Electronic Supporting Information to:
Synthesis and High-Throughput Characterization of Structural Analogues of Molecular Glassformers: 1,3,5-Trisarylbenzenes

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General Methods

All reactions were carried out under a nitrogen atmosphere with oven-dried glassware employing standard vacuum line techniques. The progress of all reactions was monitored by thin-layer chromatography. THF was dried over sodium benzophenone. Unless otherwise specified, all chemicals were obtained from Acros, Aldrich, or GFS Chemicals, and all solvents were purchased from Fischer Scientific. The ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra were obtained on a Brüker AM-500 Fourier transform NMR spectrometer at 500 and 125 MHz, respectively. Chemical shifts are reported in units of parts per million downfield from tetramethylsilane, and all coupling constants are reported in hertz. Thin-layer chromatography was performed on Whatman precoated silica gel 60 F-254 plates and visualized by ultra-violet light. Silica gel (230-400 mesh, Silicycle) was used for air-flashed chromatography. High resolution mass spectra were measured using a Waters 2695 Separations Module. The mass spectra for many of these compounds did not give the desired molecular ion using ESI or CI. 1-Naphthyl boronic acid,[1] 2-naphthyl boronic acid,[2] and 9-anthracene boronic acid[3] were synthesized according to previously reported methods. 1-Bromo-3-chloro-5-iodobenzene was synthesized using a literature method[4,5] by students at the University of Pennsylvania enrolled in the Introductory Organic Chemistry Laboratory (Chemistry 245). The trihalobenzene was further purified by dissolving in dichloromethane and filtering. The filtrate was concentrated and the solid was recrystallized using hot methanol.

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Synthesis of α-α-β TNB and its derivatives

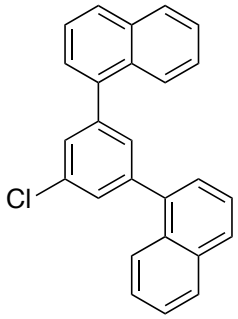
Below is an overview of the synthetic methods employed to prepare the substrates utilized in this study. The advantage of using 1-bromo-3-chloro-5-iodobenzene is that each of the three halogens has different reactivity toward palladium catalysts. Ligands for palladium catalyzed Suzuki reactions are chosen to maximize chemoselectivity in reaction at the C–halogen bonds. General procedures for each of the reactions in the overview are outlined below.

General Procedure A: Cross-Coupling of 1-Bromo-3-chloro-5-iodobenzene with 2 equiv of Boronic Acid. A dry 100 mL round bottom flask equipped with a stir bar was charged with 1-bromo-3-chloro-5-iodobenzene (1.29 g, 4.07 mmol, 1.0 equiv) and 1-naphthyl boronic acid (1.54 g, 8.95 mmol, 2.2 equiv) before purging the flask with nitrogen. Toluene (40.7 mL), ethanol (25 mL), and Na_2CO_3 (64 mL, 2 M solution in H_2O, 0.13 mol) were added to the flask before the addition of $Pd(PPh_3)_4$ (0.141 g, 0.12 mmol, 3 mol %). The reaction mixture was heated to 90 ^oC for 12 h. Upon completion by TLC analysis, the reaction was cooled to RT and distilled water was added. The organic and aqueous layers were separated, the aqueous layer was extracted with Et_2O three times, and the combined organics were washed with brine and dried over $MgSO_4$. The filtrate was concentrated and the residue was chromatographed on silica gel to afford the title compound.

General Procedure B: Cross-Coupling of Aryl Chloride with Boronic Acid. A dry 25 mL round bottom flask equipped with a stir bar was charged with aryl chloride **(a)** (0.622 g, 1.71 mmol, 1.0 equiv), 2-naphthyl boronic acid (0.440g, 2.56 mmol, 1.5 equiv), $Pd(OAc)_2$ (10 mg, 0.043 mmol, 2.5 mol %), DavePhos (34 mg, 0.085 mmol, 5 mol %), and K_3PO_4 (0.724 g, 3.41 mmol, 2.0 equiv) before flushing with nitrogen. THF (8.5 mL) and H_2O (1.7 mL) were added before warming to 50 ^oC. After 4 hours, the aryl chloride was completely consumed by TLC analysis. The reaction mixture was cooled to room temperature and diluted with distilled water. The organic and aqueous layers were separated, the aqueous layer was extracted with Et_2O three times, and the combined organic layers were washed with brine and dried over $MgSO_4$. The filtrate was concentrated and the residue was chromatographed on silica gel to afford the title compound.

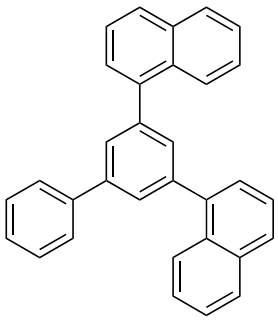
General Procedure C: Single Coupling of Aryl Halide with Boronic Acid. A dry 50 mL round bottom flask equipped with a stir bar was charged with 1-bromo-3-chloro-5-iodobenzene (0.50 g, 1.58 mmol, 1.1 equiv) and 1-naphthyl boronic acid (0.247 g, 1.43 mmol, 1.0 equiv) before purging the flask with nitrogen. THF (14 mL) and K_2CO_3 (28.4 mL, 2 M solution in H_2O, 57 mmol) were added to the flask before the addition of $Pd(PPh_3)_4$ (25 mg, 0.022 mmol, 1.5 mol %) as a solution in 14 mL of THF. The reaction flask was equipped with a condenser and heated to reflux for 12 h, and then cooled to room temperature. The organic and aqueous layers were separated, the aqueous layer was extracted with CH_2Cl_2 three times, and the combined organics were washed with brine and dried over $MgSO_4$. The filtrate was concentrated and the residue was chromatographed on silica gel to afford the title compound.

General Procedure D. The following compounds were synthesized according to previously reported methods.[6] An oven-dried 10 mL reaction vial equipped with a stir bar was charged with aryl chloride (0.109 g, 0.30 mmol, 1.0 equiv), bis(pinacolato)diboron (38 mg, 0.15 mmol, 0.5 equiv), Pd_2dba_3 (4 mg, 0.0045 mmol, 1.5 mol %), SPhos (15 mg, 0.036 mmol, 12 mol %), and K_3PO_4 (0.127 g, 0.6 mmol, 2.0 equiv) before purging with nitrogen. 1,4-Dioxane (0.6 mL) was added to the reaction vial before heating to 110 ^oC for 6 h. The reaction mixture was cooled to RT before adding H_2O (0.15 mL) followed by heating to 110 ^oC for an additional 15 h. At this point, the reaction was cooled to RT and filtered through a thin pad of celite using ethyl acetate. The filtrate was concentrated and the residue was recrystallized using hexanes/dichloromethane to provide the title compound.

