Supplementary Material (ESI) for Organic & Biomolecular Chemistry

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**Supporting Information for**

# Introduction of methyl groups on vinylene segments of phenylene vinylene systems: Synthesis and properties

Khai Leok Chan,[a] and Alan Sellinger[a,b*]

*a) Institute of Materials Research and Engineering (IMRE) and the Agency for Science, Technology and Research (A*STAR), 3 Research Link, Singapore 117602, Republic of Singapore*

*b) Current address: Department of Materials Science and Engineering and the Center for Advanced Molecular Photovoltaics (CAMP), Geballe Laboratory for Advanced Materials, 476 Lomita Mall, Stanford University, Stanford, CA 94305-4045, USA*

*Authors to whom correspondence should be addressed. E-mail: aselli@stanford.edu

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**General Methods**

$^{1}H$ and $^{13}C$ NMR data were performed on a Bruker DPX 400 MHz spectrometer with chemical shifts referenced to residual $CHCl_3$ in $CDCl_3$. Matrix assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectra were obtained on a Bruker Autoflex TOF/TOF instrument without the use of matrix. Differential scanning calorimetry (DSC) was carried out under nitrogen on a TA Instrument DSC Q100 instrument (scanning rate of 20 °C $min^{-1}$). Thermal gravimetric analysis (TGA) was carried out using a TA Instrument TGA Q500 instrument (heating rate of 10 °C $min^{-1}$). UV–vis spectra were recorded on a Shimadzu model 2501-PC. Photoluminescence (PL) spectra were measured on a Perkin-Elmer (LS50B) spectrofluorimeter. Gas chromatography-mass spectrometry (GCMS) was carried out on a Varian Chrompack 3800 gas chromatograph coupled to a Varian 4000MS mass spectrometer detector.

All commercially available materials were used as received unless otherwise noted. All reactions were carried out using Schlenk techniques in an argon or nitrogen atmosphere with anhydrous solvents. Column chromatography was carried out on silica gel [Merck Kieselgel 60 (230-400 mesh)]. TLC was performed on 0.25 mm thick plates precoated with Merck Kieselgel 60 $F_{254}$ silica gel, and visualised by UV light (254 and 366 nm) and cerium(VI) sulfate solution.

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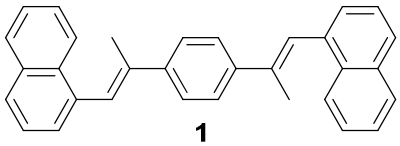
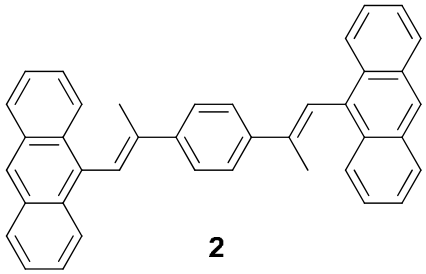
**1,4-bis((E)-1-(naphthalen-1-yl)prop-1-en-2-yl)benzene (1)**



**1**

To a mixture of 1,4-di(prop-1-en-2-yl)benzene (200 mg, 1.26 mmol, 1 equiv.), 1-bromo-naphthalene (523 mg, 2.52 mmol, 2 equiv.) and Pd[P(*t*-Bu)$_3$]$_2$ (32 mg, 63 $\mu$mol) in argon was added a degassed solution of dicyclohexylmethylamine (0.68 cm$^3$, 3.16 mmol, 2.5 equiv.) in toluene (15 cm$^3$). The resulting mixture was stirred at 100 ºC for 60 hours and cooled to room temperature whereupon white precipitates were formed. The precipitates were filtered and the residue was washed with copious amount of distilled water followed by toluene to yield the *title compound* as an off-white solid (345 mg, 66%); mp 215–218 °C; Anal. Calcd. for $C_{32}H_{26}$: C, 93.62; H, 6.38. Found: C, 93.59; H, 6.41; $^1$H NMR (400 MHz, $CDCl_3$) δ 2.19 (6H, s, CC*H*$_3$), 7.37 (2H, s, C=C*H*), 7.46–7.54 (8H, m, Ar*H*), 7.72 (4H, s, Ar*H*), 7.82 (2H, d, *J* = 8.0, Ar*H*), 7.89–7.91 (2H, m, Ar*H*), 8.05–8.08 (2H, m, Ar*H*); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 17.8, 125.6, 125.7, 125.8, 126.2, 126.3, 126.4, 127.1, 127.7, 128.9, 132.6, 134.0, 136.1, 138.8, 142.6; MALDI-TOF-MS m/z: 410.1780; calcd for $C_{32}H_{26}$ = 410.2035.

**1,4-bis((E)-1-(anthracen-9-yl)prop-1-en-2-yl)benzene (2)**

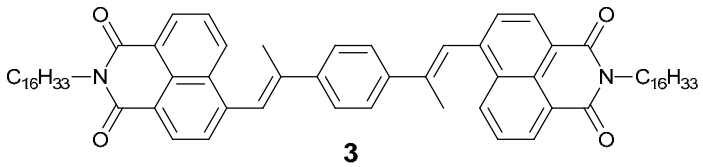


**2**

To a mixture of 1,4-di(prop-1-en-2-yl)benzene (200 mg, 1.26 mmol, 1 equiv.), 9-bromo-anthracene (650 mg, 2.52 mmol, 2 equiv.) and Pd[P(*t*-Bu)$_3$]$_2$ (32 mg, 63 $\mu$mol) in argon was added a degassed solution of dicyclohexylmethylamine (0.68 cm$^3$, 3.16 mmol, 2.5 equiv.) in toluene (15 cm$^3$). The resulting mixture

was stirred at 100 ºC for 48 hours and cooled to room temperature whereupon yellow precipitates were formed. The precipitates were filtered and the residue was washed with copious amount of distilled water followed by toluene to yield the *title compound* as a yellow solid (456 mg, 70%); mp 300–305 °C; Anal. Calcd. for $C_{40}H_{30}$: C, 94.08; H, 5.92. Found: C, 94.08; H, 5.92; $^1$H NMR (400 MHz, $CDCl_3$) δ 1.91 (6H, s, CC*H*$_3$), 7.59 (2H, s, C=C*H*), 7.48–7.53 (8H, m, Ar*H*), 8.06–8.08 (8H, m, Ar*H*), 8.20–8.22 (8H, m, Ar*H*), 8.46 (2H, s, Ar*H*); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 18.0, 124.2, 125.6, 125.9, 126.5, 126.6, 129.2, 130.2, 131.9, 133.3, 140.9, 142.2; MALDI-TOF-MS m/z: 510.2010; calcd for $C_{40}H_{30}$ = 510.2348.

**4,4'-(1*E*,1'*E*)-2,2'-(1,4-phenylene)bis(prop-1-ene-2,1-diyl)bis(*N*-hexadecyl-1,8-naphthalimide) (3)**




**3**

To a mixture of 1,4-di(prop-1-en-2-yl)benzene (200 mg, 1.26 mmol, 1 equiv.), 2-bromo-9,9-dimethyl-9*H*-fluorene (1.27 g, 2.52 mmol, 2 equiv.) and Pd[P(*t*-Bu)$_3$]$_2$ (32 mg, 63 $\mu$mol) in argon was added a degassed solution of dicyclohexylmethylamine (0.68 cm$^3$, 3.16 mmol, 2.5 equiv.) in toluene (15 cm$^3$). The resulting mixture was stirred at 100 ºC for 48 hours, cooled to room temperature and quenched with distilled water (20 cm$^3$). The product was then extracted into dichloromethane (3 × 30 cm$^3$) and the organic layer washed with dried with anhydrous $MgSO_4$ and evaporated. Purification by column chromatography (hexane:dichloromethane 1:1) followed by slow precipitation in hexane:dichloromethane (2:1) yielded the *title compound* as a pale green solid (350 mg, 28%); mp 59–62 °C; Anal. Calcd. for $C_{68}H_{88}N_2O_4$: C, 81.88; H, 8.89; N, 2.81. Found: C, 81.45; H, 8.73; N, 2.48; $^1$H NMR (400 MHz, $CDCl_3$) δ 0.88 (6H, t, *J* = 7.6, $CH_2CH_3$), 1.20–1.48 (56H, m, C*H*$_2$), 1.70–1.80 (4H, s, $NCH_2CH_2$), 2.22 (6H, s, CC*H*$_3$), 4.20 (4H, d, *J* = 7.6, NC*H*$_2$), 7.39 (2H, s, C=C*H*), 7.51–7.78 (8H, m, Ar*H*), 8.40 (2H, d, *J* = 8.8, Ar*H*), 8.63–8.68 (4H, m, Ar*H*); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 14.5, 18.1, 23.1, 27.6, 28.6, 29.8, 32.3, 40.9, 121.9, 123.6, 124.3, 126.7, 127.1, 128.1, 128.9, 131.0, 131.1, 131.6, 131.7, 141.6, 142.5, 142.9, 164.5, 164.7; MALDI-TOF-MS m/z: 996.6890; calcd for $C_{68}H_{88}N_2O_4$ = 996.6744.

