separations

Supplementary Materials

Enhancement of Thermal Stability and Selectivity by Introducing Aminotriazine Comonomer to Poly(Octadecyl Acrylate)-Grafted Silica as Chromatography Matrix

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Experimental

Preparation

Immobilization of MPS onto Silica

Dried silica gel (3.50 g) was placed to a dried flask and dispersed in dry toluene (25 mL). Then MPS (1.20 g, 6.11 mmol) was added and the dispersed mixture was refluxed for 72 h. The suspension was filtered and the solid was washed with toluene, methanol, water, methanol and diethyl ether successively to obtain the MPS-modified silica (Sil-MPS) as shown in Figure 1. After drying the particles were characterized by elemental analysis.

Immobilization of ODA and AT copolymer onto Silica

To a reaction flask containing Sil-MPS (3.50 g) a mixture of ODA (4.65 g, 14.32 mmol), AT (1.96 g, 14.32 mmol), 100 mg of radical initiator AIBN and dimethyl sulfoxide (DMSO) (10 mL) was added. The polymerization mixture was gently stirred for 6 h at 70 °C. Then the reaction mixture was filtered and washed successively with DMSO, chloroform, and methanol to obtain Sil-ODA_5-AT_5. Another reaction was carried out using to same procedure only changing monomer molar ratio (ODA:AT=10:1) to get Sil-ODA_{10}-AT_1.

Calculation

The ODA contents in Sil-ODA_{10}-AT_1 and Sil-ODA_5-AT_5 were calculated from elemental analyses (EA) result showed in Table 1 in the manuscript with the following values.

	Rational formula	Molecular weight of a unit	Carbon wt % for a unit
MPS moiety in Sil-MPS	C3H7S	75.1	47.9
AT unit in copolymer	C5H7N5	137.1	43.8
ODA unit in copolymer	C21H40O2	324.3	77.7

Step 1. Calculation of the amount of carbon originates from MPS moiety (C_{MPS}) in prepared stationary phase based on the obtained C% in Sil-MPS (from Table 1).

$$C_{MPS}\ [g/1g\ Sil\text{-}MPS] = (C\%\ in\ Sil\text{-}MPS\ /100) \times 1 \quad (1)$$

Step 2. Calculation of the amount of carbon originates originates from AT moiety (C_{AT}) in prepared stationary phase.

$$\text{Theoretical C/N value of AT} = \frac{\text{Atomic weight of carbon} \times \text{The number of carbon in AT unit}}{\text{Atomic weight of nitrogen} \times \text{The number of nitrogen in AT unit}} = \boldsymbol{X} \quad (2)$$

$$\text{Carbon \% from AT} = \boldsymbol{X} \times \text{Nitrogen \% obtained by elemental analysis} = \boldsymbol{Y} \quad (3)$$

$$C_{AT}\ [g/1g\ Sil\text{-}ODA_x\text{-}AT_y] = (\boldsymbol{Y}/100) \times 1 \quad (4)$$

Step 3. Calculation of the amount of carbon originates from ODA moiety (C_{ODA}) in prepared stationary phase.

$$C\%\ obtained\ by\ EA = 100 \times (C_{MPS} + C_{AT} + C_{ODA}) \quad (5)$$

$$C_{ODA}\ [g/1g\ Sil\text{-}ODA_x\text{-}AT_y] = (C\%\ obtained\ by\ EA/100) - (C_{MPS} + C_{AT}) \quad (6)$$

Step 4. Calculation of ODA content [wt %] in Sil-ODA_xAT_y.

$$Contents\ of\ ODA\ [wt\ \%] = 100 \times C_{ODA}/Carbon\ wt\ \%\ for\ a\ unit \quad (7)$$

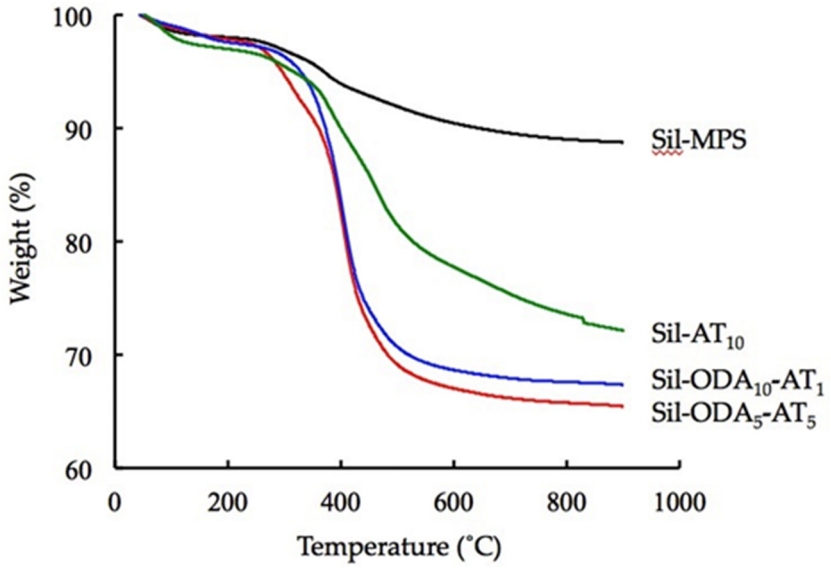

Figure S1. TGA curves of Sil-MPS, Sil-AT10, Sil-ODA10-AT1, and Sil-ODA5-AT5.