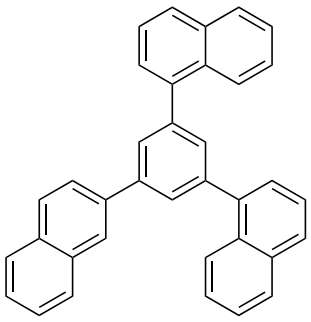


1,1'-(5-Chloro-1,3-phenylene)dinaphthalene (a). The product was prepared using General Procedure A by adding $Pd(PPh_3)_4$ (0.141 g, 0.12 mmol, 3 mol %) to a mixture of 1-bromo-3-chloro-5-iodobenzene (1.29 g, 4.07 mmol, 1.0 equiv), 1-naphthyl boronic acid (1.54 g, 8.95 mmol, 2.2 equiv), toluene (40.7 mL), ethanol (25 mL), and Na_2CO_3 (64 mL, 2 M solution in H_2O, 0.13 mol). The filtrate was concentrated and the residue was chromatographed on silica gel (10% ethyl acetate in hexanes) to afford the title compound in 80% yield (1.19 g, 3.26 mmol). ^1H NMR ($CDCl_3$, 500 MHz) δ 7.99 (d, J = 8.2 Hz, 2H), 7.89-

7.82 (m, 4H), 7.56 (d, J = 1.5 Hz, 2H), 7.51 (t, J = 1.5 Hz, 1H), and 7.50-7.42 (m, 8H); ^{13}C {^{1}H} ($CDCl_3$, 125 MHz) δ 142.5, 138.6, 134.1, 133.8, 131.4, 130.1, 128.9, 128.4, 128.3, 127.1, 126.4, 126.0, 125.6, 125.3; IR (neat) 3047, 1930, 1815, 1590, 1565, 1507, 1440, 1390, 1335, 1309, 1271, 1210, 1189, 1161, 1143, 1126, 1107, and 1019 cm^{-1}; HRMS *m/z* 364.1008 [M^+; calcd for $C_{26}H_{17}Cl$: 364.1019].

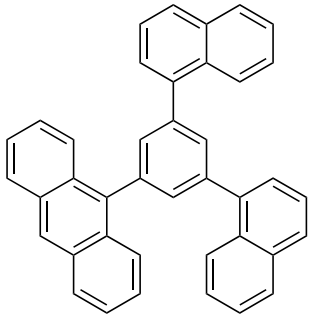


3,5-Di(naphthalen-1-yl)-1-phenylbenzene (b). The product was prepared by General Procedure B using aryl chloride **a (**2.0 g, 5.50 mmol, 1.0 equiv), phenylboronic acid (1.000 g, 8.25 mmol, 1.5 equiv), $Pd(OAc)_2$ (32 mg, 0.138 mmol, 2.5 mol %), DavePhos (109 mg, 0.273 mmol, 5 mol %), K_3PO_4 (2.328 g, 10.96 mmol, 2.0 equiv), THF (15 mL), and H_2O (3.0 mL). The filtrate was concentrated and the residue was chromatographed on silica gel (5% EtOAc in hexanes) to afford the title compound in 90% yield (2.0 g, 4.95 mmol). ^1H NMR ($CDCl_3$, 500 MHz) δ 8.15 (d, J = 7.0 Hz, 2H), 7.93 (d, J = 7.0 Hz, 2H), 7.90 (d, J = 7.0 Hz, 2H), 7.85 (s, 2H), 7.74 (d, J = 7.0 Hz, 2H), 7.67 (s, 1H), 7.58-7.46 (m, 10H), 7.38 (t, J = 7.0 Hz, 1H). $^{13}C\{^1H\}$ ($CDCl_3$, 125 MHz) δ 141.3, 141.1, 140.8, 133.9, 133.9, 131.6, 130.7, 128.9, 128.4, 127.9, 127.8, 127.5, 127.3, 127.1, 126.2, 126.0, 125.9, 125.4 (Due to signals with similar chemical shifts, not all peaks are observed); IR (neat) 3045, 2302, 1934, 1818, 1589, 1506, 1441, 1417, 1387, 1336, 1264, 1160, 1124, 1077, 1029, 1019, 1012 cm^{-1}.

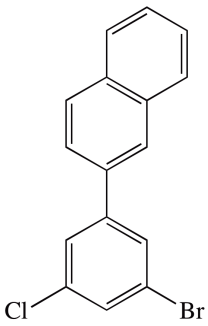


1,3-Bis(1-naphthyl)-5-(2-naphthyl)benzene (c). The product was prepared by General Procedure B using aryl chloride **a** (0.622 g, 1.71 mmol, 1.0 equiv), 2-naphthyl boronic acid (0.440 g, 2.56 mmol, 1.5 equiv), $Pd(OAc)_2$ (10 mg, 0.043 mmol, 2.5 mol %), DavePhos (34 mg, 0.085 mmol, 5 mol %), K_3PO_4 (0.724 g, 3.41 mmol, 2.0 equiv), THF (8.5 mL), and H_2O (1.7 mL). The filtrate was concentrated and the residue was chromatographed on silica gel (10% to 40% dichloromethane in hexanes) to afford

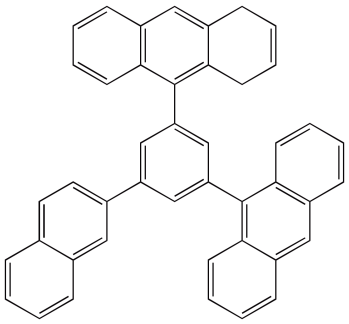
the title compound in 92% yield (0.718 g, 1.57 mmol). ^{1}H NMR and ^{13}C{^{1}H} NMR for this compound match previously reported literature data.[1]



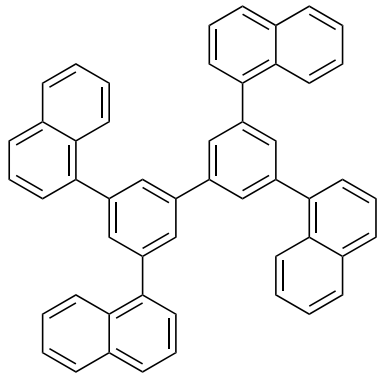
9-(3,5-Di(naphthalen-1-yl)phenyl)anthracene (d). The product was prepared by General Procedure B at 80 ^{o}C using aryl chloride **a** (73 mg, 0.20 mmol, 1.0 equiv), 9-anthracene boronic acid (52 mg, 0.30 mmol, 1.5 equiv), $Pd(OAc)_2$ (2 mg, 0.01 mmol, 5 mol %), DavePhos (8 mg, 0.02 mmol, 10 mol %), K_3PO_4 (85 mg, 0.40 mmol, 2.0 equiv), THF (1.0 mL), and H_2O (0.2 mL). The filtrate was concentrated and the residue was chromatographed on silica gel (10% dichloromethane in hexanes) to afford the title compound in 60% yield (61 mg, 0.12 mmol). mp = 236 ^{o}C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.51 (s, 1H), 8.28-8.25 (m, 2H), 8.06 (d, *J* = 8.4 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.92-7.85 (m, 5H), 7.70 (d, *J* = 1.6 Hz, 2H), 7.66 (dd, *J* = 7.1, 1.1 Hz, 2H), 7.57-7.53 (m, 2H), and 7.52-7.43 (m, 8H); ^{13}C {^{1}H} ($CDCl_3$, 125 MHz) δ 140.9, 139.7, 138.8, 133.9, 131.9, 131.6, 131.4, 130.9, 130.3, 128.5, 128.4, 127.9, 127.4, 126.8, 126.3, 125.9, 125.8, 125.6, 125.4, and 125.1 (Due to signals with similar chemical shifts, not all peaks are observed.); IR (neat) 3047, 1589, 1507, 1481, 1460, 1443, 1389, 1361, 1334, 1310, 1264, 1244, and 1013 cm^{-1}.



