Electronic Supplementary Information (ESI)

Defection-Selective Solubilization and Chemically-Responsive Solubility Switching of Single-Walled Carbon Nanotubes with Cucurbit[7]uril

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Experimental

Materials. All solvents and reagents were used as supplied except the following. Milli-Q water was used for preparation of aqueous solutions. Hipco Single-Walled Carbon Nanotube (Hipco SWCNT) (d ～ 1 nm) was purchased from Carbon Nanotechnologies, Inc., Texas, USA. CoMoCAT SWCNT (d ～ 0.8 nm) was obtained from Southwest Nanotechnologies, Inc., Norman, OK. CarboLex SWCNT (d ～ 1.3 nm) was purchased from Aldrich.

Measurements. The ^{1}H NMR spectra were recorded at 270 MHz with a JEOL-JNM EX270 spectrometers. UV-Vis absorption spectra were recorded with a JASCO V-630 spectrophotometer. Tapping mode atomic force microscopy (TM-AFM) was taken on multimode SPA 400 (SEIKO Instruments). Nanoprobe cantilevers (SI-DF20, SEIKO Instruments) were utilized. The sample was prepared by slow evaporation on substrate overnight at room temperature. Mica was used as a substrate for TM-AFM measurement. Raman spectra were measured using a JASCO NRS-2000 micro-Raman spectrometer equipped with an Ar laser. The Ar laser was operated at 514.5 nm, and the spectra were collected at a resolution of 1 cm^{-1}.

Purification of Hipco SWCNTs. The purification of Hipco SWCNTs followed literature method.[1]

Cucurbit[5]uril (**CB5**) and **cucurbit[7]uril** (**CB7**) were prepared according to previous paper.[2]

Solubilization of SWCNTs with CB7. CB7 (20 mg) was dissolved in aqueous solution (5 mL). To the mixture, purified SWCNTs (1 mg) were added and sonicated in low-energy ultrasonic bath (Bransonic 2510) for 3 h, followed by centrifugation.

UV-Vis Spectra of Hipco SWCNTs Suspended with CB7 and SDBS

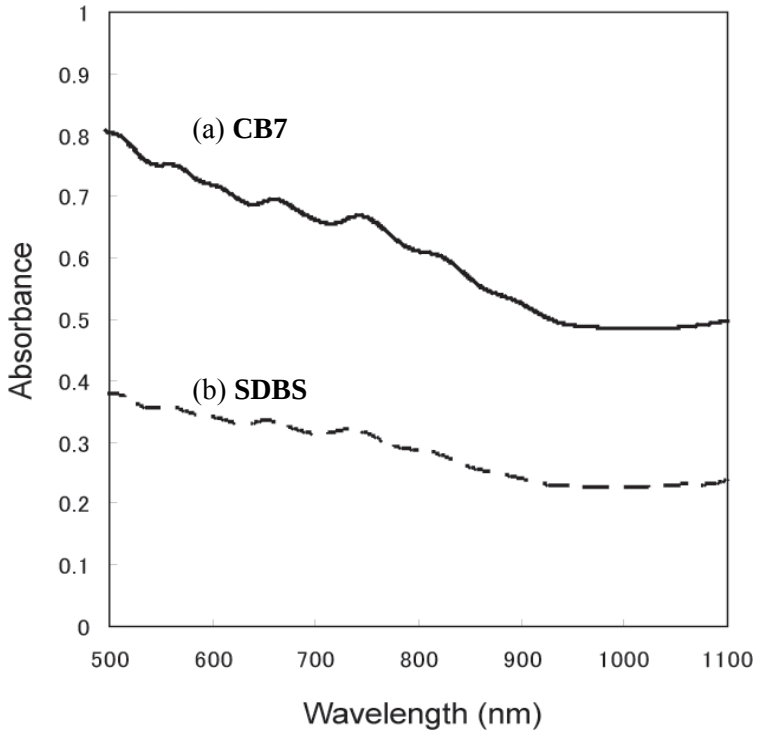


Figure 1S. UV-Vis spectra of the aqueous supernatants (5 mL) containing Hipco SWCNTs with (a) **CB7** (solid line) and (b) sodium dodecylbenzene sulfonate (**SDBS**, dash line) after sonication. Weight of solubilizer and Hipco SWCNTs was 20 and 1 mg, respectively. Solubility of SWCNTs with **CB7** and **SDBS** was 3.42×10^{-2} and 1.61×10^{-2} mg/mL, respectively.