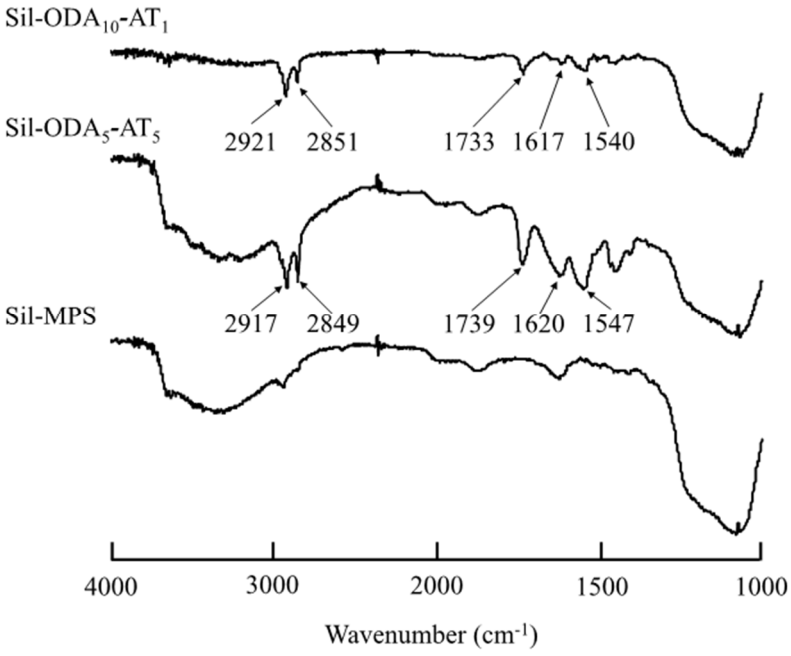

Figure S2. DRIFT spectra of Sil-MPS, Sil-ODA$_5$-AT$_5$ and Sil-ODA$_{10}$-AT$_1$.

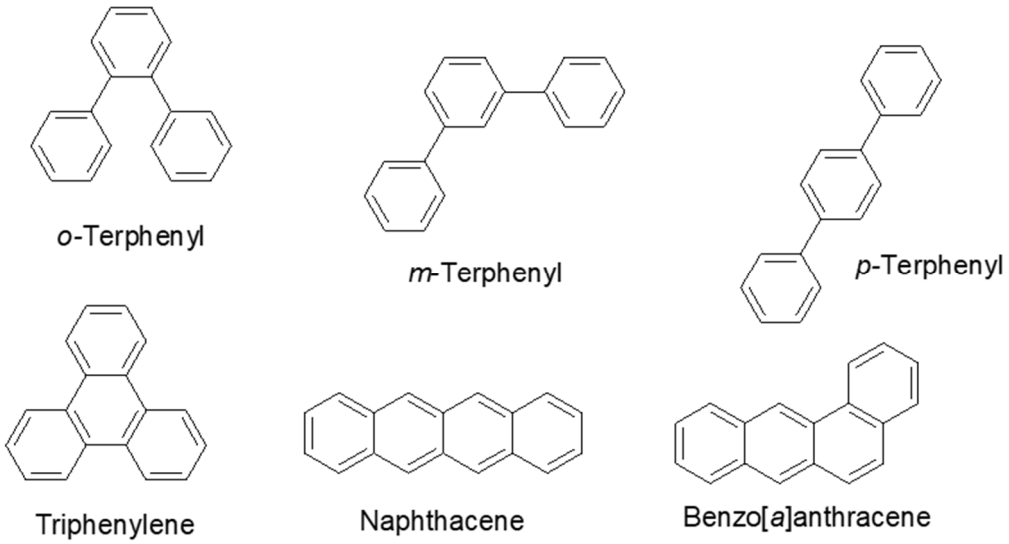

Figure S3. Structures of the studied PAHs.

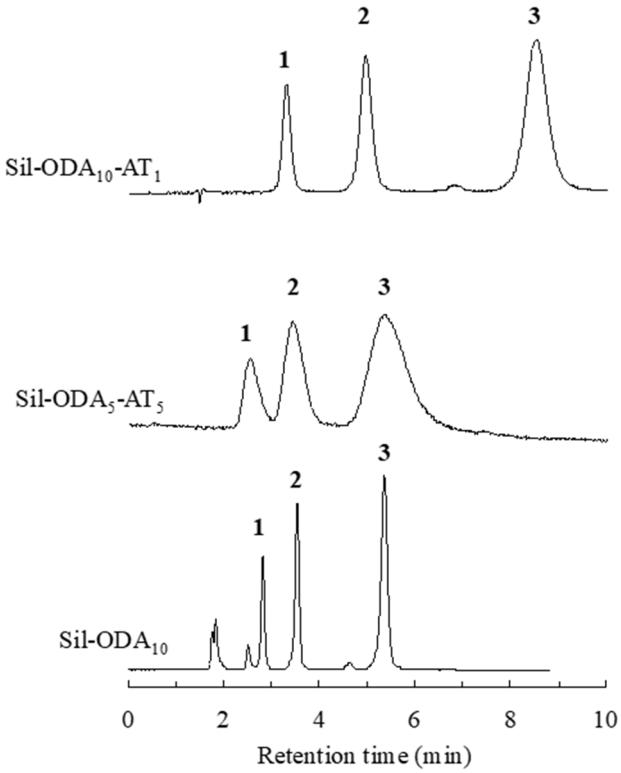

Figure S4. Chromatograms for the separation of *o*-terphenyl, **1**, *m*-terphenyl, **2**, and triphenylene, **3**, on Sil-ODA$_{10}$-AT$_1$, Sil-ODA$_5$-AT$_5$ and Sil-ODA$_{10}$, respectively. Column temperature: 30 °C, Mobile phase: MeOH-H$_2$O (90:10). Flow rate: 1.0 mL min^{-1}.