2-(3-Bromo-5-chlorophenyl)naphthalene (e). The product was prepared using General Procedure C by adding $Pd(PPh_3)_4$ (25 mg, 0.022 mmol, 1.5 mol %) in 14 mL of THF to a mixture of 1-bromo-3-chloro-5-iodobenzene (0.50 g, 1.58 mmol, 1.1 equiv), 2-naphthyl boronic acid (0.247 g, 1.43 mmol, 1.0 equiv), THF (14 mL), and K_2CO_3 (28.4 mL, 2 M solution in H_2O, 57 mmol). The filtrate was concentrated and the residue was chromatographed on silica gel (100% hexanes) to afford the title compound in 65% yield (0.295 g, 0.93 mmol). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.98 (s, 1H), 7.93-7.84 (m, 3H), 7.75-7.72 (m, 1H), 7.66-7.61 (m, 2H), and 7.55-7.47 (m, 3H); ^{13}C {^{1}H} ($CDCl_3$, 125 MHz) δ 144.4, 135.7, 135.5, 133.5, 133.1, 130.0, 128.9, 128.8, 128.3, 127.7, 126.7, 126.6, 126.4, 126.3, 124.8, and 123.2; IR (neat) 3058, 1587, 1552, 1506, 1438, 1407, 1337, 1269, and 1107 cm^{-1}; HRMS *m/z* 315.9650 [M^{+}; calcd for $C_{16}H_{10}BrCl$: 315.9654].



9,9'-(5-(Naphthalen-2-yl)-1,3-phenylene)dianthracene (f). The product was prepared by General Procedure B using aryl chloride **e** (0.100 g, 0.32 mmol, 1.0 equiv), 9-anthracene boronic acid (0.163 g, 0.95 mmol, 3.0 equiv), $Pd(OAc)_2$ (7 mg, 0.032 mmol, 10 mol %), DavePhos (25 mg, 0.063 mmol, 20 mol %), K_3PO_4 (0.267 g, 1.26 mmol, 4.0 equiv), THF (1.6 mL), and H_2O (0.32 mL). The reaction mixture was heated at 80 ^oC for 24 h. The filtrate was concentrated and the residue was chromatographed on silica gel (10% to 50% dichloromethane in hexanes) to afford the title compound in 56% yield (98 mg, 0.18 mmol). ^1H NMR ($CDCl_3$, 500 MHz) δ 8.52 (s, 2H), 8.21 (s, 1H), 8.09-8.02 (m, 10H), 7.89 (d, J = 1.0 Hz, 2H), 7.85-7.80 (m, 2H), 7.57 (t, J = 1.5 Hz, 1H), and 7.52-7.43 (m, 10H); ^{13}C {^1H} ($CDCl_3$, 125 MHz) δ 141.1, 139.6, 137.6, 136.5, 133.7, 133.3, 132.8, 131.4, 130.3, 129.3, 128.6, 128.5, 128.2, 128.1, 127.6, 126.8, 126.8, 126.4, 126.1, 125.7, 125.4, and 125.1; IR (neat) 3054, 2925, 2854, 1669, 1623, 1590, 1519, 1508, 1482, 1461, 1443, 1411, 1349, 1334, 1268, 1199, and 1014 cm^{-1}.



3,3',5,5'-tetra(naphthalen-1-yl)-1,1'-biphenyl (g). The product was prepared by General Procedure D using aryl chloride **a** (0.109 g, 0.30 mmol, 1.0 equiv), bis(pinacolato)diboron (38 mg, 0.15 mmol, 0.5 equiv), Pd_2dba_3 (4 mg, 0.0045 mmol, 1.5 mol %), SPhos (15 mg, 0.036 mmol, 12 mol %), K_3PO_4 (0.127 g, 0.6 mmol, 2.0 equiv), 1,4-dioxane (0.6 mL), and H_2O (0.15 mL). The filtrate was concentrated and the residue was recrystallized using hexanes/dichloromethane to provide the title compound in 71% yield (70 mg, 0.11 mmol). ^1H NMR ($CDCl_3$, 500 MHz) δ 8.11 (d, J = 8.0 Hz, 4H), 7.94 (d, J = 1.7 Hz, 4H), 7.91-7.85 (m, 8H), 7.68-7.66 (m, 2H), and 7.59-7.43 (m, 16H); ^{13}C {^1H} ($CDCl_3$, 125 MHz) δ 141.4, 140.9, 139.8, 133.9, 131.6, 131.0, 128.3, 127.9, 127.8, 127.2, 126.3, 126.0, 125.8, and 125.4; IR (neat) 3045, 2927, 1587, 1576, 1507, 1392, 1335, 1264, 1161, 1113, and 1020 cm^{-1}.

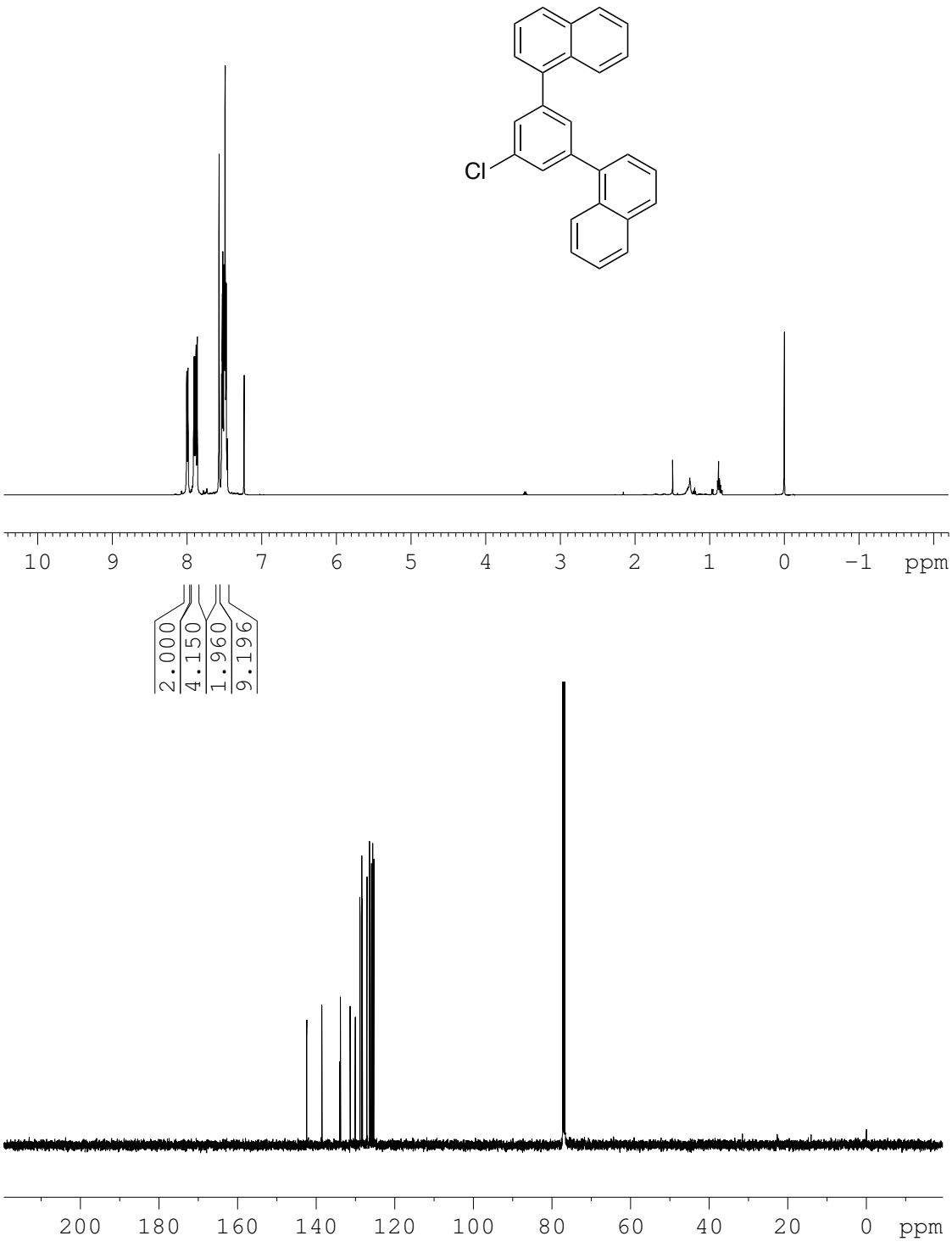


Fig. S1 500 MHz ^{1}H NMR and 125 MHz $^{13}C\{^{1}H\}$ NMR of **a** in $CDCl_3$.