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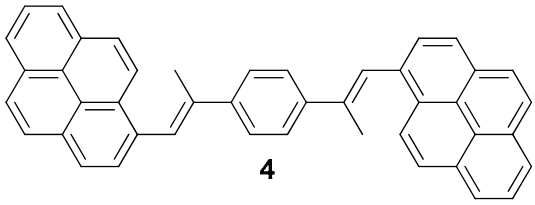
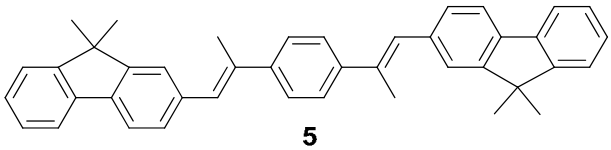
**1,4-bis((E)-1-(pyren-1-yl)prop-1-en-2-yl)benzene (4)**



**4**

To a mixture of 1,4-di(prop-1-en-2-yl)benzene (200 mg, 1.26 mmol, 1 equiv.), 1-bromo-pyrene (708 mg, 2.52 mmol, 2 equiv.) and Pd[P(*t*-Bu)$_3$]$_2$ (32 mg, 63 $\mu$mol) in argon was added a degassed solution of dicyclohexylmethylamine (0.68 cm$^3$, 3.16 mmol, 2.5 equiv.) in toluene (15 cm$^3$). The resulting mixture was stirred at 100 ºC for 24 hours, cooled to room temperature and quenched with distilled water (20 cm$^3$). The product was then extracted into dichloromethane (3 × 30 cm$^3$) and the organic layer washed with dried with anhydrous $MgSO_4$ and evaporated. Purification by column chromatography (hexane:dichloromethane 4:1) followed recrystallisation in toluene solution yielded the *title compound* as a yellow solid (56 mg, 8 %); mp 234–237 °C; Anal. Calcd. for $C_{44}H_{30}$: C, 94.59; H, 5.41. Found: C, 94.22; H, 5.78; $^1$H NMR (400 MHz, $CDCl_3$) δ 2.26 (6H, s, CC*H*$_3$), 7.69 (2H, s, C=C*H*), 7.83 (4H, s, Ar*H*), 7.00–7.04 (4H, m, Ar*H*), 8.10–8.14 (6H, m, Ar*H*), 8.20–8.23 (6H, m, Ar*H*), 8.31 (2H, d, *J* = 8.0, Ar*H*); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 17.9, 124.9, 125.2, 125.3, 125.4, 125.5, 126.3, 126.4, 126.5, 127.6, 127.7, 127.8, 129.6, 130.8, 131.5, 131.9, 133.9, 139.2, 142.7; MALDI-TOF-MS m/z: 558.1760; calcd for $C_{44}H_{30}$ = 558.2348.

**1,4-bis((*E*)-1-(9,9-dimethyl-9H-fluoren-2-yl)prop-1-en-2-yl)benzene (5)**



**5**

To a mixture of 1,4-di(prop-1-en-2-yl)benzene (200 mg, 1.26 mmol, 1 equiv.), 2-bromo-9,9-dimethyl-9*H*-

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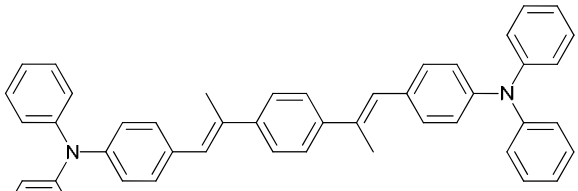
fluorene (688 mg, 2.52 mmol, 2 equiv.) and Pd[P(*t*-Bu)$_3$]$_2$ (32 mg, 63 $\mu$mol) in argon was added a degassed solution of dicyclohexylmethylamine (0.68 cm$^3$, 3.16 mmol, 2.5 equiv.) in toluene (15 cm$^3$). The resulting mixture was stirred at 100 ºC for 48 hours, cooled to room temperature and quenched with distilled water (20 cm$^3$). The product was then extracted into dichloromethane (3 × 30 cm$^3$) and the organic layer washed with dried with anhydrous $MgSO_4$ and evaporated. Purification by column chromatography (hexane:dichloromethane 2:1) followed by recrystallisation in hexane:dichloromethane (4:1) yielded the *title compound* as a pale green solid (112 mg, 14%); mp 248–250 °C; Anal. Calcd. for $C_{42}H_{38}$: C, 92.94; H, 7.06. Found: C, 92.93; H, 7.07; $^1$H NMR (400 MHz, $CDCl_3$) δ 1.53 (12H, s, C(C*H*$_3$)$_2$), 2.39 (6H, s, CC*H*$_3$), 7.00 (2H, s, C=C*H*), 7.30–7.48 (8H, m, C*H*$_2$), 7.59 (4H, s, Ar*H*), 7.74 (2H, d, *J* = 8.0, Ar*H*); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 18.0, 27.6, 47.2, 120.1, 120.4, 123.0, 123.8, 126.3, 127.4, 127.5, 128.5, 128.6, 137.0, 137.9, 138.1, 139.4, 143.2, 154.0, 154.3; MALDI-TOF-MS m/z: 542.2780; calcd for $C_{42}H_{38}$ = 542.2974

**Synthesis of 4,4'-(1*E*,1'*E*)-2,2'-(1,4-phenylene)bis(prop-1-ene-2,1-diyl)bis(N,N-diphenylaniline) (6)**




**6**

To a mixture of 1,4-di(prop-1-en-2-yl)benzene (200 mg, 1.26 mmol, 1 equiv.), 4-bromotriphenylamine (820 mg, 2.52 mmol, 2 equiv.) and Pd[P(*t*-Bu)$_3$]$_2$ (32 mg, 63 $\mu$mol) in argon was added a degassed solution of dicyclohexylmethylamine (0.68 cm$^3$, 3.16 mmol, 2.5 equiv.) in toluene (15 cm$^3$). The resulting mixture was stirred at 100 ºC for 48 hours, cooled to room temperature and quenched with distilled water (20 cm$^3$). The product was then extracted into dichloromethane (3 × 30 cm$^3$) and the organic layer washed with dried with anhydrous $MgSO_4$ and evaporated. Purification by column chromatography (hexane:dichloromethane 2:1) followed by recrystallisation in hexane:dichloromethane (4:1) yielded the *title compound* as a pale green solid (177 mg, 22%); mp 243–245 °C; Anal. Calcd. for $C_{48}H_{40}N_2$: C, 89.40; H, 6.25; N, 4.34. Found: C, 89.53; H, 6.37; N, 4.10; $^1$H NMR (400 MHz, $CDCl_3$) δ 1.52 (6H, s, C*H*$_3$), 6.82 (2H, s, C=C*H*), 7.00–7.18 (16H, m, Ar*H*), 7.25–7.30 (12H, m, Ar*H*), 7.52 (4H, s, Ar*H*); $^{13}$C

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NMR (100 MHz, CDCl3) δ 18.0, 123.3, 123.7, 124.8, 126.2, 12.5, 129.7, 130.5, 133.0, 136.2, 143.2, 136.6, 148.1; MALDI-TOF-MS m/z: 644.3190; calcd for $C_{48}H_{40}N_2$ = 644.3191

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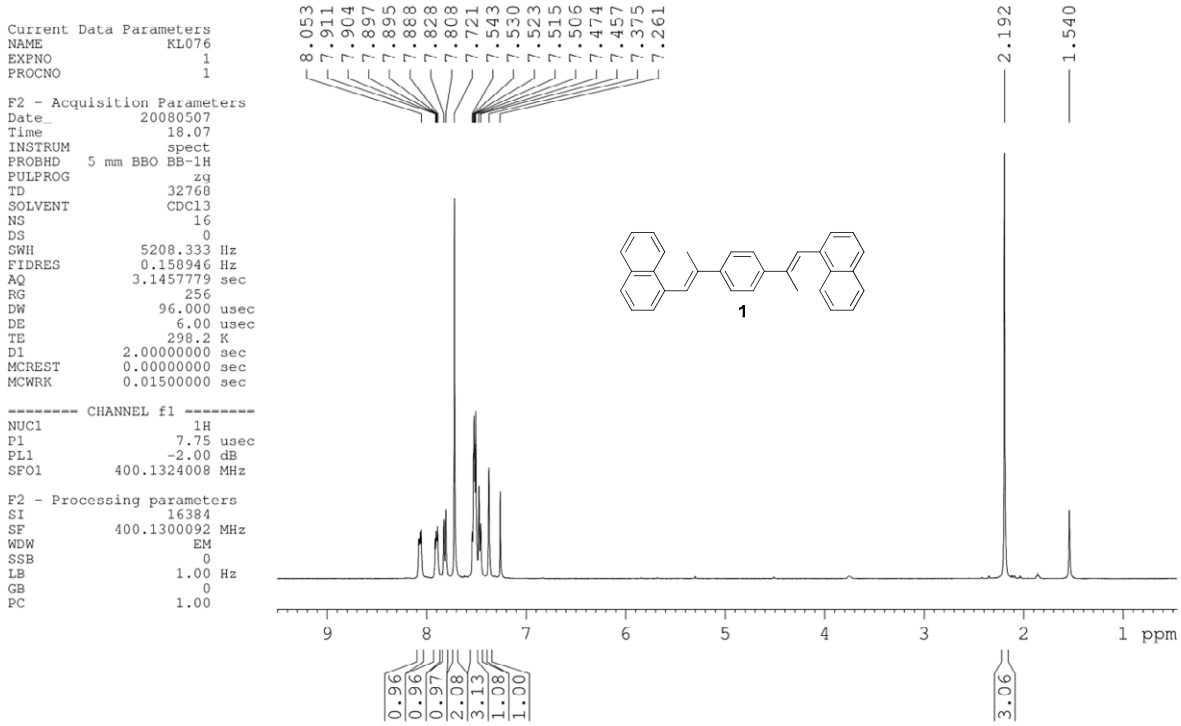


