Supporting Information

for

Line Tension and Line Activity in Mixed Monolayers Composed of Aliphatic and Terphenyl-Containing Surfactants

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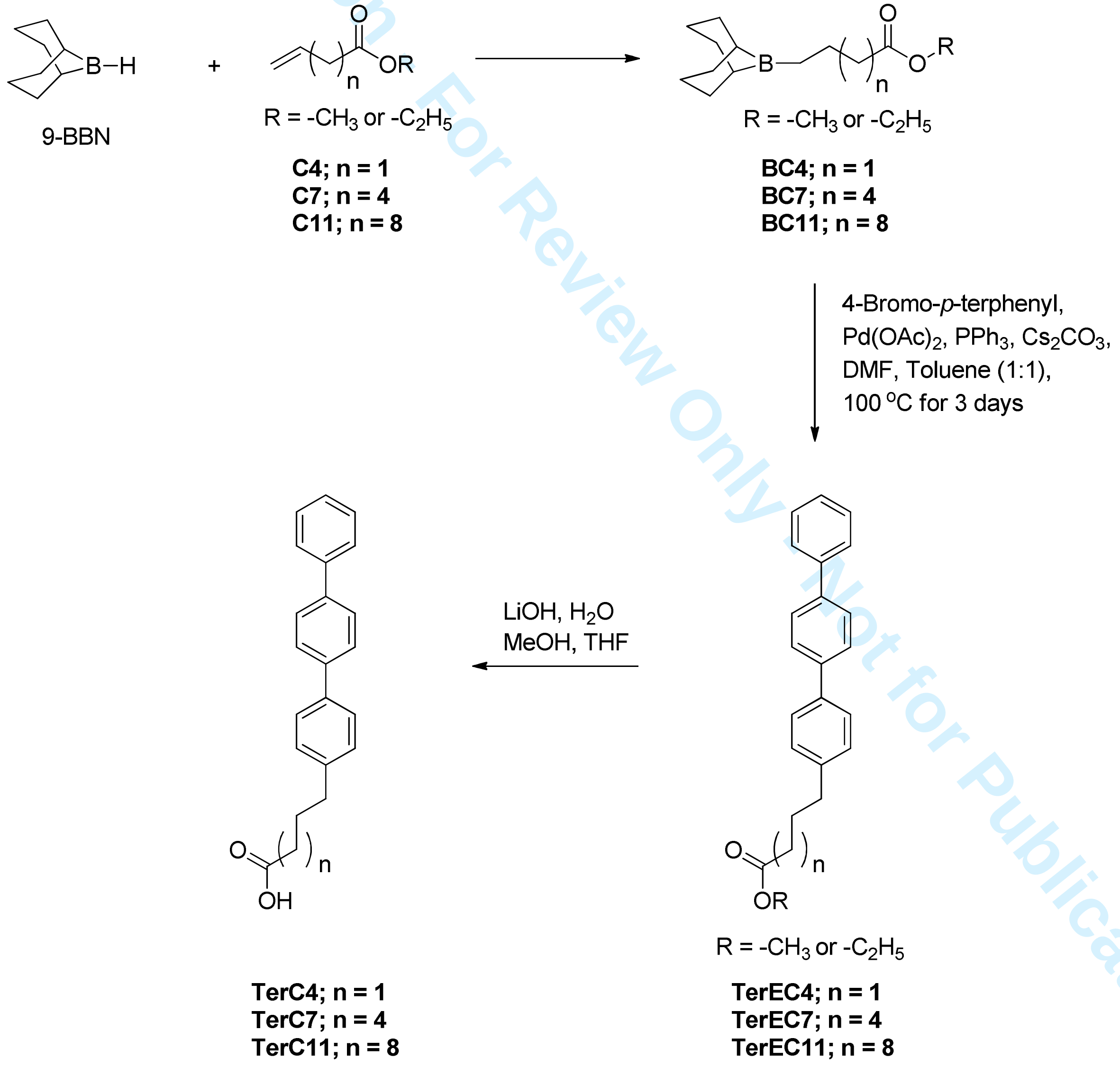
Materials

The starting material 4-bromo-*p*-terphenyl (>94%) was purchased from TCI America, pentadecanoic acid (**PDA**, ≥99.5%) was purchased from Fluka, and *p*-terphenyl-4-carboxylic acid (**Ter**, 97%), 9-borabicyclo[3.3.1]nonane (9-BBN) solution (0.5 M in THF), cesium carbonate (Cs_2CO_3, 99%), palladium(II) acetate ($Pd(OAc)_2$, reagent grade, 98%), triphenylphosphine (PPh_3, 99%), methyl 3-butenoate (95%), ethyl 6-heptenoate (98%) and methyl 10-undecenoate (99%) were purchased from Sigma-Aldrich. All chemicals were used without further purification.