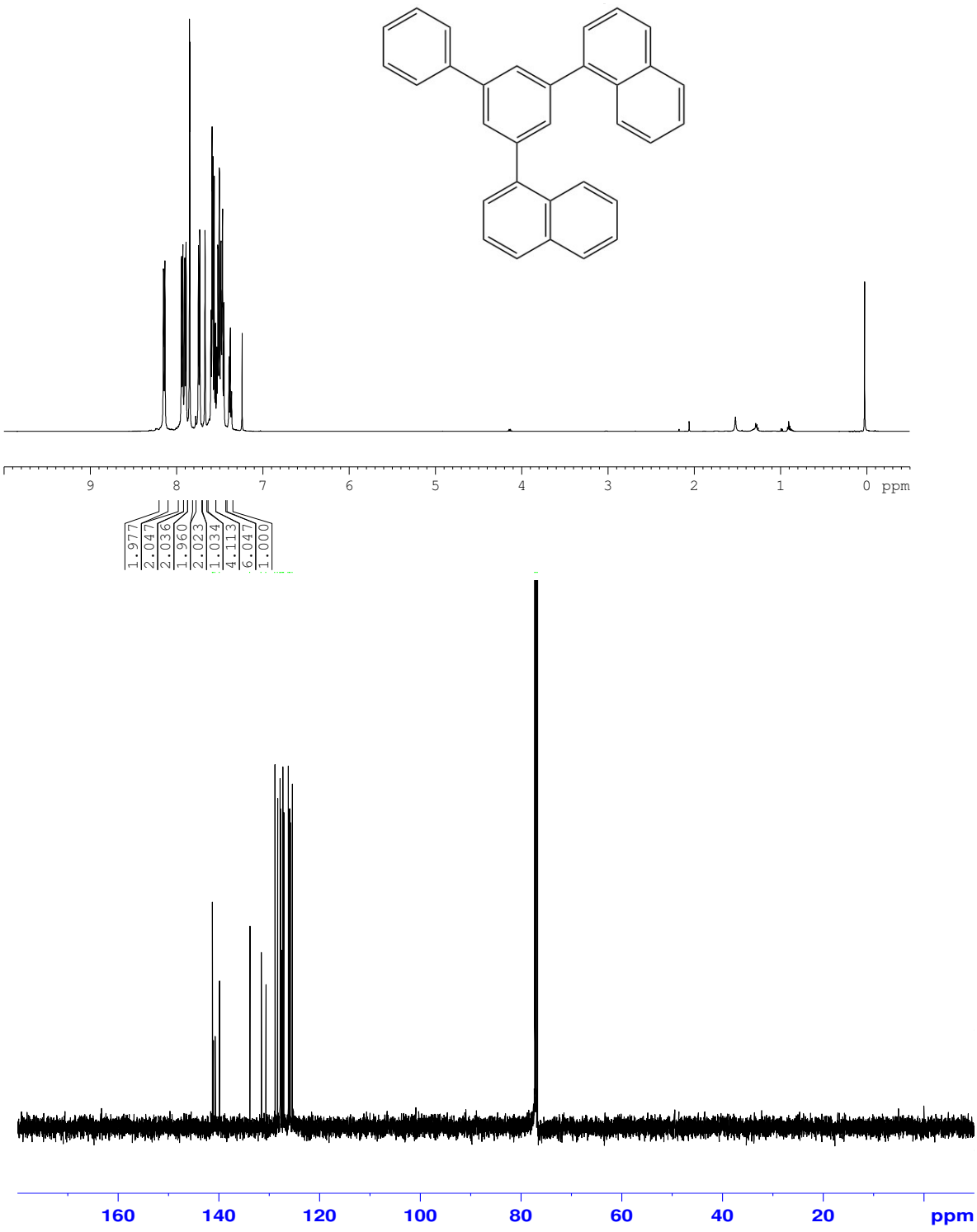


Fig. S2 500 MHz ^{1}H NMR and 125 MHz $^{13}C\{^{1}H\}$ NMR of **b** in $CDCl_3$.

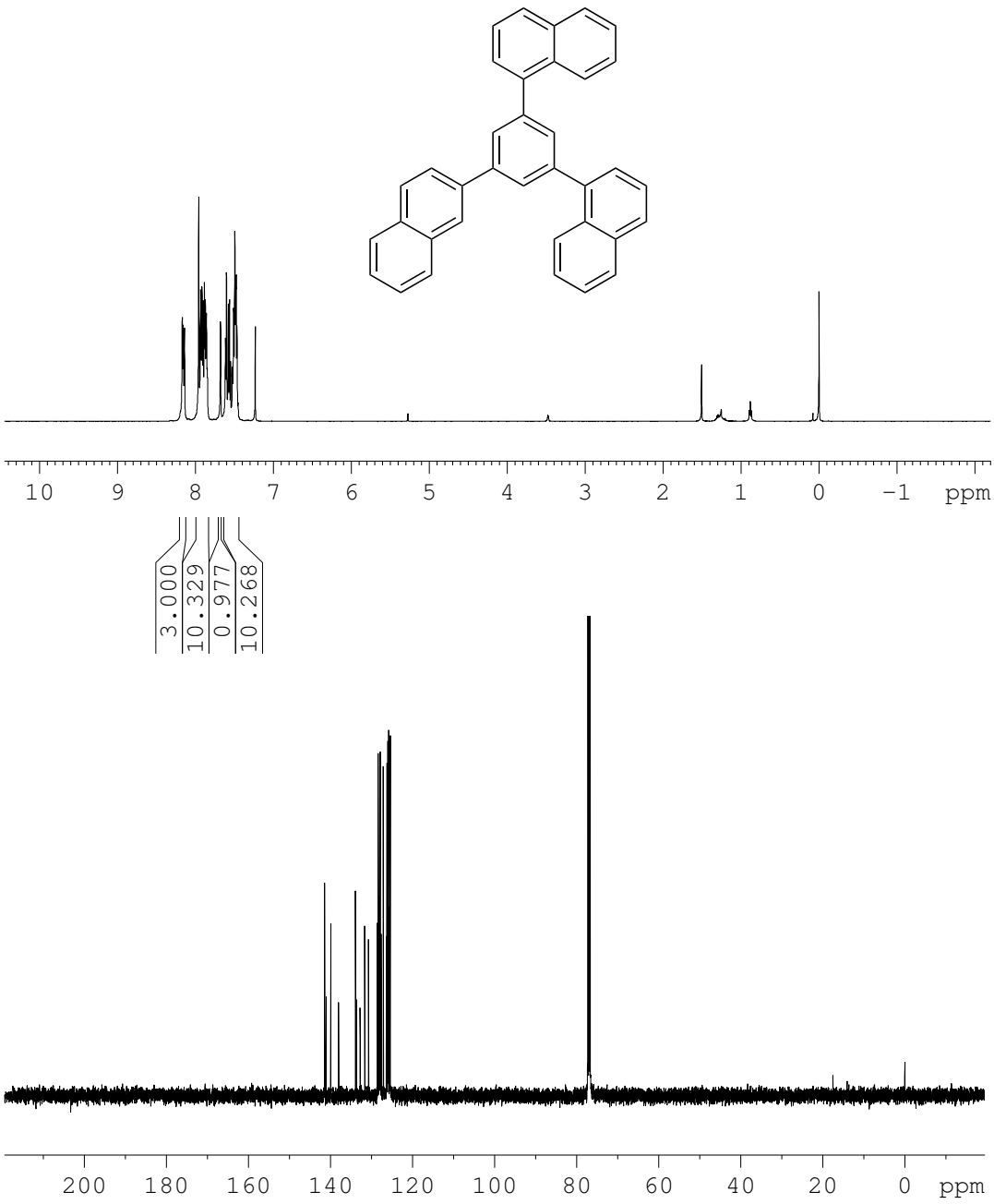


Fig. S3 500 MHz ^{1}H NMR and 125 MHz $^{13}C\{^{1}H\}$ NMR of **c** in $CDCl_3$.