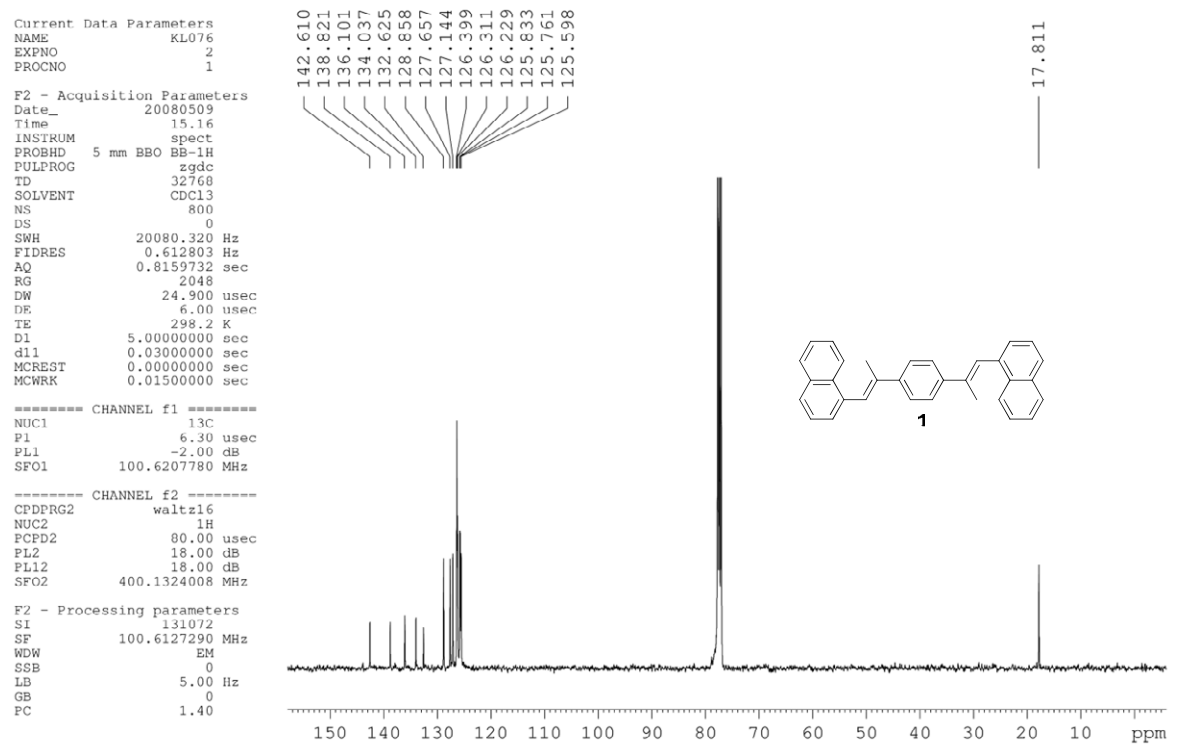

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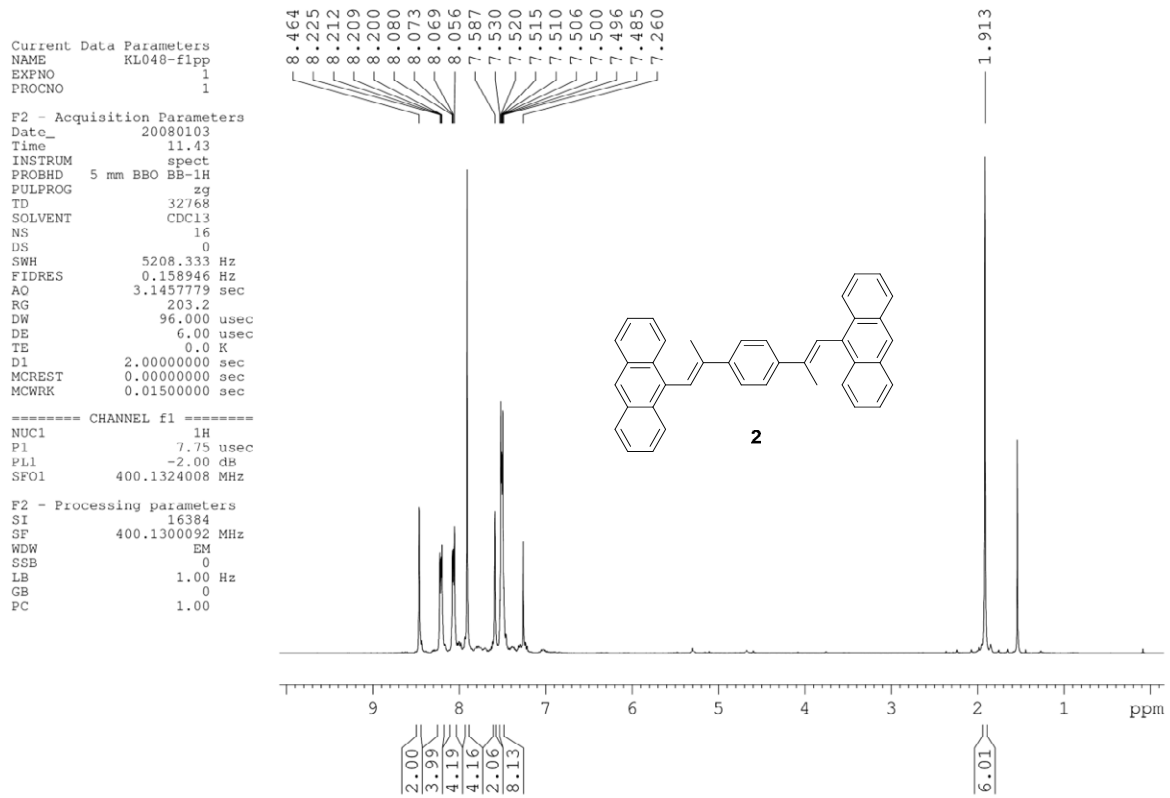
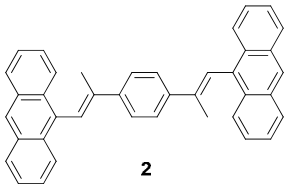
**Figure S1**. $^{1}H$ and $^{13}C$ NMR spectra of compound **1**.



