

## New Journal of Chemistry

### Ring-opening reactions of epoxidized SWCNT with nucleophilic agents: a convenient way for sidewall functionalization

K H Markiewicz, A Z Wilczewska, O Chernyayeva and K Winkler

#### Supplementary Information

#### Functionalization of SWCNT

##### *Synthesis of SWCNT-H (Birch reduction)*

100 mg of CNT and 100 mg of Li was mixed in a dried 100-mL three-neck round-bottom flask. Dried  $\text{NH}_3$  (25 mL) was condensed into the reaction mixture from a  $\text{Na}/\text{NH}_3$  solution. After the solvent became colorless, the reaction mixture was gradually heated to ambient temperature to evaporate  $\text{NH}_3$ . After a second condensation of 25 mL of  $\text{NH}_3$ , 10 mL of methanol was slowly added to the reactants. Then, the suspension was filtered through a 0.2  $\mu\text{m}$  polytetrafluoroethylene (PTFE) membrane filter. The black product (SWCNT-H) was washed with water (20 mL), hydrochloric acid (10%, 20 mL), water (20 mL), and methanol (20 mL). Finally, the sample was dried in a vacuum oven at ambient temperature overnight.

#### Raman spectroscopy

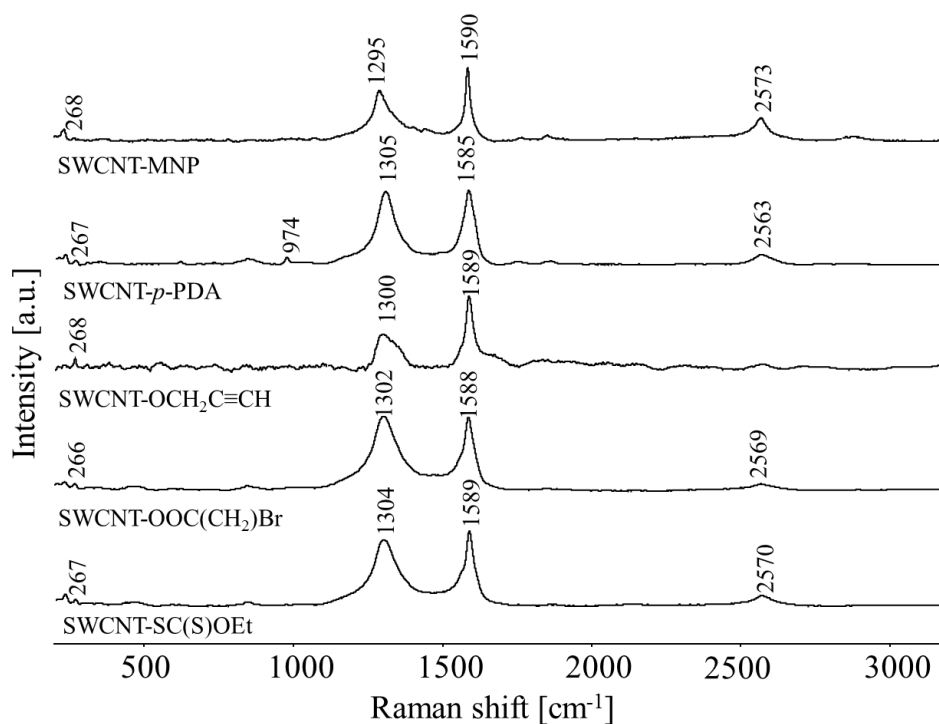
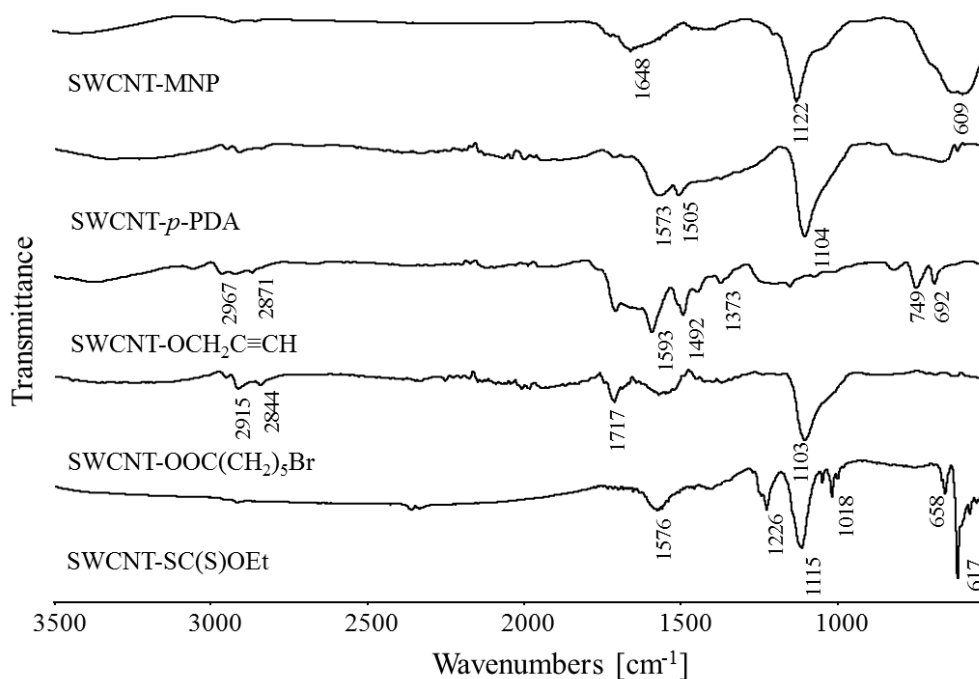