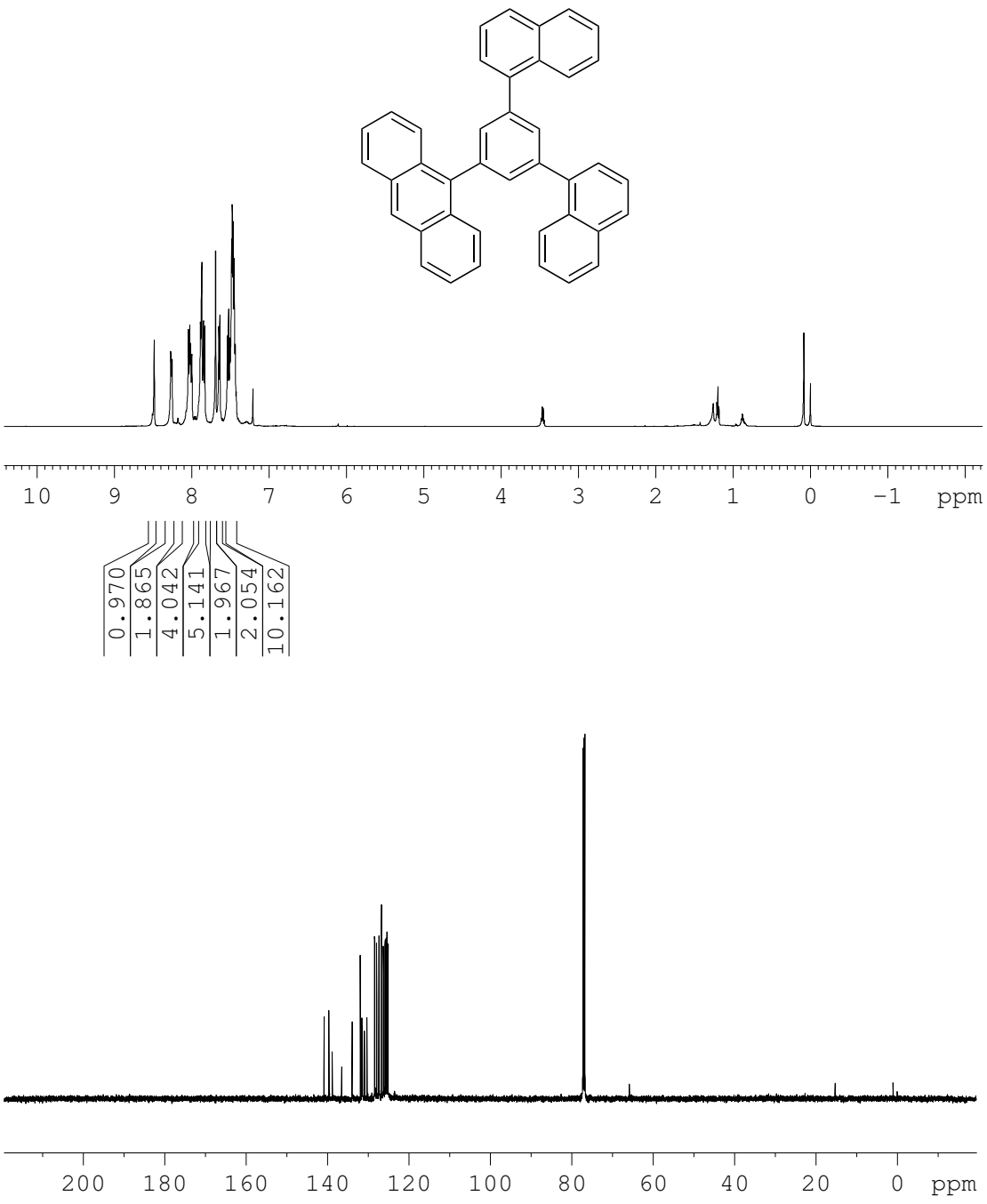


Fig. S4 500 MHz ^{1}H NMR and 125 MHz $^{13}C\{^{1}H\}$ NMR of **d** in $CDCl_3$.