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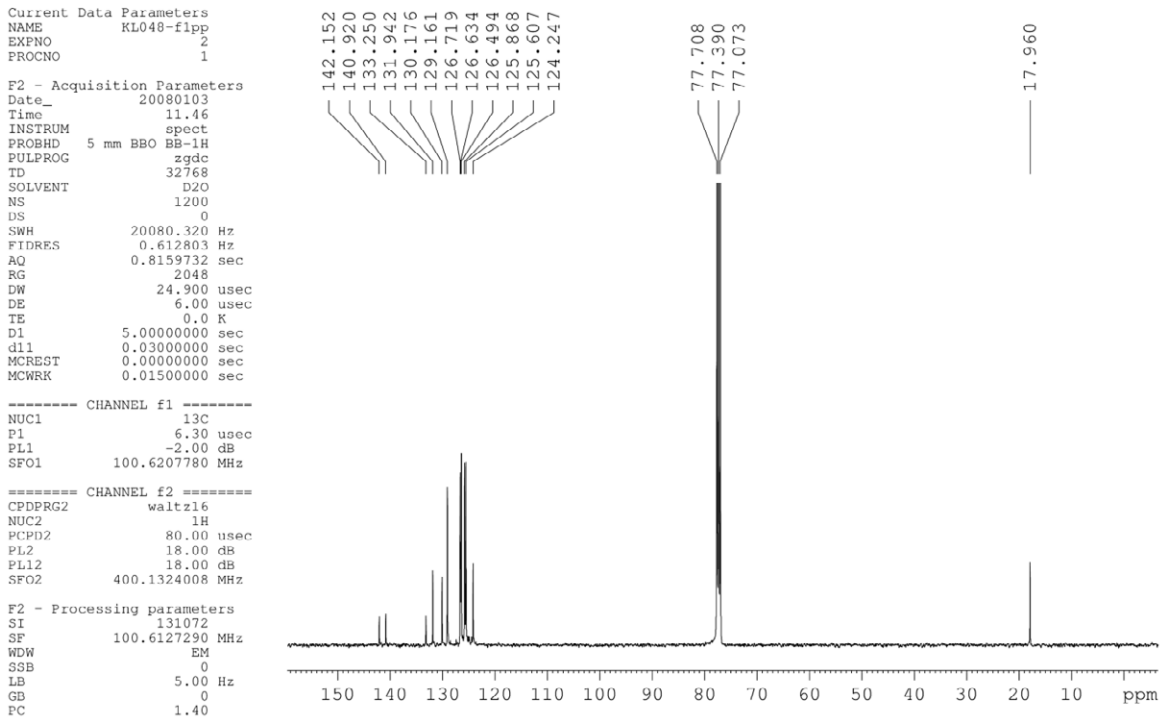
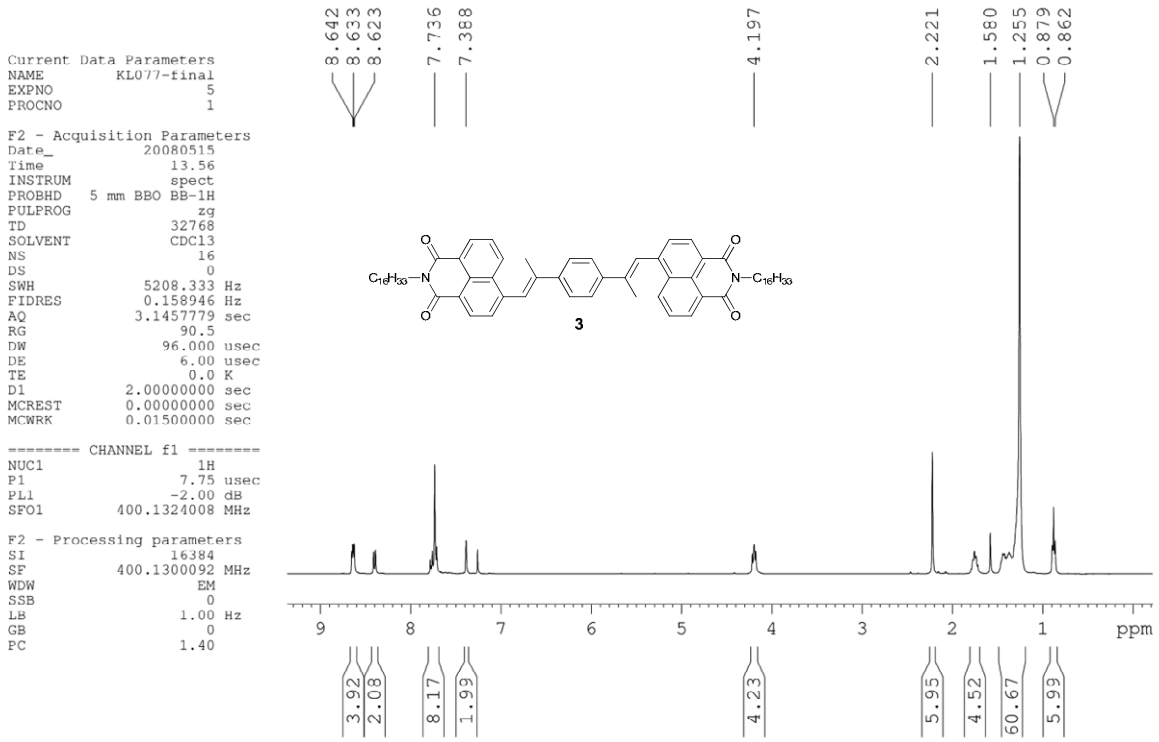



**Figure S2**. $^{1}H$ and $^{13}C$ NMR spectra of compound **2**.



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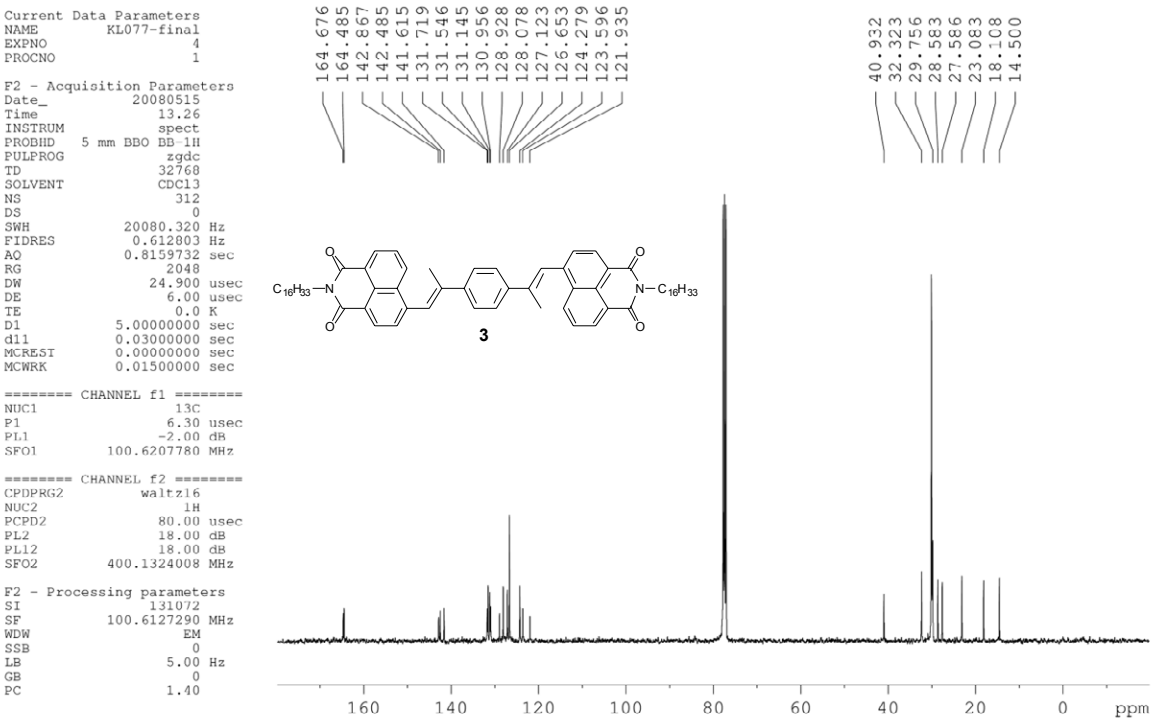


**Figure S3**. $^{1}H$ and $^{13}C$ NMR spectra of compound **3**.

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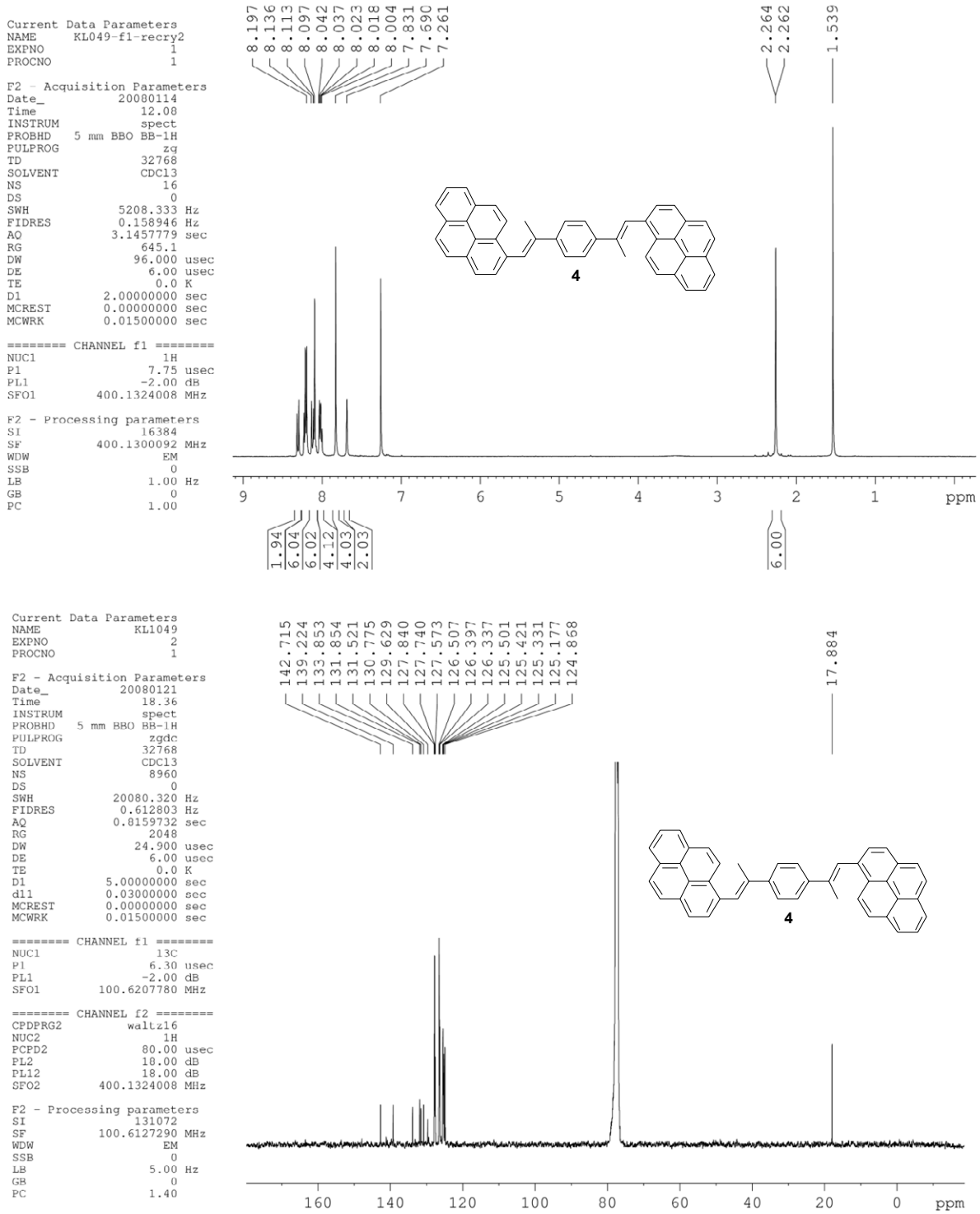