*Synthesis of **TerC4**, **TerC7**, and **TerC11***

We synthesized **TerC4**, **TerC7**, and **TerC11** using Suzuki coupling as a key step followed by hydrolysis of the Suzuki products with aqueous base (see Scheme S1).

Scheme S1. Illustration of the Strategy Used to Prepare **TerC4**, **TerC7**, and **TerC11**



Methyl 4-(9-borabicyclo[3.3.1]nonan-9-yl)butanoate (**BC4**). This intermediate was prepared by adding 1.0 g (10 mmol) of methyl 3-butenoate to 1.2 g (9.8 mmol) of 9-borabicyclo[3.3.1]nonane (9-BBN). The mixture was stirred at room temperature for 3 h, and the crude borane adduct was used immediately in the next step.

Methyl 4-([1,1':4',1''-terphenyl]-4-yl)butanoate (**TerEC4**). A two-necked round-bottomed flask was cleaned and dried in the oven at >100 °C for at least 4 h before cooling to rt under nitrogen. An aliquot (1.48 g; 4.79 mmol) of 4-bromo-*p*-terphenyl was added to the flask together with 15 mL (7.2 mmol) of **BC4** and 4.70 g (14.4 mmol) of Cs_2CO_3. The mixture was placed under vacuum and then purged with nitrogen for 3 cycles before adding a 200 mL mixture of 1:1 v:v dimethylformamide (DMF):toluene. After the mixture was placed under vacuum and purged with nitrogen for 3 cycles again to remove oxygen, 0.22 g (0.98 mmol) of $Pd(OAc)_2$ and 0.75 g (2.9 mmol) of PPh_3 were immediately added under nitrogen. The reaction was stirred at 100 °C for 3 d and then cooled to rt. The resulting mixture was filtered through a celite pad and was washed with dichloromethane (3 × 50 mL). The organic phase was evaporated and the crude product was recrystallized with dichloromethane (DCM) and MeOH (1:1) to obtain 0.75 g (2.3 mmol, 47% yield) of **TerEC4** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61–7.77 (m, 6H), 7.54–7.69 (m, 2H), 7.42–7.49 (m, 2H), 7.32–7.38 (m, 1H), 7.24–7.29 (m, 2H), 3.67 (s, 3H), 2.70 (t, J = 8.0 Hz, 2H), 2.37 (t, J = 8.0 Hz, 2H), 2.00 (quin, J = 8.0 Hz, 2H).

4-([1,1':4',1''-terphenyl]-4-yl)butanoic acid (**TerC4**). An aliquot of **TerEC4** (0.75 g; 2.3 mmol) was added to LiOH (0.17 g; 7.1 mmol) in MeOH (4.6 mL), THF (4.6 mL), and water (4.6 mL). After the reaction was refluxed overnight, the reaction was cooled to rt, and the volatiles were evaporated. Water (20 mL) was added to dissolve the residue, and 6 N HCl was added to adjust the pH of the resultant aqueous phase to a value of 2. The mixture was then extracted with DCM (3 × 20 mL), and the layers were separated. The organic phase was dried with Na_2SO_4, filtered, and evaporated to afford the crude product. After recrystallization from DCM, 0.60 g (1.9 mmol; 83% yield) of a pale yellow solid was obtained (**TerC4**). ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.11 (s, 1H), 7.70–7.79 (m, 6H), 7.63–7.66 (m, 2H), 7.46–7.53 (m, 2H), 7.35–7.40 (m, 1H), 7.28–7.33 (m, 2H), 2.64 (t, J = 5.0 Hz, 2H), 2.26 (t, J = 5.0 Hz, 2H), 1.85 (quin, J = 5.0 Hz, 2H). ^{13}C-NMR (400 MHz, DMSO-d_6): δ 174.84, 141.54, 140.16, 139.40, 137.68, 129.53, 128.02, 127.69, 127.51, 127.08, 127.04, 34.55, 33.61, 26.77. IR (neat): 3150–2700 (br), 2922, 1688, 1484, 759, 690. HRMS (ESI): m/z Calcd for $C_{22}H_{20}O_2$ $[M+Na]^+$: 339.1356; Found: 339.1357.

The compounds **BC7**, **TerEC7**, **TerC7**, **BC11**, **TerEC11**, and **TerC11** were prepared as described above, respectively, but involving the starting materials, amounts, and characterization data provided below.

Ethyl 7-(9-borabicyclo[3.3.1]nonan-9-yl)heptanoate (**BC7**). This intermediate was prepared by adding 0.50 g (3.2 mmol) of ethyl 6-heptenoate and 0.43 g (3.5 mmol) of 9-BBN to give the crude borane adduct.