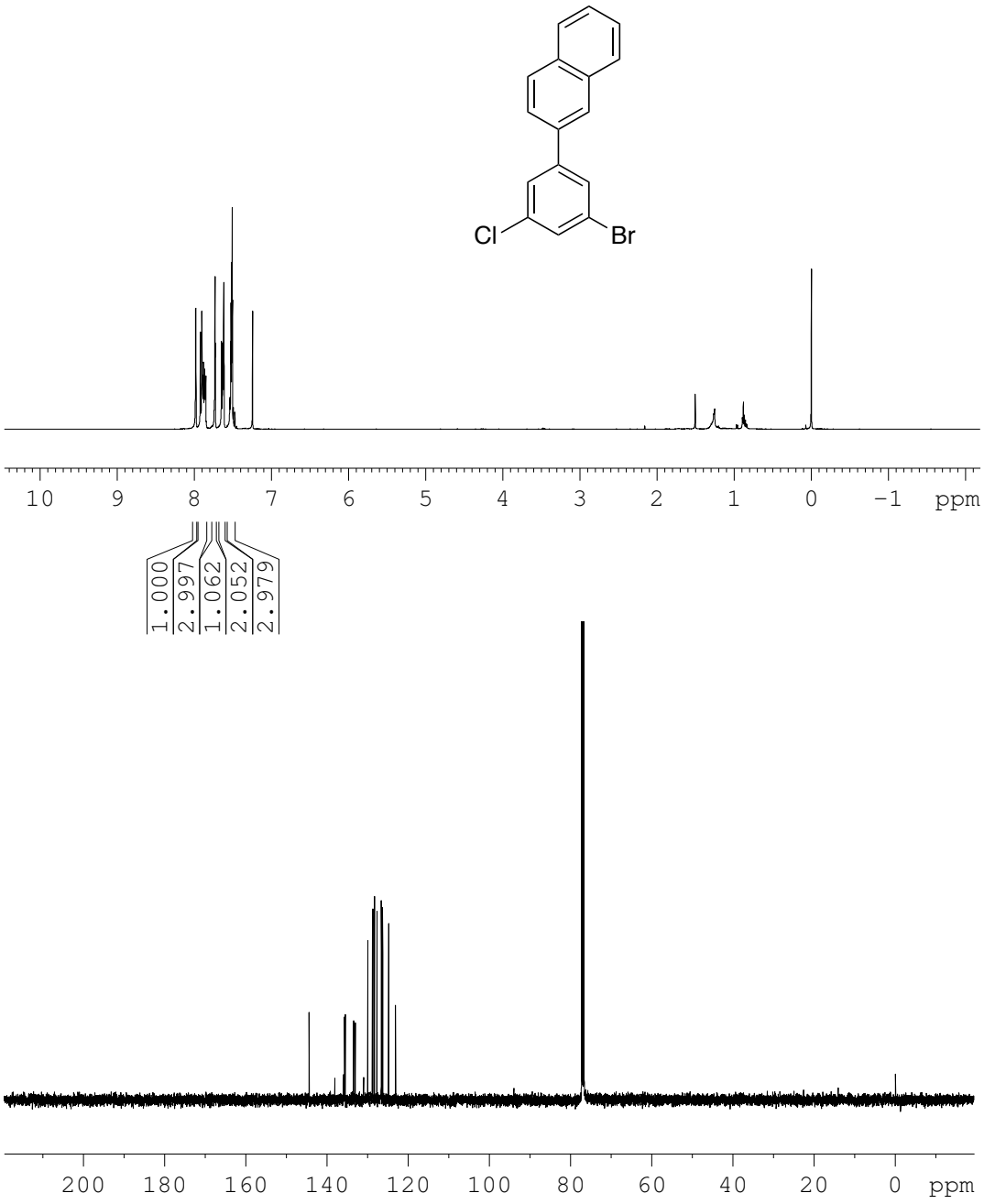


Fig. S5 500 MHz ^{1}H NMR and 125 MHz $^{13}C\{^{1}H\}$ NMR of **e** in $CDCl_3$.

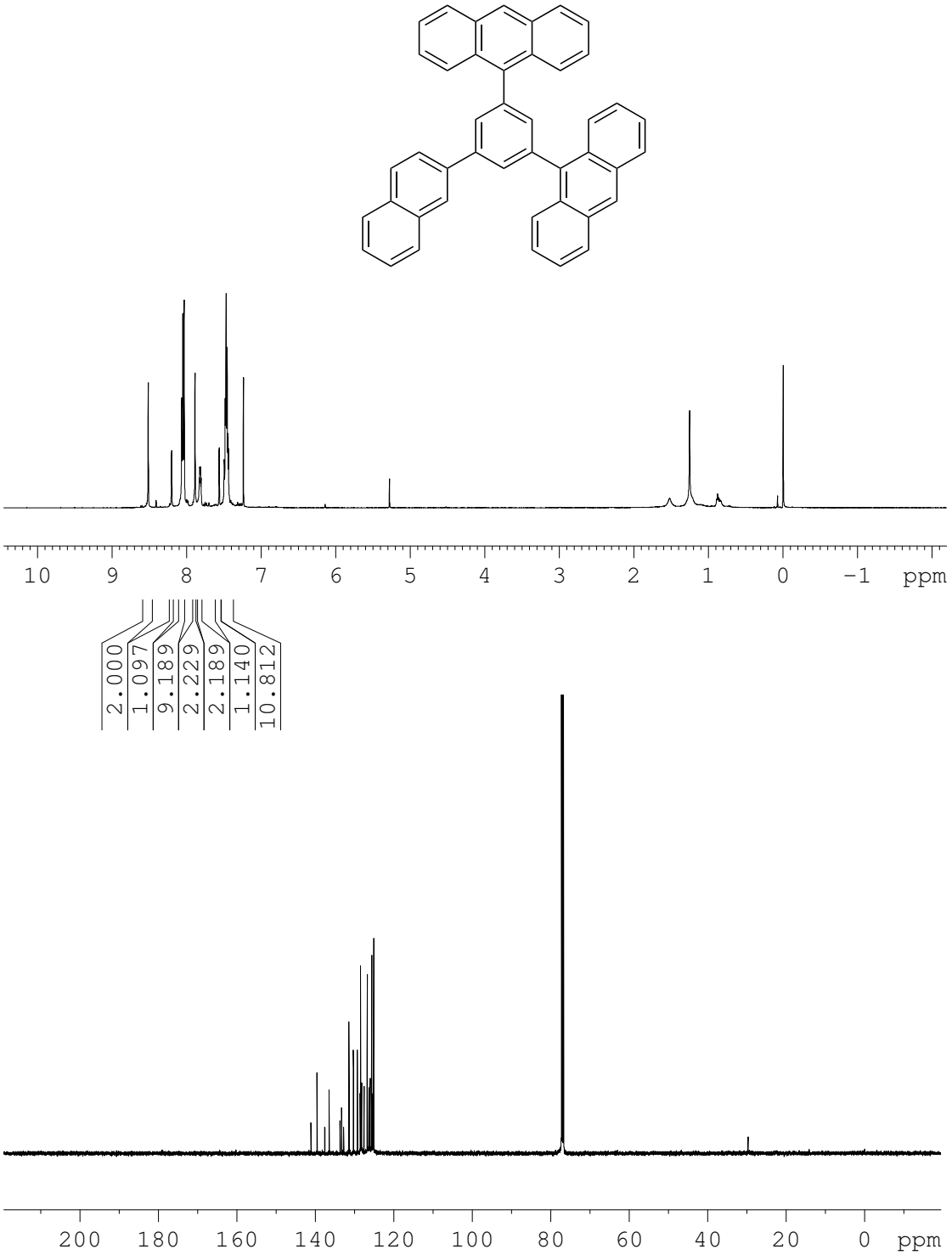


Fig. S6 500 MHz ^{1}H NMR and 125 MHz $^{13}C\{^{1}H\}$ NMR of **f** in $CDCl_3$.