**Figure S4**. $^{1}H$ and $^{13}C$ NMR spectra of compound **4**.

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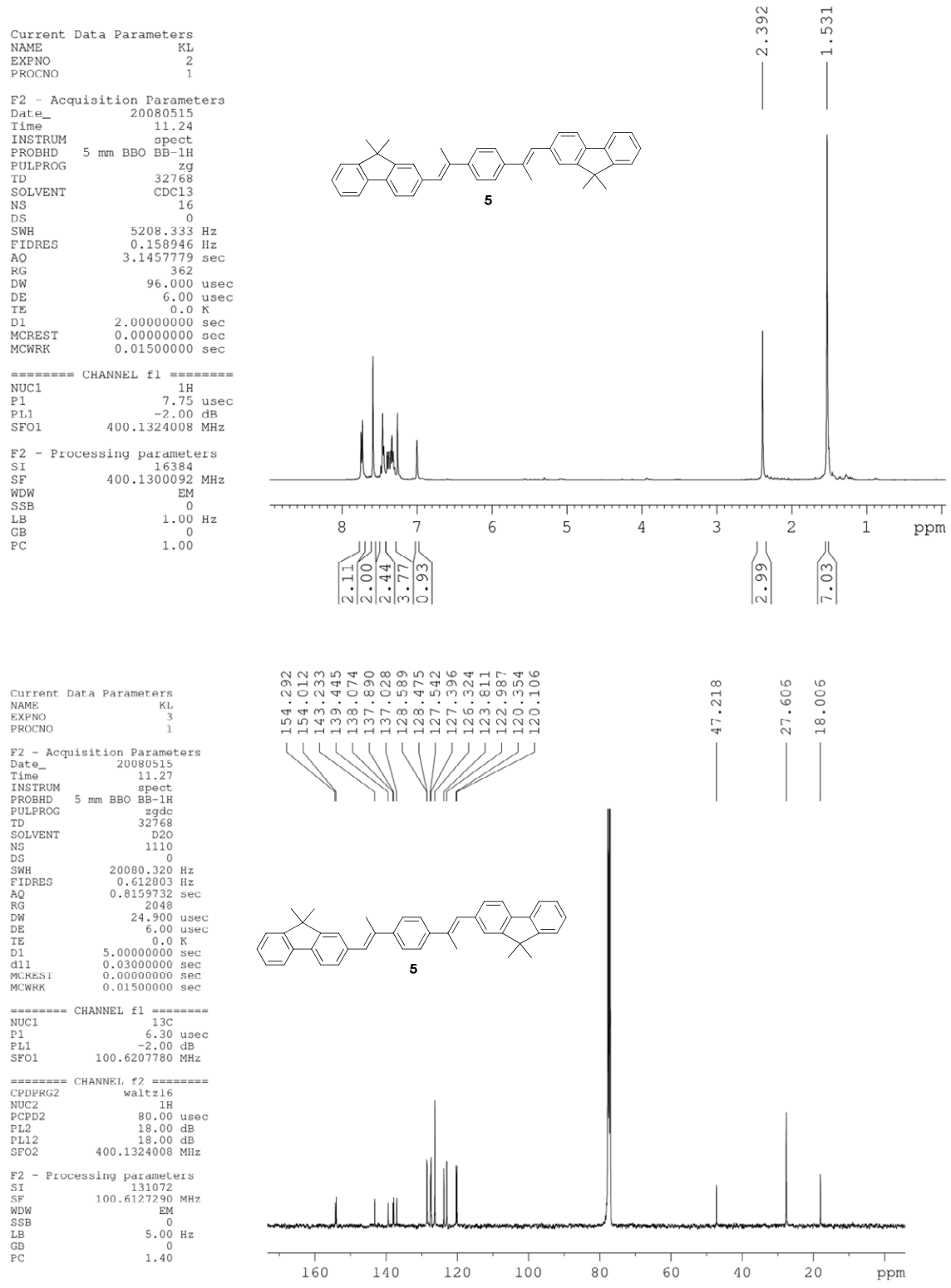


**Figure S5**. $^{1}H$ and $^{13}C$ NMR spectra of compound **5**.

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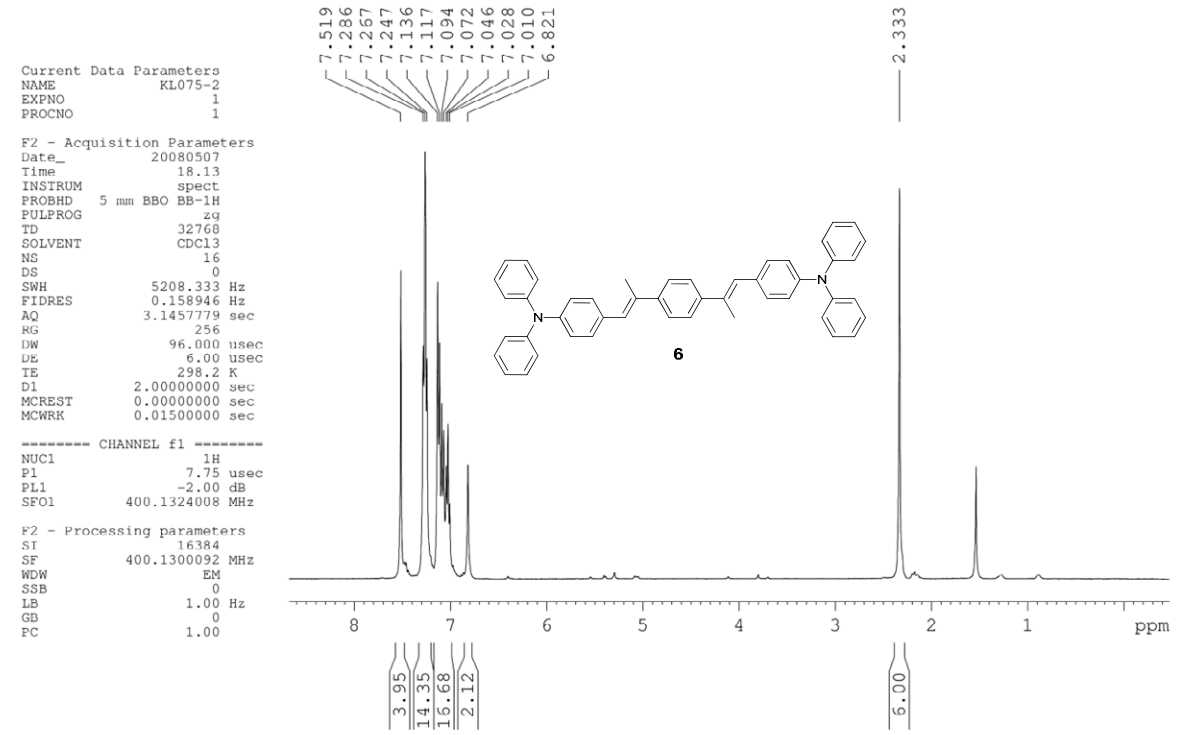