Ethyl 7-([1,1':4',1''-terphenyl]-4-yl)heptanoate (**TerEC7**). The indicated quantities of 4-bromo-*p*-terphenyl (1.0 g; 3.2 mmol), **BC7** (1.98 g; 7.49 mmol), Cs_2CO_3 (2.90 g; 8.90 mmol), $Pd(OAc)_2$ (0.13 g; 0.58 mmol), and PPh_3 (0.46 g; 1.8 mmol) were used to prepare **TerEC7** as a white solid (0.55 g; 1.4 mmol; 44% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.62–7.67 (m, 6H), 7.54–7.58 (m, 2H), 7.42–7.50 (m, 2H), 7.33–7.38 (m, 1H), 7.24–7.28 (m, 2H), 4.12 (q, J = 5.0, 2H), 2.65 (t, J = 10.0 Hz, 2H), 2.30 (t, J = 10.0 Hz, 2H), 1.60–1.70 (m, 4H), 1.34–1.43 (m, 4H), 1.25 (t, J = 5.0 Hz, 3H).

7-([1,1':4',1''-terphenyl]-4-yl)heptanoic acid (**TerC7**). The indicated quantities of **TerEC7** (0.55 g; 1.4 mmol), LiOH (0.15 g; 6.3 mmol) in MeOH (5 mL), THF (5 mL) and water (5 mL) were used to give **TerC7** as a white solid (0.48 g; 1.3 mmol; 94% yield). ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.00 (s, 1H), 7.70–7.77 (m, 6H), 7.61–7.65 (m, 2H), 7.46–7.51 (m, 2H), 7.35–7.40 (m, 1H), 7.27–7.32 (m, 2H), 2.61 (t, J = 5.0 Hz, 2H), 2.20 (t, J = 5.0 Hz, 2H), 1.54–1.64 (m, 2H), 1.45–1.54 (m, 2H), 1.27–1.35 (m, 4H). ^{13}C-NMR (500 MHz, DMSO-d_6): δ 175.04, 142.29, 140.18, 139.63, 139.36, 137.48, 129.52, 129.47, 128.01, 127.68, 127.49, 127.07, 126.96, 35.24, 34.18, 31.34, 28.95, 28.91, 24.99. IR (neat): 3150–2750 (br), 2922, 1696, 1485, 759, 690. HRMS (ESI): m/z Calcd for $C_{25}H_{26}O_2$ $[M+Na]^+$: 381.1825; Found: 381.1829.

Methyl 11-(9-borabicyclo[3.3.1]nonan-9-yl)undecanoate (**BC11**). This intermediate was prepared by adding 1.01 g (5.09 mmol) of methyl 10-undecenoate and 0.63 g (5.2 mmol) of 9-BBN to give the crude borane adduct.

Methyl 11-([1,1':4',1''-terphenyl]-4-yl)undecanoate (**TerEC11**). The indicated quantities of 4-bromo-1,1':4',1''-terphenyl (0.88 g; 2.8 mmol), **BC11** (1.80 g; 5.62 mmol), Cs_2CO_3 (3.10 g; 9.51 mmol), $Pd(OAc)_2$ (0.13 g; 0.58 mmol), and PPh_3 (0.46 g; 1.8 mmol) were used to prepare **TerEC11** as a white solid (0.40 g; 0.93 mmol, 33% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.62–7.67 (m, 6H), 7.54–7.58 (m, 2H), 7.42–7.50 (m, 2H), 7.43–7.49 (m, 2H), 7.33–7.38 (m, 1H), 7.25–7.28 (m, 2H), 3.66 (s, 3H), 2.65 (t, J = 5.0 Hz, 2H), 2.30 (t, J = 5.0 Hz, 2H), 1.58–1.68 (m, 4H), 1.18–1.36 (m, 12H).

11-([1,1':4',1''-terphenyl]-4-yl)undecanoic acid (**TerC11**). The indicated quantities of **TerEC11** (0.395 g; 0.922 mmol), LiOH (0.206 g; 8.60 mmol) in MeOH (5 mL), THF (5 mL) and water (5 mL) were used to give **TerC11** as a pale yellow solid (0.330 g; 0.796 mmol; 87% yield). ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.94 (s, 1H), 7.70–7.77 (m, 6H), 7.61–7.65 (m, 2H), 7.46–7.51 (m, 2H), 7.35–7.40 (m, 1H), 7.27–7.32 (m, 2H), 2.61 (t, J = 5.0 Hz, 2H), 2.18 (t, J = 5.0 Hz, 2H), 1.55–1.64 (m, 2H), 1.43–1.57 (m, 2H), 1.21–1.34 (m, 12H). ^{13}C-NMR (500 MHz, DMSO-d_6): δ 175.05, 142.19, 139.64, 139.36, 137.47, 129.53, 129.47, 128.01, 127.69, 127.49, 127.08, 126.95, 35.30, 34.19, 31.47, 29.49, 29.44, 29.38, 29.27, 29.23, 29.08, 25.03. IR (neat): 3250–2750 (br), 2918, 1697, 1485, 760, 689. HRMS (ESI): m/z: Calcd for $C_{29}H_{34}O_2$ $[M+Na]^+$: 437.2451; Found: 437.2448.