Figure S1. Raman spectra of functionalized SWCNT.

## FT IR spectroscopy



**Figure S2.** FTIR spectra of functionalized SWCNT.

SWCNT-MNP: 3500-3300 ( $\nu(\text{N-H})$ ); 1648 ( $\nu(\text{N-H})$ ); 1122 ( $\nu(\text{C-O})$ ); 609 ( $\nu(\text{Fe-O})$ )

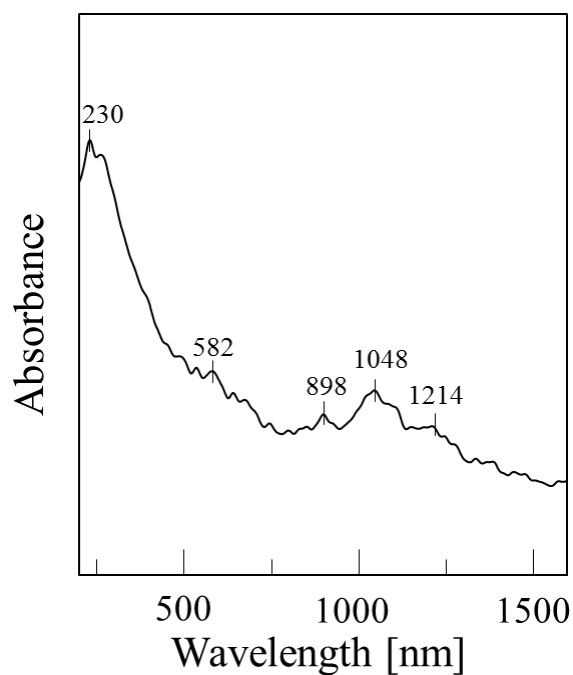
SWCNT-*p*-PDA: 3500-3200 ( $\nu(\text{N-H})$ ); 2965-2850 ( $\nu(\text{C-H})$ ); 1505, 1573 ( $\nu(\text{N-H})$ ); 1104 ( $\nu(\text{C-O})$ )

SWCNT-OCH<sub>2</sub>C≡CH: 2500-3670 ( $\nu(\text{O-H})$ ); 2965-2850 ( $\nu(\text{C-H})$ ); 1540-1000 ( $\delta(\text{O-H})$ ); 1300-1020 ( $\nu(\text{C-O})$ ); 700-600 ( $\delta(\equiv\text{CH})$ )