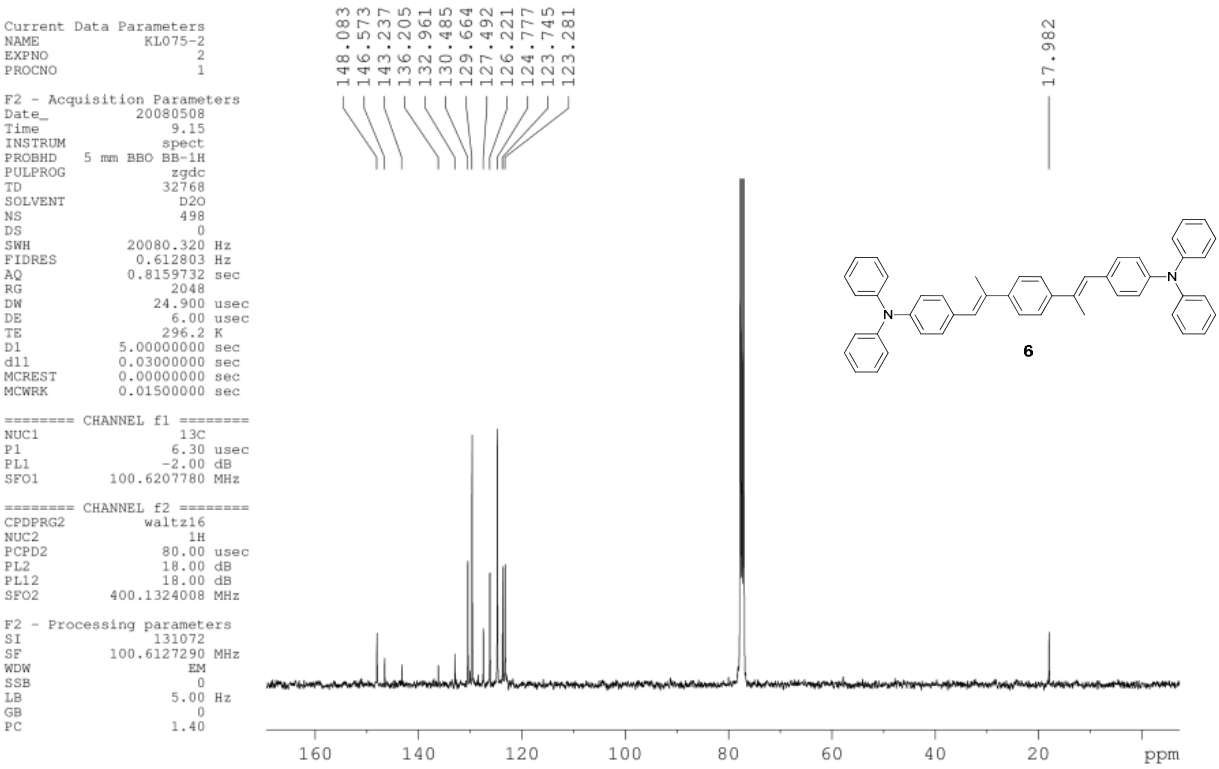

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**Figure S6**. $^{1}H$ and $^{13}C$ NMR spectra of compound **6**.

**2D NOESY NMR of compound 6**

A 2D NOESY $^{1}H$ NMR was recorded of compound 6 to confirm the *trans,trans*-conformation (Figure S7a). The hydrogens have been assigned to the respective peaks on the NMR spectrum. Figure S7b shows an expansion of the same spectrum with focus on the NOEs of the aliphatic hydrogen ($H_g$). No interactions can be observed between $H_g$ and $H_f$, indicating that the two hydrogens are not on the same side of the double bond, and that the double bond adopts a trans-configuration.

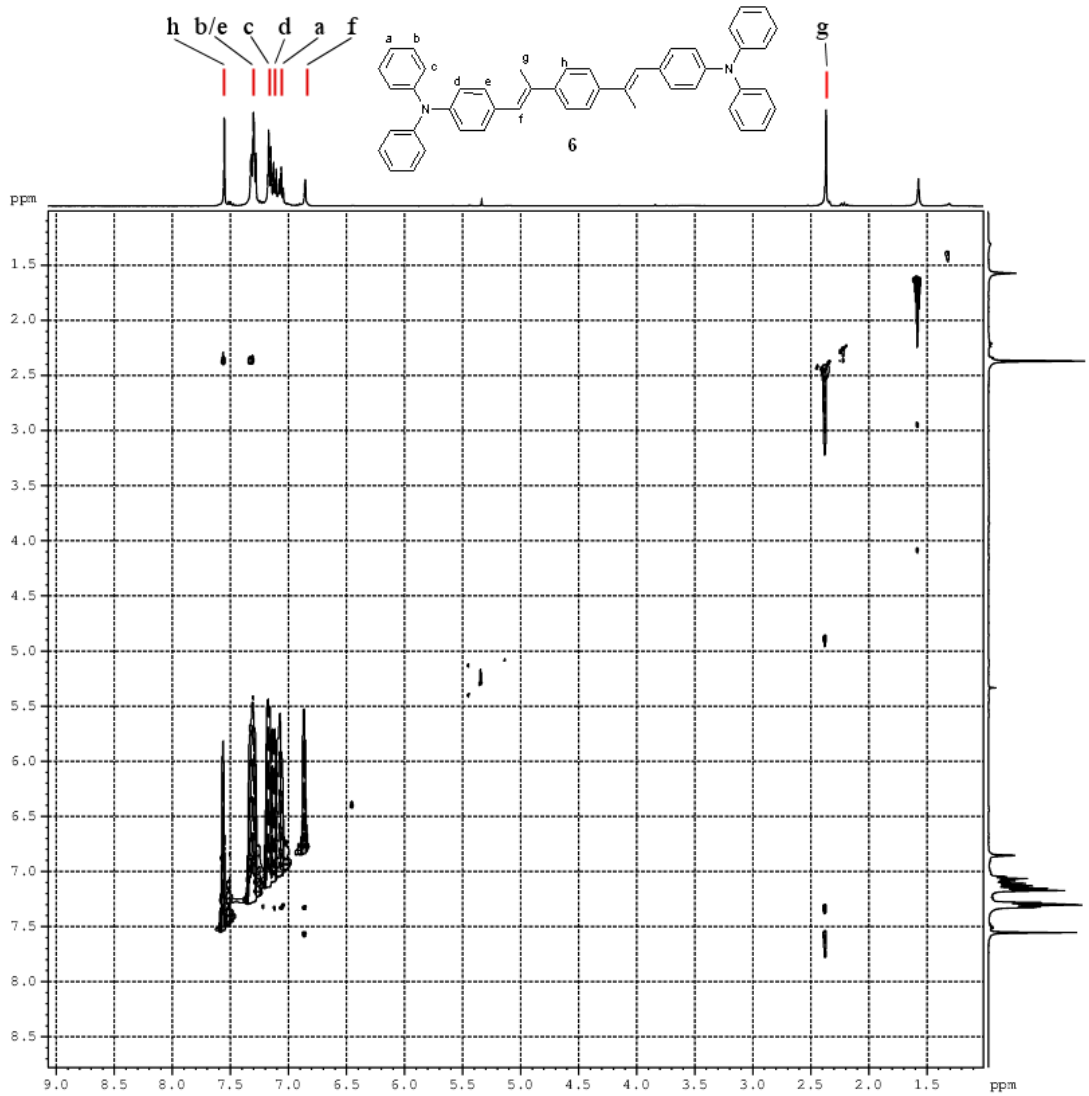


**Figure S7a**. 2D NOESY $^{1}H$ NMR spectrum of compound **6**.

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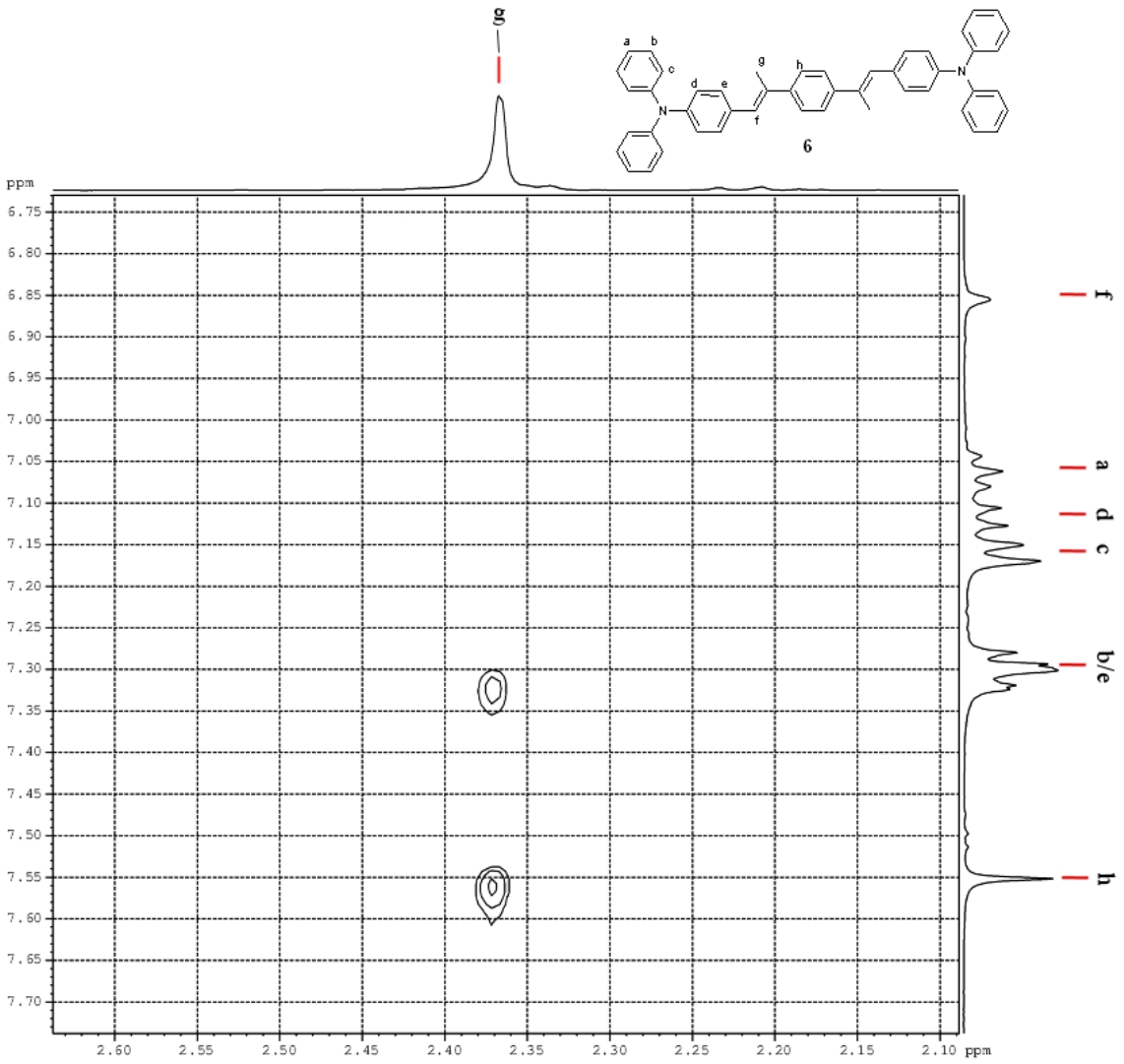