UV-Vis Spectra of Soluble Hipco SWCNTs with the Increasing of CB7 Concentration

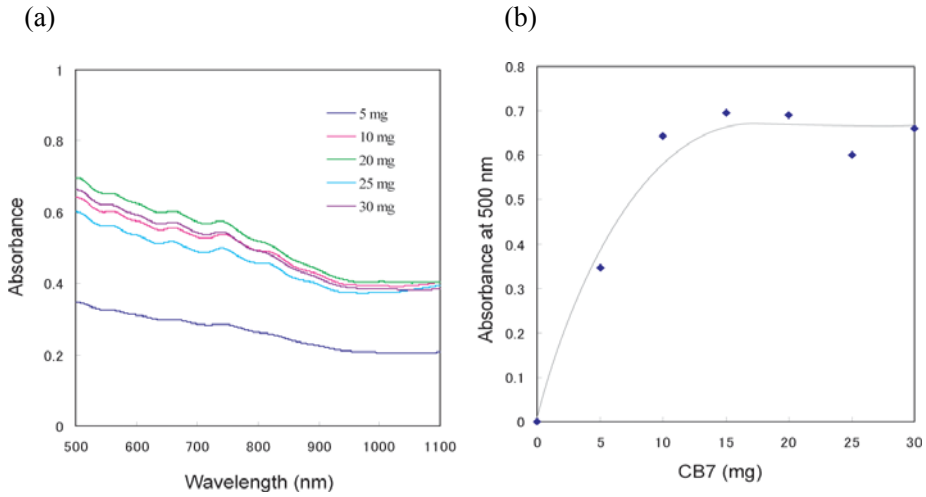


Figure 2S. (a) UV-Vis spectra of the aqueous supernatants (5 mL) containing Hipco SWCNTs by adding **CB7** (0 – 30 mg). Weight of Hipco SWCNTs was 1 mg. (b) Changes in absorbance intensities from soluble Hipco SWCNTs at 500 nm by adding **CB7** (0 – 30 mg).

