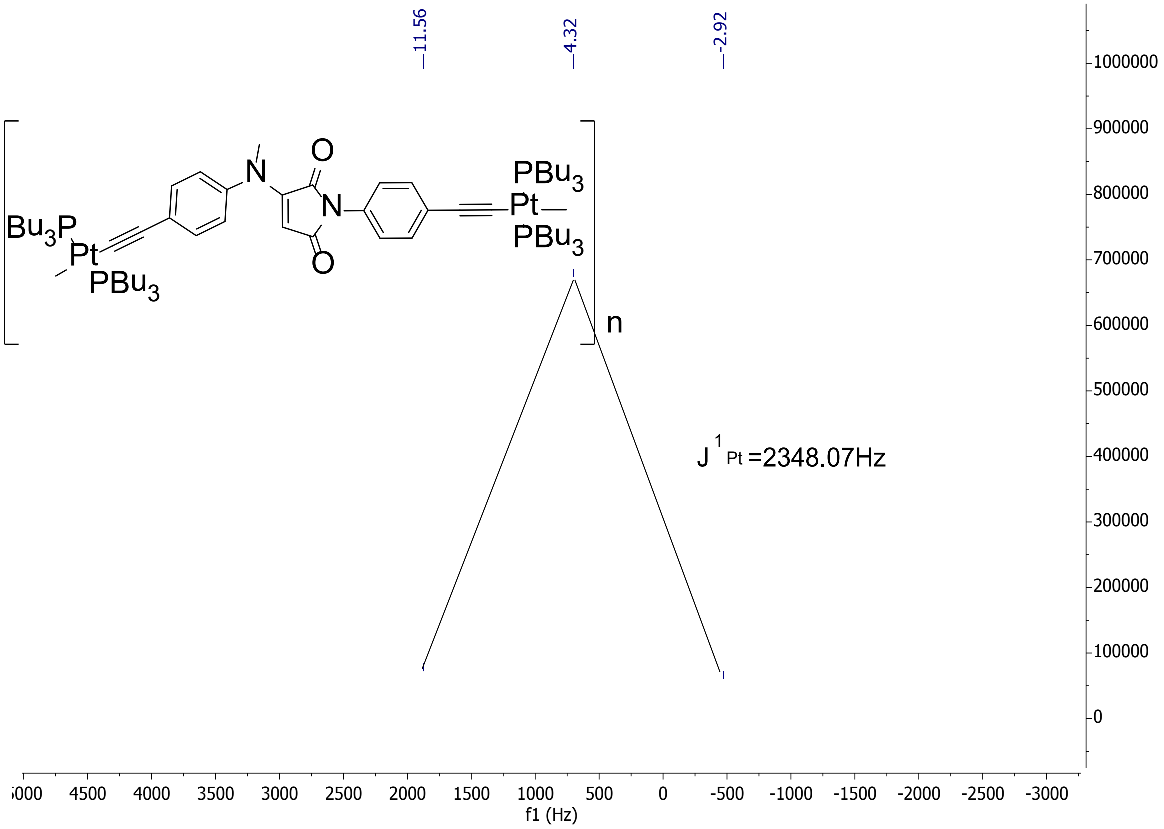


Fig. S30. ^{13}C NMR spectrum of the compound **2** in $CDCl_3$.