**Figure S7b**. 2D NOESY $^{1}$H NMR spectrum of compound **6**. There is no evidence of interaction between between $H_g$ and $H_f$, indicating that the double bond configuration has to be *trans*, and not *cis*.

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**Oxidative Stability study**

Thin films of compounds **6** and **14** were drop cast on quartz plates from toluene solutions and left to dry in the dark. Photoluminescence spectra were recorded on a Perkin Elmer LS55 Fluorescence Spectrometer under ambient conditions with the following settings: scan rate = 10 nm/s; excitation wavelength = 400 nm; excitation slit width = 2.5 nm; emission slit width = 2.5 nm. Successive measurements (20 in total) were taken with the same settings at intervals of 1 min, while the sample remains in the spectrometer chamber (Figure S8). The emission intensities at the emission peaks (461 nm for **6**, 516nm for **14**) of each measurement were then noted, and plotted against each measurement (Figure 3 in main text).

a) b)

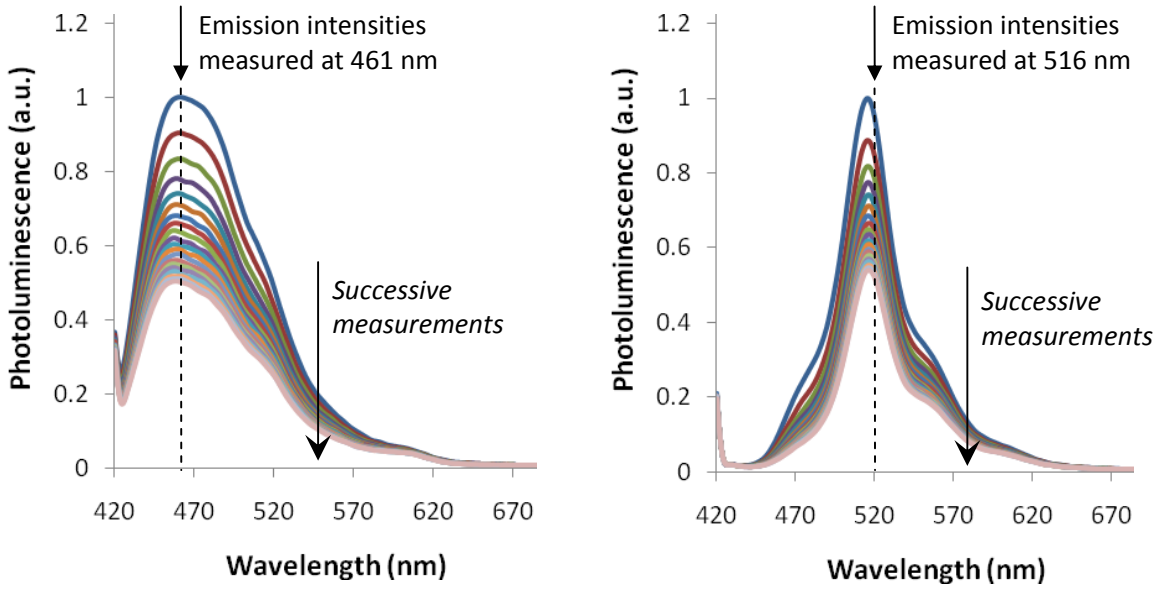


**Figure S8**. Photoluminescence spectra of (a) compound **6** and (b) compound **14** in solid state, excited at 400 nm and recorded over 1 minute intervals.

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**Density Functional Theory (DFT) calculations**

The DFT calculations were performed using the DMol[3] module in the Materials Studio Modeling software package (Accelrys Inc.).[1, 2] DFT calculations were carried out in the generalized gradient approximation with nonlocal exchange and correlation functions according to Perdew–Wang (GGA–PW91),[3] and using the Double Numerical plus polarization (DNP) as the basis set. The convergence tolerances for energy change, maximum force, and maximum displacement between optimization cycles were set as $10^{-5}$ hartree, 0.002 hartree/Å, and 0.005 Å, respectively. Self-consistent-field (SCF) density convergence was $10^{-6}$. The orbital cutoff of 4 Å was used for all atoms.

**Table S1**. Table of Cartesian coordinates and total energy for geometrically optimized compound **14**.
Total Energy = –1883.9951068 Ha

| | Atom | X | Y | Z | | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|---|---|
| 1 | C | -1.432105 | 0.136187 | 0.083974 | 43 | C | 12.082088 | 0.008635 | -1.206874 |
| 2 | C | -0.812280 | -1.064568 | 0.494371 | 44 | C | 11.319396 | -0.547255 | -0.182916 |
| 3 | C | 0.565352 | -1.204057 | 0.533490 | 45 | C | 9.524153 | -2.307944 | 2.946330 |
| 4 | C | 1.415949 | -0.141643 | 0.163837 | 46 | C | 10.153188 | -3.000059 | 3.978581 |
| 5 | C | 0.796045 | 1.060614 | -0.241512 | 47 | C | 11.232843 | -3.844980 | 3.712670 |
| 6 | C | -0.581153 | 1.200193 | -0.280334 | 48 | C | 11.673775 | -3.995922 | 2.396577 |
| 7 | C | 2.864826 | -0.217830 | 0.172580 | 49 | C | 11.040369 | -3.321394 | 1.354863 |
| 8 | C | 3.630530 | -1.280503 | 0.525573 | 50 | H | 8.721381 | -1.735726 | -2.035850 |
| 9 | C | 5.080077 | -1.357734 | 0.523885 | 51 | H | 10.070488 | -0.719579 | -3.849209 |
| 10 | C | 5.925642 | -0.298417 | 0.129829 | 52 | H | 12.233322 | 0.404728 | -3.326559 |
| 11 | C | 7.304967 | -0.426014 | 0.147377 | 53 | H | 13.023815 | 0.499973 | -0.964375 |
| 12 | C | 7.912953 | -1.629389 | 0.551397 | 54 | H | 11.660137 | -0.494942 | 0.849655 |
| 13 | C | 7.087659 | -2.695234 | 0.944646 | 55 | H | 8.691691 | -1.638396 | 3.156736 |
| 14 | C | 5.706841 | -2.551590 | 0.935030 | 56 | H | 9.802939 | -2.866107 | 5.001609 |
| 15 | H | -1.442777 | -1.905753 | 0.786565 | 57 | H | 11.725407 | -4.380977 | 4.522367 |
| 16 | H | 0.990170 | -2.153317 | 0.856890 | 58 | H | 12.508929 | -4.659578 | 2.174104 |
| 17 | H | 1.426245 | 1.901215 | -0.535872 | 59 | H | 11.379856 | -3.449925 | 0.328291 |
| 18 | H | -1.005436 | 2.148707 | -0.606274 | 60 | N | -9.321108 | 1.746151 | -0.621268 |
| 19 | H | 3.132935 | -2.197550 | 0.850483 | 61 | C | -9.895856 | 2.529415 | -1.659894 |
| 20 | H | 5.495262 | 0.651221 | -0.184920 | 62 | C | -10.162494 | 1.102144 | 0.325062 |
| 21 | H | 7.932786 | 0.411334 | -0.153681 | 63 | C | -9.390619 | 2.452786 | -2.967113 |
| 22 | H | 7.538285 | -3.635482 | 1.258158 | 64 | C | -9.945300 | 3.229696 | -3.980876 |
| 23 | H | 5.084203 | -3.393940 | 1.239715 | 65 | C | -11.019152 | 4.081922 | -3.714019 |
| 24 | C | -2.881067 | 0.209150 | 0.049239 | 66 | C | -11.529410 | 4.151859 | -2.416074 |
| 25 | C | -3.637280 | 1.276814 | -0.309587 | 67 | C | -10.972303 | 3.389191 | -1.392290 |
| 26 | C | -5.085238 | 1.353837 | -0.367101 | 68 | C | -9.815109 | 1.076906 | 1.685370 |
| 27 | C | -5.945432 | 0.273779 | -0.074438 | 69 | C | -10.639829 | 0.438861 | 2.608157 |
| 28 | C | -7.322924 | 0.398420 | -0.155064 | 70 | C | -11.829880 | -0.166433 | 2.199250 |
| 29 | C | -7.914971 | 1.619389 | -0.529529 | 71 | C | -12.181543 | -0.134237 | 0.847987 |
| 30 | C | -7.074204 | 2.706914 | -0.818134 | 72 | C | -11.355729 | 0.487501 | -0.085296 |
| 31 | C | -5.695557 | 2.566442 | -0.746152 | 73 | H | -8.560305 | 1.780400 | -3.177069 |
| 32 | H | -3.129125 | 2.199556 | -0.599922 | 74 | H | -9.543966 | 3.155730 | -4.991018 |
| 33 | H | -5.526116 | -0.691245 | 0.206964 | 75 | H | -11.455724 | 4.684100 | -4.509359 |
| 34 | H | -7.960565 | -0.457606 | 0.059942 | 76 | H | -12.362157 | 4.818578 | -2.193746 |
| 35 | H | -7.512686 | 3.661384 | -1.104451 | 77 | H | -11.363198 | 3.456608 | -0.378436 |
| 36 | H | -5.062832 | 3.426554 | -0.969035 | 78 | H | -8.894021 | 1.558902 | 2.009529 |
| 37 | N | 9.322987 | -1.755718 | 0.567628 | 79 | H | -10.355615 | 0.430400 | 3.660073 |
| 38 | C | 10.101666 | -1.182046 | -0.473469 | 80 | H | -12.475204 | -0.657978 | 2.925829 |