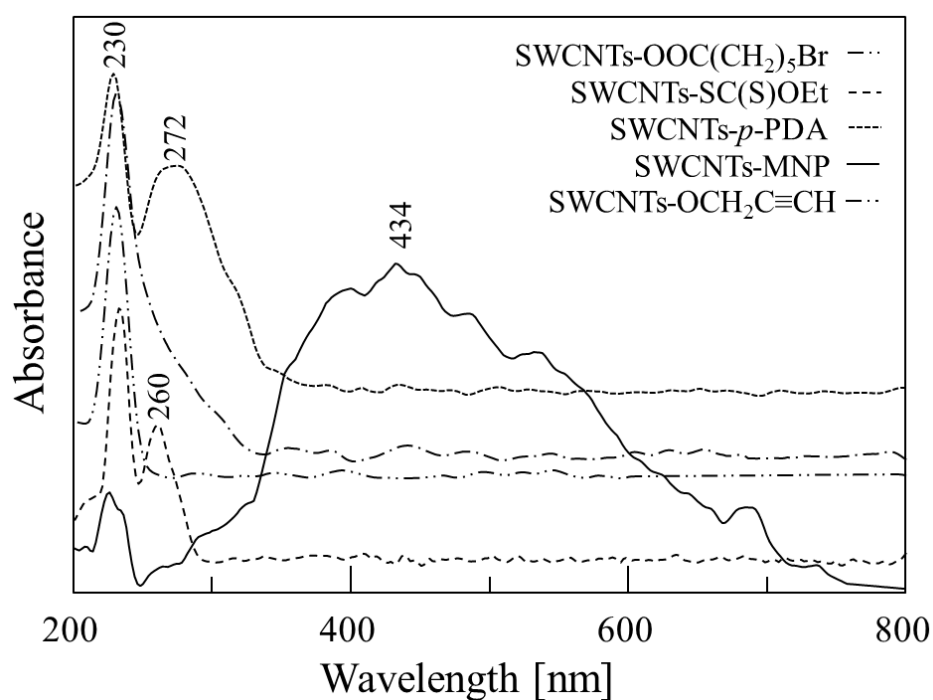
SWCNT-OOC(CH<sub>2</sub>)<sub>5</sub>Br: 2965-2850 ( $\nu(\text{C-H})$ ); 1717 ( $\nu(\text{C=O})$ ); 1103 ( $\nu(\text{C-O})$ )

SWCNT-SC(S)OEt: 1226 ( $\delta(\text{C-O})$ ); 1115 ( $\nu(\text{C=S})$ ); 1200-1050 ( $\nu(\text{C=S})$ ); 800-570 ( $\nu(\text{C-S})$ )

