Supporting Information

Pseudopolyrotaxanes based polyhedral oligomeric silsesquioxanes and cucurbit[7]uril

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Experiment

Materials

γ-Chloropropyltrimethoxysilane was purchased from Shandong Qiquan Silicon Co., Ltd. 1-Methylimidazole was purchased from Aladdin Chemical Reagent Co., Ltd. Glycoluril, paraformaldehyde, glycerol, concentrated hydrochloric acid, methanol, toluene were obtained from Sinopharm Chemical Reagent Beijing Co., Ltd. Methanol was purified by published methods before use. The other regents were used as received. Triply distilled water was used to prepare all the solutions.

Characterization

^{1}H and ^{29}Si NMR spectrums were recorded using a Bruker AV 300 spectrometer in chloroform-d, D_2O or methanol-d. Fourier transform infrared (FT-IR) spectrum was measured with a Nicolet FT-IR spectrometer using anhydrous KBr pellets. Thermogravimetric analysis (TGA) measurement was performed with a METTLER

TOLEDO TGA/DSC-1 thermogravimetric analyzer over temperature range from 25 to 800 ^{o}C at heating rate of 10 ^{o}C/min under nitrogen atmosphere. Before TGA experiment, an isothermal segment was carried out first (125 ^{o}C for 20 min). Powder X-ray Diffraction (XRD) patterns were measured on a Max 2200PC power X-ray diffractometer with Cu-Ka (1.54051 Å) radiation (40 kV, 20 mA). Powder samples were mounted on a sample holder and scanned with a step size of 2 θ = 0.02 ^{o} between 5 ^{o} and 50 ^{o}. Transmission electron microscopy (TEM) experiments were performed with a JEOL JEM-100 CXII (Japan) operating at 80 kV. TEM samples were prepared by dipping a copper TEM grid into the POSS/CB[7] solution and dried at room temperature. The microanalyses of C, H, and N were performed with Elementar Vario EI III.

Preparation of CB[7]

CB[7] was prepared according to the literature [10c].

Preparation of POSS-min-Cl (octaimidazolium-based POSS)

POSS-min-Cl was prepared according to the literature: octakis(3-chloropropyl)octasilsesquioxane (4.0 g, 0.004 mol) and 1-methylimidazole (7.8 g, 0.095 mol) was added to toluene (15 ml) at nitrogen atmosphere with a reflux condenser, then the solution was heated to 90 ^{o}C in an oil bath. After 3 h, the reaction was completed, the liquid descent from and the residual wash with hot toluene and hexane several times. Finally, a transparent product was obtained by dried at 60 ^{o}C in

vacuum. ^{1}H NMR: 7.40, 7.36 ppm (C**H**=C**H**, 2H), 4.15-4.10 ppm (NC**H**$_2$, 2H), 3.82 ppm (C**H**$_3$， 3H), 1.95-1.85 ppm ($CH_2C\mathbf{H}_2CH_2$), 0.56-0.52 ppm ($CH_2CH_2C\mathbf{H}_2$) ^{29}Si NMR: 64.97 ppm. FT-IR (KBr, cm^{-1}): 3102, 2955, 2896, 1640, 1574, 1456, 1130, 762.

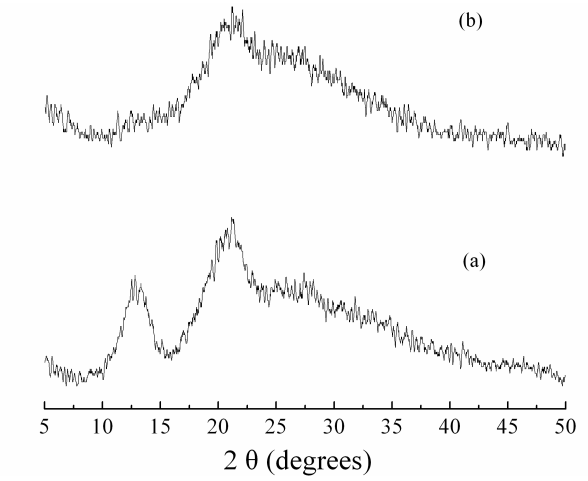

Figure S1 X-ray diffraction of (a) CB[7], (b) POSS/CB[7]