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| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 39 | C | 9.962166 | -2.463177 | 1.622032 | 81 | H | -13.104226 | -0.607002 | 0.512284 |
| 40 | C | 9.661948 | -1.238292 | -1.805484 | 82 | H | -11.628733 | 0.500760 | -1.139401 |
| 41 | C | 10.424137 | -0.664377 | -2.820270 | 83 | H | 3.363761 | 0.699239 | -0.149711 |
| 42 | C | 11.638508 | -0.039803 | -2.530084 | 84 | H | -3.386450 | -0.712477 | 0.347738 |

**Table S2**. Table of Cartesian coordinates and total energy for geometrically optimized compound **6.**

Total Energy = –1962.6030057 Ha

| | Atom | X | Y | Z | | Atom | X | Y | Z |
|---|---|---|---|---|---|---|---|---|---|
| 1 | C | -1.357570 | 0.521143 | 0.171922 | 46 | N | -8.764796 | 2.155930 | 2.559426 |
| 2 | C | -1.042957 | -0.822597 | -0.125052 | 47 | C | 9.862997 | -2.155306 | -1.601482 |
| 3 | C | 0.244531 | -1.224192 | -0.450196 | 48 | C | 9.026846 | -2.366721 | -3.904986 |
| 4 | C | 1.310695 | -0.301898 | -0.477692 | 49 | C | -8.949136 | 2.163649 | 3.969983 |
| 5 | C | 0.995870 | 1.043177 | -0.191792 | 50 | C | -9.893514 | 2.151004 | 1.699041 |
| 6 | C | -0.291460 | 1.444618 | 0.136299 | 51 | C | -9.896758 | 1.376743 | 0.527187 |
| 7 | C | 2.691052 | -0.643928 | -0.805130 | 52 | C | -11.011475 | 1.373970 | -0.308133 |
| 8 | C | 3.393771 | -1.782177 | -0.543901 | 53 | C | -12.144739 | 2.123622 | 0.014300 |
| 9 | C | 4.776517 | -1.914063 | -1.052448 | 54 | C | -12.145497 | 2.890116 | 1.181756 |
| 10 | C | 5.166618 | -1.314506 | -2.267091 | 55 | C | -11.030209 | 2.912974 | 2.015632 |
| 11 | C | 6.467261 | -1.397925 | -2.746139 | 56 | C | -8.143825 | 2.975291 | 4.784794 |
| 12 | C | 7.445697 | -2.112546 | -2.035361 | 57 | C | -8.321118 | 2.976643 | 6.166245 |
| 13 | C | 7.069772 | -2.739528 | -0.837880 | 58 | C | -9.309535 | 2.185860 | 6.755845 |
| 14 | C | 5.767289 | -2.639915 | -0.363709 | 59 | C | -10.115601 | 1.382494 | 5.945973 |
| 15 | H | -1.846396 | -1.560200 | -0.118927 | 60 | C | -9.935722 | 1.362740 | 4.564842 |
| 16 | H | 0.422338 | -2.262745 | -0.722389 | 61 | C | 8.211920 | -3.200625 | -4.687872 |
| 17 | H | 1.799245 | 1.780802 | -0.197497 | 62 | C | 8.462740 | -3.351456 | -6.049574 |
| 18 | H | -0.464410 | 2.482989 | 0.410087 | 63 | C | 9.534414 | -2.691164 | -6.654059 |
| 19 | H | 3.245402 | 0.168978 | -1.280453 | 64 | C | 10.350513 | -1.867055 | -5.875724 |
| 20 | H | 4.422360 | -0.786364 | -2.862043 | 65 | C | 10.098057 | -1.696067 | -4.516889 |
| 21 | H | 6.732385 | -0.920752 | -3.688421 | 66 | C | 9.856934 | -1.235468 | -0.542151 |
| 22 | H | 7.809651 | -3.308974 | -0.277208 | 67 | C | 10.918802 | -1.196001 | 0.358365 |
| 23 | H | 5.525441 | -3.137084 | 0.573746 | 68 | C | 12.008407 | -2.056034 | 0.208973 |
| 24 | C | 2.847724 | -2.912491 | 0.287109 | 69 | C | 12.020499 | -2.965444 | -0.849950 |
| 25 | H | 2.619878 | -3.793757 | -0.332240 | 70 | C | 10.955542 | -3.024008 | -1.745792 |
| 26 | H | 1.939646 | -2.622919 | 0.824038 | 71 | H | -9.021260 | 0.778797 | 0.279510 |
| 27 | H | 3.580390 | -3.242467 | 1.035292 | 72 | H | -10.997980 | 0.765202 | -1.211941 |
| 28 | C | -2.732454 | 0.844163 | 0.532580 | 73 | H | -13.016045 | 2.112561 | -0.639139 |
| 29 | C | -3.439020 | 2.003244 | 0.402406 | 74 | H | -13.018811 | 3.487339 | 1.442699 |
| 30 | C | -4.808827 | 2.071563 | 0.957430 | 75 | H | -11.030777 | 3.519400 | 2.919967 |
| 31 | H | -3.284040 | -0.009681 | 0.932673 | 76 | H | -7.382118 | 3.602239 | 4.323484 |
| 32 | C | -5.159830 | 1.340420 | 2.111310 | 77 | H | -7.690244 | 3.614381 | 6.784965 |
| 33 | C | -6.447711 | 1.354050 | 2.628057 | 78 | H | -9.451833 | 2.195162 | 7.835594 |
| 34 | C | -7.452901 | 2.125980 | 2.023215 | 79 | H | -10.882921 | 0.751976 | 6.394686 |
| 35 | C | -7.117090 | 2.880753 | 0.888167 | 80 | H | -10.557417 | 0.727795 | 3.935468 |
| 36 | C | -5.825576 | 2.852075 | 0.375214 | 81 | H | 7.385884 | -3.731997 | -4.217979 |
| 37 | H | -4.394504 | 0.758867 | 2.623361 | 82 | H | 7.820974 | -4.005547 | -6.639139 |
| 38 | H | -6.682110 | 0.776095 | 3.520544 | 83 | H | 9.732438 | -2.816453 | -7.717335 |
| 39 | H | -7.878962 | 3.493654 | 0.408516 | 84 | H | 11.184884 | -1.336586 | -6.333663 |
| 40 | H | -5.615281 | 3.448214 | -0.510906 | 85 | H | 10.730664 | -1.042602 | -3.918267 |
| 41 | C | -2.908685 | 3.217326 | -0.311503 | 86 | H | 9.013475 | -0.555865 | -0.429980 |
| 42 | H | -3.679667 | 3.677752 | -0.941763 | 87 | H | 10.901370 | -0.475631 | 1.175514 |
| 43 | H | -2.059534 | 2.970827 | -0.956982 | 88 | H | 12.839708 | -2.020191 | 0.911480 |
| 44 | H | -2.587464 | 3.994057 | 0.400000 | 89 | H | 12.860575 | -3.648186 | -0.975361 |
| 45 | N | 8.775432 | -2.206814 | -2.516430 | 90 | H | 10.961167 | -3.740707 | -2.565132 |

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