Photos and ^{1}H NMR spectra of the supernatant after addition of $AdNH_2$

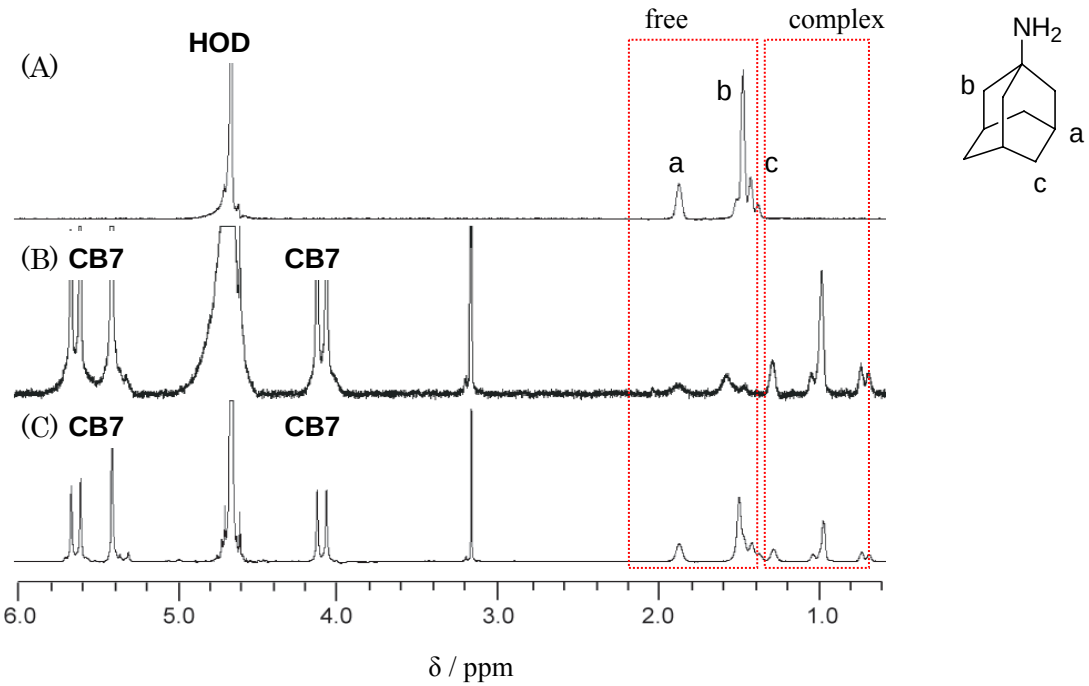
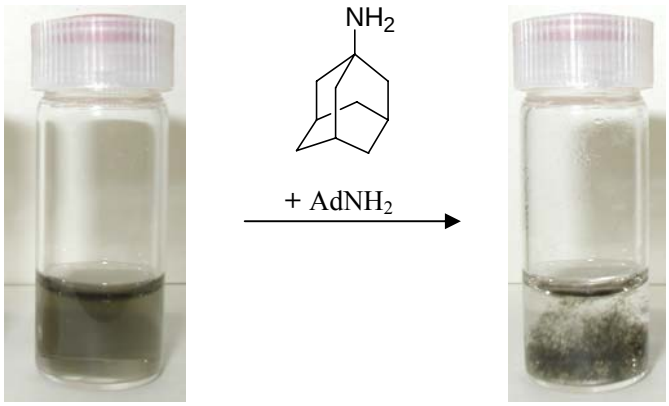


Figure 3S. ^{1}H NMR spectra of (A) $AdNH_2$ (4 mM), (B) $AdNH_2$ (1 mM) with **CB7** (1 mM) and (C) a supernatant of **CB7** (4 mM) upon addition of $AdNH_2$ (4 mM) in D_2O at 25 ^oC. Both free and complex signals from adamantyl group of $AdNH_2$ were observed with **CB7**.



(a) **CB7/Hipco SWCNT hybrids** (b) **CB7/Hipco SWCNT hybrids** with $AdNH_2$

Figure 4S. Photos of (a) the supernatant of **CB7/Hipco SWCNT hybrids** and (b) **CB7/Hipco SWCNT hybrids** upon addition of $AdNH_2$ (1 eq. to **CB7**).

UV-Vis spectra of the supernatant of CB7 / Hipco SWCNT hybrids with $AdNH_2$

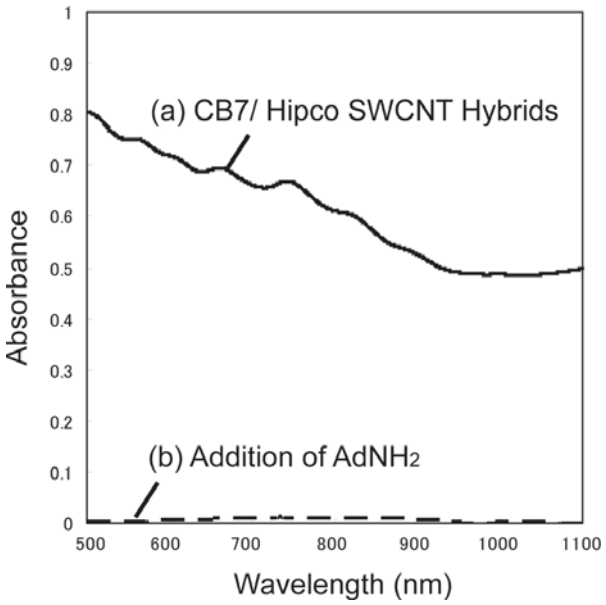


Figure 5S. UV-Vis spectra of the supernatants of (a) **CB7** / **Hipco SWCNT hybrids** (solid line) and (b) **CB7 / Hipco SWCNT hybrids** upon addition of $AdNH_2$ (dash line).