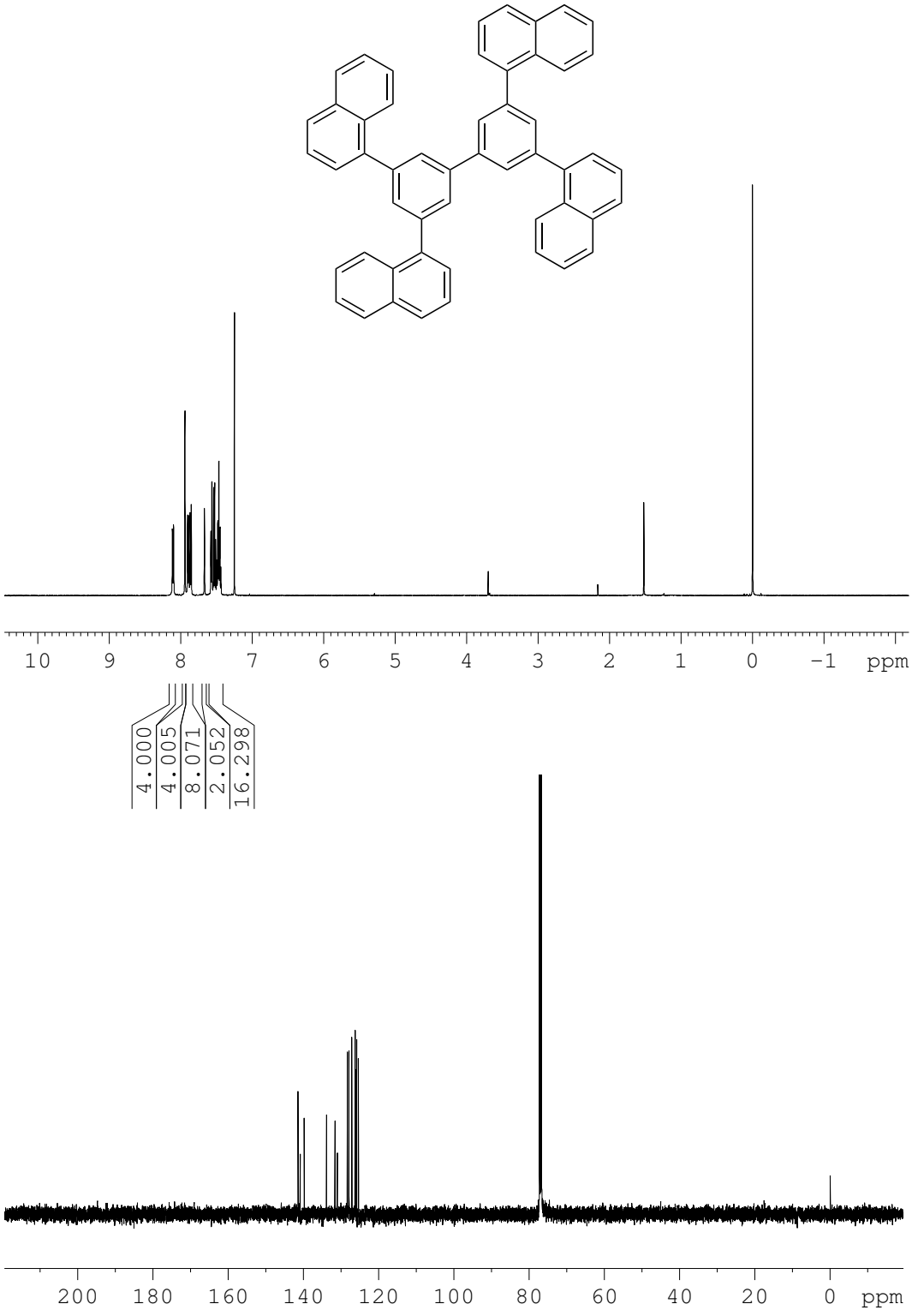


Fig. S7 500 MHz ^{1}H NMR and 125 MHz ^{13}C $\{^{1}$H$\}$ NMR of **g** in $CDCl_3$.

Table S1 Deposition temperatures and film thicknesses for as-deposited glasses of various compounds.

	α,α-P	TNB	α,α-A	β -AA	α,α,α,α –TNBP
T_{dep} (K)	274	323	311	329	340
h (nm)	202	197	193	187	189

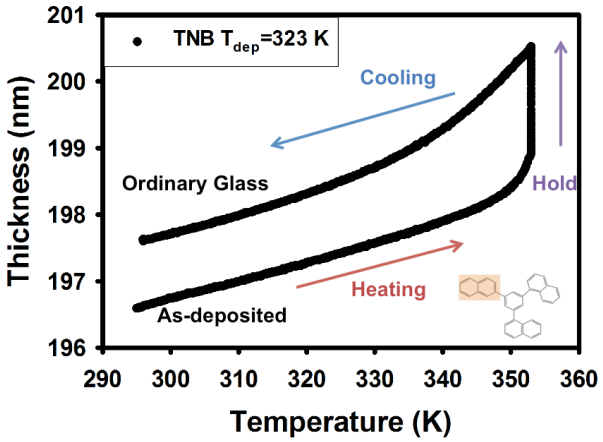


Fig. S8 Transformation by heating of an as-deposited stable glass to ordinary glass of a 197 nm thick film of α,α,β-TNB deposited at 306 K (0.9 T_g).

Details of ellipsometry measurements

Each sample was mounted onto a temperature-controlled stage (Linkam THMSEL350V, temperature range between 77 K to 623 K) using a thermally conductive paste (Arctic Silver Ceramic polysynthetic thermal compound) and was immobilized by two Teflon screws. The temperature during heating/cooling ramps was controlled by the system controller (Linkam PE95/T95). Temperature profiles were written using temperature control and video capture software (Linkam Linksys32). Prior to the experiments, the temperature of the stage was calibrated by measuring the melting point of indium (Sigma Aldrich), and the error was determined to be at most ± 0.6 K. Dilatometry measurements were performed using a spectroscopic ellipsometer (J.A. Woollam spectroscopic ellipsometer M-2000V). The acquisition angle of the incidence was set to 70 degrees and the spectroscopic wavelength range of 500–

1600 nm was chosen. A total of 486 data points in this range were acquired and used for data fitting. The ellipsometer is equipped with a rotating compensator with a frequency of about 20 Hz, and a high-speed CCD detection that allows rapid averaging of the data over a short period of time. An acquisition time of 1 second was chosen with zone averaging enabled to eliminate possible systematic errors due to offsets of the polarizer's angle. As such, the total acquisition time was slightly longer than 1 second. After the initial alignment, focusing optics were attached to reduce the spot size of the beam to 30 µm. Calibrations were the performed on silicon with a thermally grown oxide layer to adjust for the effects of focusing the beam. During measurements, nitrogen gas was flown across the samples to prevent oxidation and water uptake.

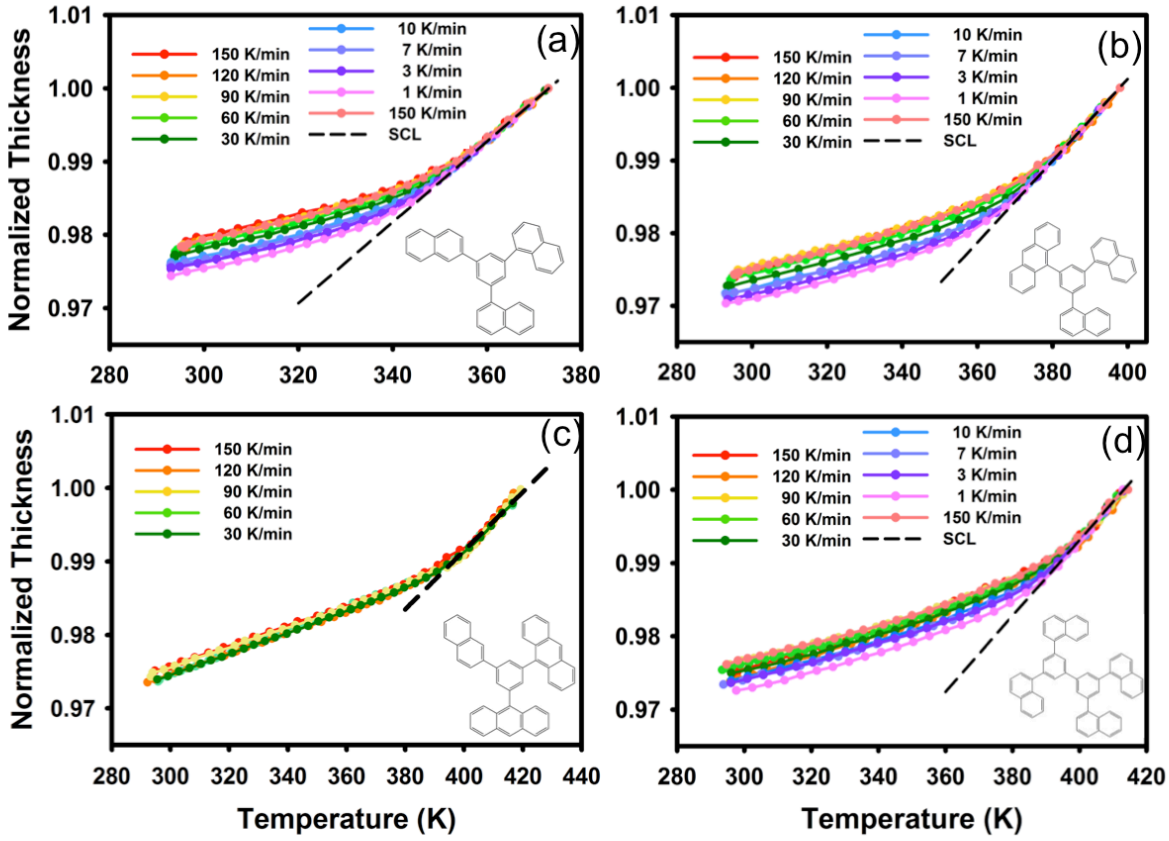


Fig. S9 CR-T_g measurements of 200 nm films of (a) α,α,β-TNB (b) α,α-A, (c) β-AA and (d) α,α,α,α-TNBP. The CR-T_g was measured in the range of 1-150 K/min for all compounds except for α,α-A (only in the limited range of 30-150 K/min) due to rapid crystallization of the film at lower cooling rates. All film thicknesses are normalized to the thickness of the corresponding SCL before the beginning of the cooling ramps.