## UV-Vis-NIR spectroscopy



**Figure S3.** UV-Vis-NIR spectrum of pristine SWCNT.



**Figure S4.** UV-Vis spectra of functionalized SWCNT.

SWCNT-MNP:  $\lambda_{\max} = 228$ ;  $\lambda_{\max} = 434$

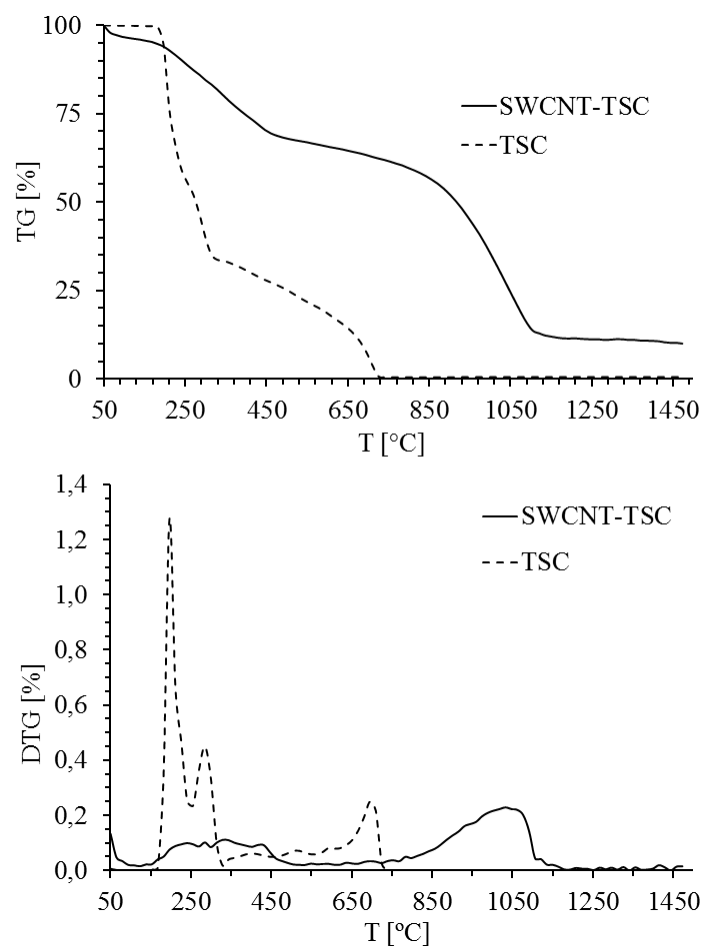
SWCNT-*p*-PDA:  $\lambda_{\max} = 230$ ;  $\lambda_{\max} = 272$

SWCNT-OCH<sub>2</sub>C≡CH:  $\lambda_{\max} = 230$

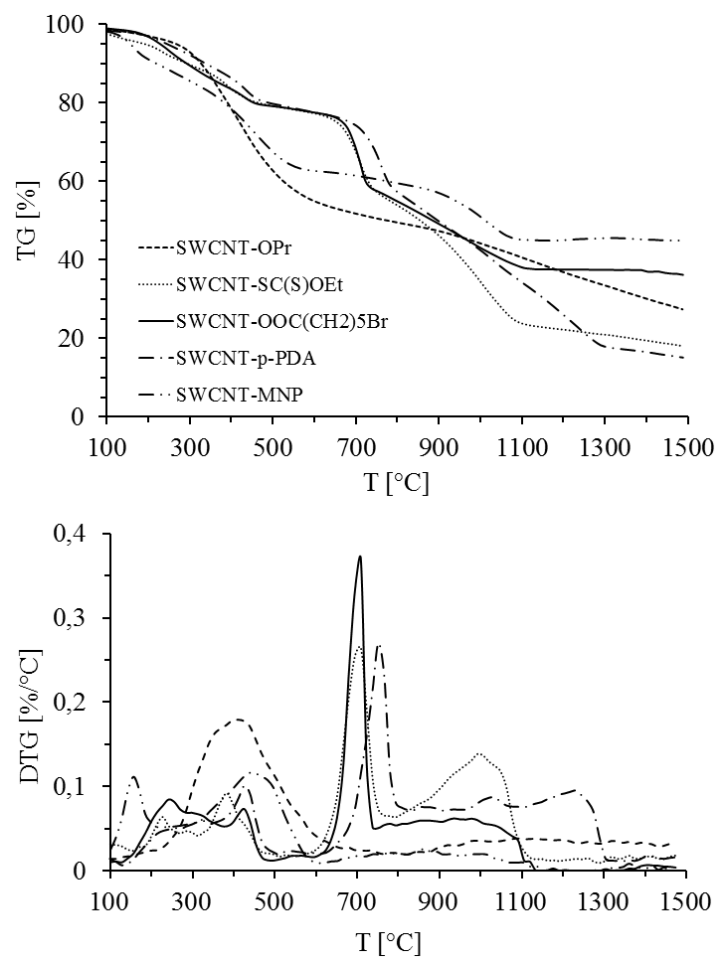
SWCNT-OOC(CH<sub>2</sub>)<sub>5</sub>Br:  $\lambda_{\max} = 230$

SWCNT-SC(S)OEt:  $\lambda_{\max} = 231$ ;  $\lambda_{\max} = 260$

## Thermogravimetric analysis



**Figure S5.** TG and DTG curves of substituted SWCNT.



**Figure S6.** TG and DTG curves of TSC and SWCNT-TSC.