

Preparation and Properties of Polymer-Wrapped Single-Walled Carbon Nanotubes**

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1: A solution of hydroquinone (6.5 g, 59 mmol), 1-chlorooctane (20 mL, 118 mmol), and K_2CO_3 (32.6 g, 236 mmol) in DMF (240 mL) was heated for 5 d at 90°C. The product was isolated by extraction with light petroleum, washed with H_2O , dried over Na_2SO_4 , and evaporated to afford **1** as white solid (14 g, 71%). M.p. 56-57°C (light petroleum); 1H NMR (360 MHz, $CDCl_3$): δ = 6.82 (s, 1H), 3.89 (t, J = 6.6 Hz, 2H), 1.75 (p, J = 6.7 Hz, 2H), 1.44 (p, J = 6.7 Hz, 2H), 1.31-1.28 (m, 8H), 0.88 (t, J = 6.6 Hz, 3H); ^{13}C NMR (90 MHz, $CDCl_3$): δ = 153.2, 115.4, 68.7, 31.8, 29.4, 29.2, 26.0, 22.6, 14.1.

2: 1,4-Bis(octyloxy)benzene (**1**) (9.5 g, 28 mmol) was added to a mixture of dioxane (80 mL), 37% aqueous formaldehyde solution (17 mL) and conc. hydrochloric acid (12 mL), saturated with hydrogen chloride. The mixture was kept at 60-70° C with continuous introduction of HCl for 9 h. After cooling, ice/water (300 mL) was added and the precipitate was filtered off. Crystallization from light petroleum yielded 1,4-bis(chloromethyl)-2,5-dioctyloxybenzene (**2**) as colorless needles (9.4 g, 77%). M.p. 80°C; 1H NMR (360 MHz, $CDCl_3$): δ = 6.91 (s, 1H), 4.63 (s, 2H), 3.98 (t, J = 6.5 Hz, 2H), 1.80 (p, J = 6.5 Hz, 2H), 1.48

(p, $J = 6.5$ Hz, 2H), 1.35-1.29 (m, 8H), 0.89 (t, $J = 6.5$ Hz, 3H); ^{13}C NMR (90 MHz, CDCl_3): $\delta = 150.6, 127.0, 114.3, 69.1, 41.3, 31.8, 29.3, 26.0, 22.6, 14.1$; EI-MS: 430.2-432.2 $[\text{M}]^+$; calcd for $\text{C}_{24}\text{H}_{40}\text{Cl}_2\text{O}_2$ (431.5): C 66.81, H 9.34; found: C 66.73, H 9.56.

3: A mixture of **2** (1.45 g, 3.36 mmol) and triphenylphosphine (2.69 g, 10 mmol) in anhydrous DMF (20 mL) was heated under reflux for 3 d. The resulting solution was added dropwise into Et_2O (100 mL) to precipitate out the product. The white precipitates (2.66 g, 83%) were collected via filtration and dried under vacuum. M.p. $> 200^\circ\text{C}$; ^1H NMR (360 MHz, CDCl_3): $\delta = 7.75\text{-}7.73$ (m, 3H), 7.66-7.63 (m, 12H), 6.68 (s, 1H), 5.34 (d, $J = 12.7$ Hz, 2H), 2.99 (t, $J = 5.8$ Hz, 2H), 1.32-1.19 (m, 5H), 1.13-1.04 (m, 5H), 0.90 (t, $J = 6.7$ Hz, 3H); ^{13}C NMR (90 MHz, CDCl_3): $\delta = 150.4, 134.7, 134.2, 134.14, 134.09, 130.0, 129.95, 129.88, 118.5, 117.5, 116.3, 115.8, 67.8, 31.7, 29.2, 29.1, 28.6, 25.7, 22.5, 14.0$.

4: A 5% NaOEt in EtOH solution (2.8 g, 6 mmol) was added dropwise to a solution of **3** (1.91 g, 2 mmol) and isophthalaldehyde (0.27 g, 2 mmol) in a mixture of anhydrous EtOH (20 mL) and THF (20 mL) at ambient temperature. The reaction mixture was stirred for additional 24 h. The resulting polymer was precipitated twice from MeOH and then dried to afford **4** (0.55 g, 60%) as yellow resin. ^1H NMR (360 MHz, CDCl_3): $\delta = 7.60\text{-}7.30$ (m, 6H), 7.20-6.50 (m, 4H), 4.09 (t, $J = 6.5$ Hz, 2H (*trans* fragment)), 3.51-3.49 (m, 2H (*cis* fragment)), 1.90 (p, $J = 6.5$ Hz, 2H), 1.56 (br, 2H), 1.25 (m, 8H), 0.86 (br, 3H).

PmPV: A sample of **4** (0.55 g) and I_2 (0.002 g) were refluxed in PhMe (20 mL) for 4h. The solvent and iodine were evaporated off under reduced pressure and the product was dissolved

in CHCl_3 and precipitated out with MeOH. The resulting precipitate was dried to afford PmPV as yellow resin (0.5 g). ^1H NMR (360 MHz, CDCl_3): $\delta = 7.64$ (s, 1H), 7.55-7.46 (m, 4H), 7.37 (t, $J = 7.5$ Hz, 1H), 7.21 (s, 1H), 7.16 (s, 3H), 4.09 (t, $J = 6.5$ Hz, 2H), 1.90 (p, $J = 6.5$ Hz, 2H), 1.55 (p, $J = 6.5$ Hz, 2H), 1.35 (m, 8H), 0.87 (t, $J = 6.5$ Hz, 3H); ^{13}C NMR (90 MHz, CDCl_3): $\delta = 151.0, 138.3, 128.5, 126.9, 125.7, 124.0, 111.1, 69.8, 31.8, 29.4, 26.3, 22.7, 14.1$; calcd for $\text{C}_{32}\text{H}_{44}\text{O}_2$ (460.7): C 83.43, H 9.63; found: C 82.59, H 9.72.

The lower molecular weight polymer corresponding to **4** made by using 3% excess of isophthalaldehyde in the preparation of PmPV. The molecular weights and polydispersity (PDI) of PmPV ($M_w=340,000$; PDI=1.9 and $M_w=19,000$; PDI=1.6) were determined in THF by using size exclusion chromatography (SEC) equipped with a UV detector. The SEC system was calibrated by using polystyrene standards prior to use. The number-average degree of polymerization was estimated to be $n \approx 380$ and $n \approx 25$ using M_n and the molecular weight of the repeating unit (460). The degree of polymerization of lower molecular weight polymer was confirmed by NMR end-group analysis.