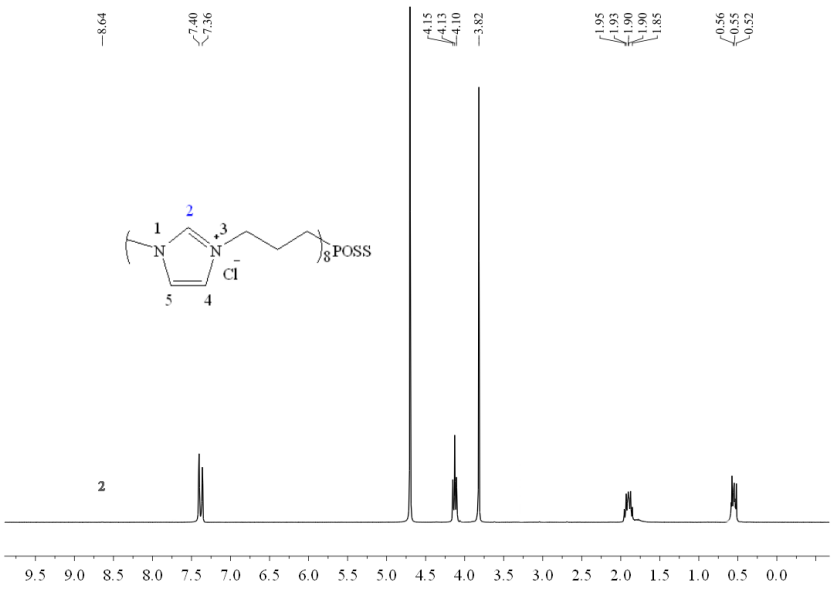

Figure S2 ^{1}H NMR spectrum of POSS-min-Cl

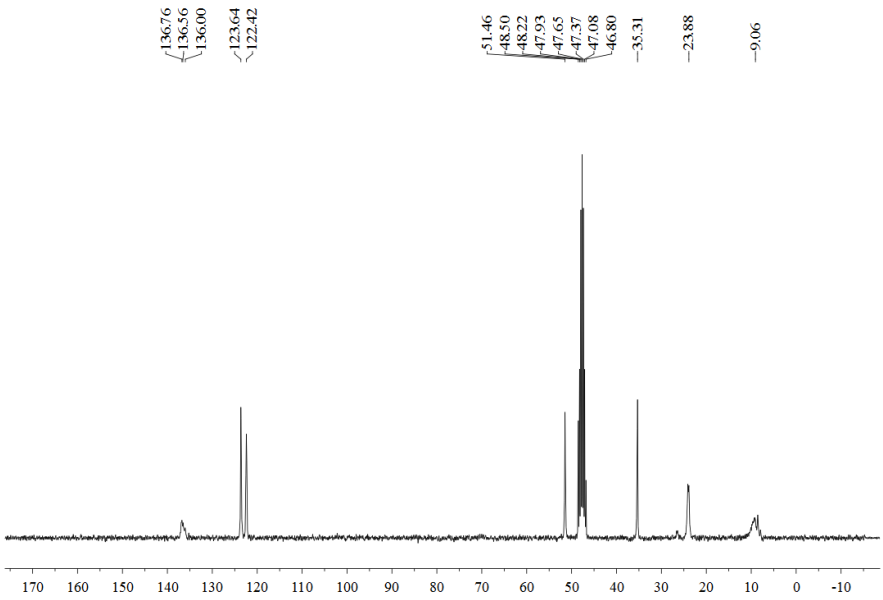

Figure S3 ^{13}C NMR spectrum of POSS-min-Cl

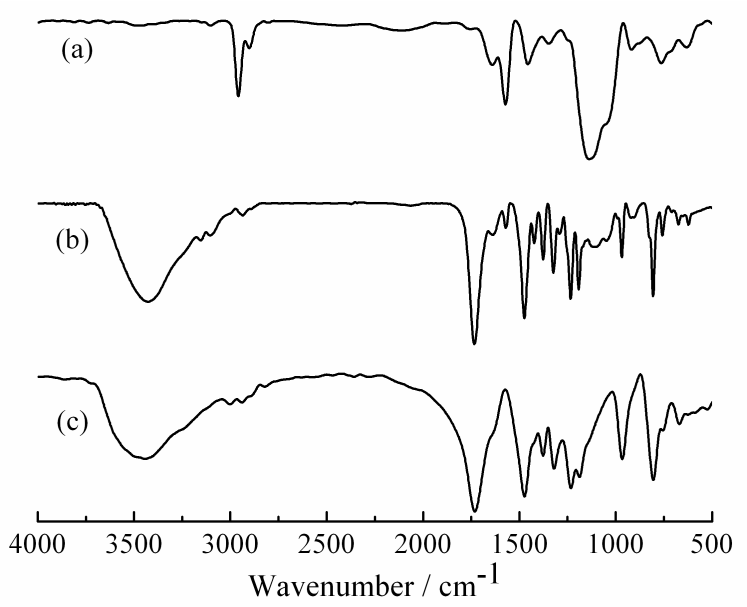

Figure S4 FT-IR spectrum of (a) POSS-min-Cl, (b) POSS/CB[7], (c) CB[7]

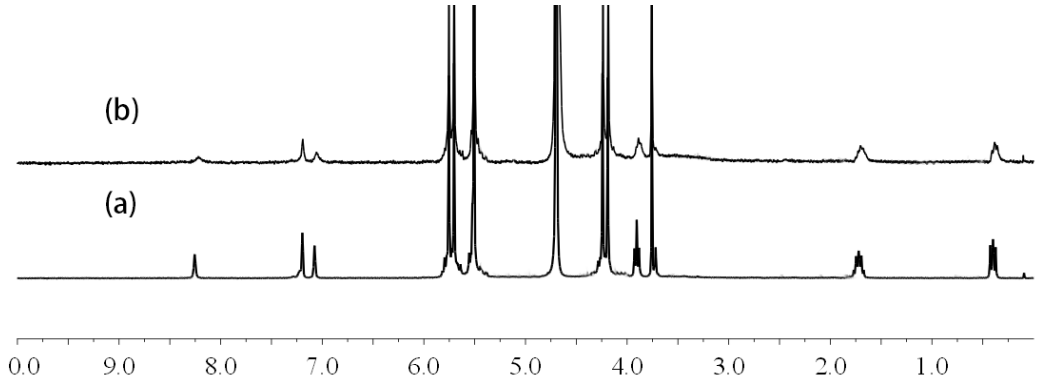

Figure S5 ^{1}H NMR spectra of POSS in the presence of 8 equiv (a) and 9 equiv(b)

Reference

[1] J. Tian, S. Q. Ma, P. K. Thallapally, D. Fowler, B. P. McGraila and J. L. Atwood, Chem. Commun., 2011, **47**, 7626–7628