UV-Vis spectra of the supernatants of CoMoCAT and CarboLex SWCNTs with CB7

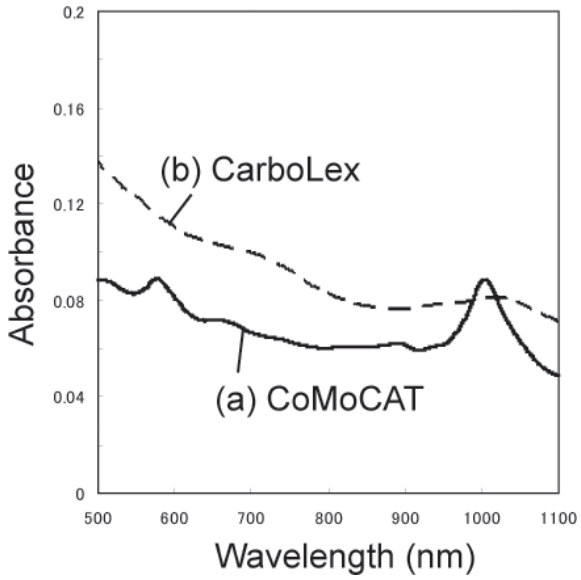


Figure 6S. UV-Vis spectra of the supernatants of (a) **CoMoCAT SWCNTs** with **CB7** (solid line) and (b) **CarboLex SWCNTs** with **CB7** (dash line).

Raman spectra of pristine Hipco SWCNTs and SWCNT-COOH

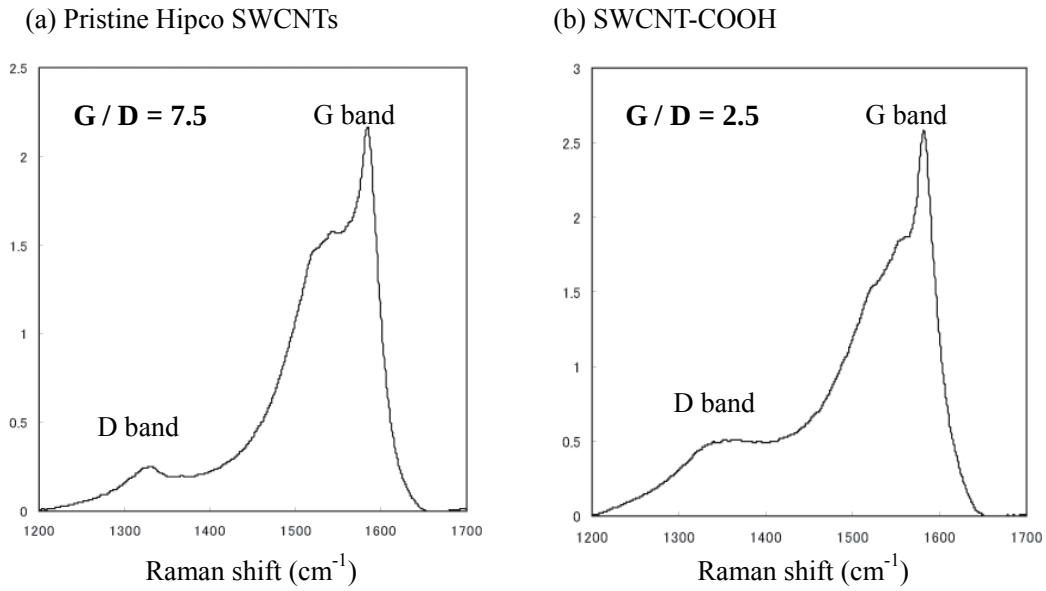


Figure 7S. (a) Raman spectra of (a) pristine Hipco SWCNTs and (b) SWCNT-COOH.

References

1) V. C. Moore, M. S. Strano, E. H. Haroz, R. H. Hauge, R. E. Smalley, J. Schmidt and Y. Talmon, *Nano Lett.*, 2003, **3**, 1379.

2) A. Day, A. P. Arnold, R. J. Blanch and B. Snushall, *J. Org. Chem.,* 2001, **66**, 8094.