Due to fast crystallization near its T_g, the cooling rate data on β-AA were gathered from 3 different samples. The last cooling ramp performed on each sample deviated from the previous ones due to prior heating above T_g, but the expansion coefficients were within experimental error. If significant crystallization happened, the slope of the curve in the glassy regime would deviate significantly from other ramps and that data set would not be used.

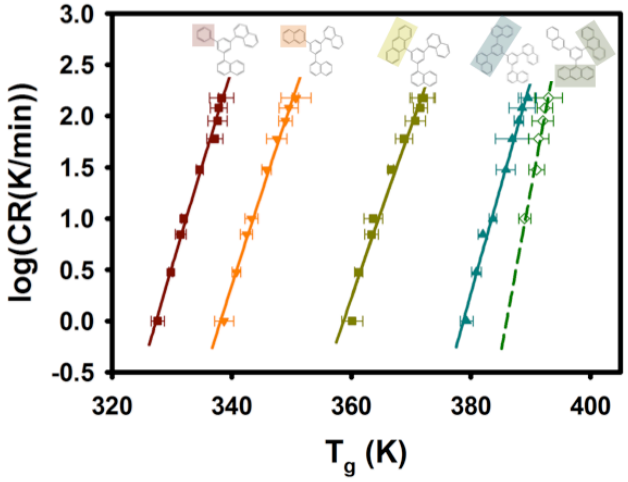


Fig. S10 Log (cooling rate) as a function of T_g; α,α-P (red); TNB (orange); α,α-A (yellow); β-AA (open green); α,α,α,α-TNBP(cyan). Dash and solid lines are reciprocal fits.

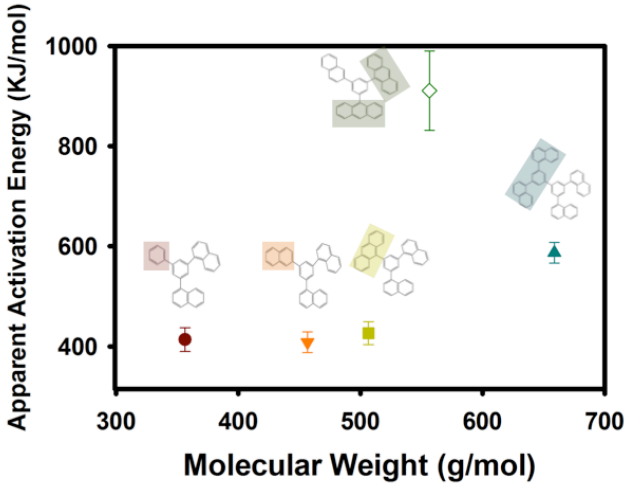


Fig. S11 Apparent activation energy of ~200 nm α,α-P (red); TNB (orange); α,α-A (yellow); β-AA (open green); α,α,α,α-TNBP(cyan).

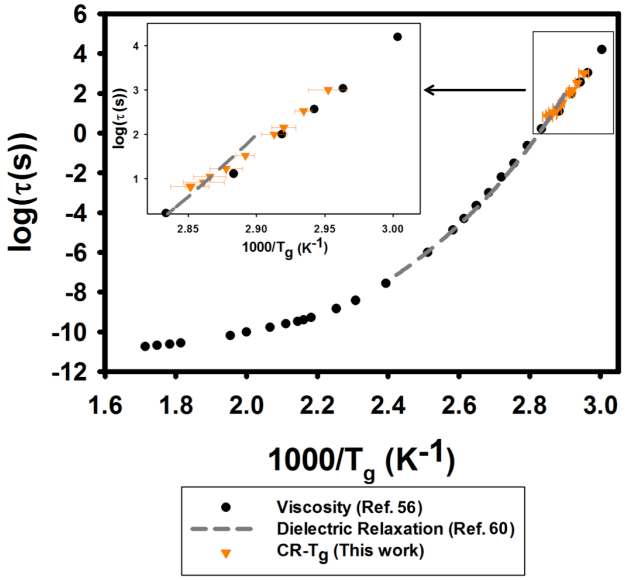


Fig. S12 Relaxation time of α,α,β-TNB probed by viscosity measurement (black dots),[7–9] dielectric relaxation measurement (grey dashed lines)[10] and CR-T_g measurement (orange triangles). Inset shows an expanded image in the temperature range where all three data sets overlap. In order to generate this plot, it was assumed that a cooling rate of 10 K/min corresponds to a relaxation time of 100 seconds and a viscosity of 10^{11} $\mathbf{g/(cm \cdot s)}$. The data was vertically shifted according to this assumption without further adjustment.

Calculation of the expansion coefficient

Values of thermal expansion coefficients were calculated using the following equation.

$$\boldsymbol{\alpha = \frac{1}{h}\frac{dh}{dT}}$$

Where α is the expansion coefficient, h is the film thickness at T equals to the mid point of the fitting range, $\frac{1}{2}\boldsymbol{(275 + T_g)K}$ for glassy region (α(G)) and $\boldsymbol{T_g + 25K}$ for SCL region (α(SCL)). Error bars were determined by the standard deviation of the fittings at different cooling rates.

References

1. P. A. Bonvallet, C. J. Breitkreuz, Y. S. Kim, E. M. Todd, K. Traynor, C. G. Fry, M. D. Ediger, and R. J. McMahon, *J. Org. Chem.*, 2007, **72**, 10051–7.

2. A. Ford, E. Sinn, and S. Woodward, *J. Organomet. Chem.*, 1995, **493**, 215–220.

3. J. Huang, J.-H. Su, X. Li, M.-K. Lam, K.-M. Fung, H.-H. Fan, K.-W. Cheah, C. H. Chen, and H. Tian, *J. Mater. Chem.*, 2011, **21**, 2957.

4. G. B. Heisig, *J. Am. Chem. Soc.*, 1928, **50**, 139–145.

5. J. Gilbert and S. Martin, *Experimental Organic Chemistry*, Thomson Brook/Cole, Belmont, CA, 4th edn., 2006.

6. K. L. Billingsley, T. E. Barder, and S. L. Buchwald, *Angew. Chem. Int. Ed. Engl.*, 2007, **46**, 5359–63.

7. J. H. Magill and D. J. Plazek, *J. Chem. Phys.*, 1967, **46**, 3757.

8. C. M. Whitaker and R. J. McMahon, *Magill in 1958 and Plazek in 1966 misidentified ααβ-TNB as ααα-TNB*.

9. C. M. Whitaker and R. J. McMahon, *J. Phys. Chem.*, 1996, **100**, 1081–1090.

10. R. Richert, K. Duvvuri, and L. T. Duong, *J. Chem. Phys.*, 2003, **118**, 1828–1836.