# Supporting information

# A simple, high yield method for the synthesis of organic wires from aromatic molecules using nitric acid as the solvent

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## 1. Elemental analysis result of the acid sonicated sample

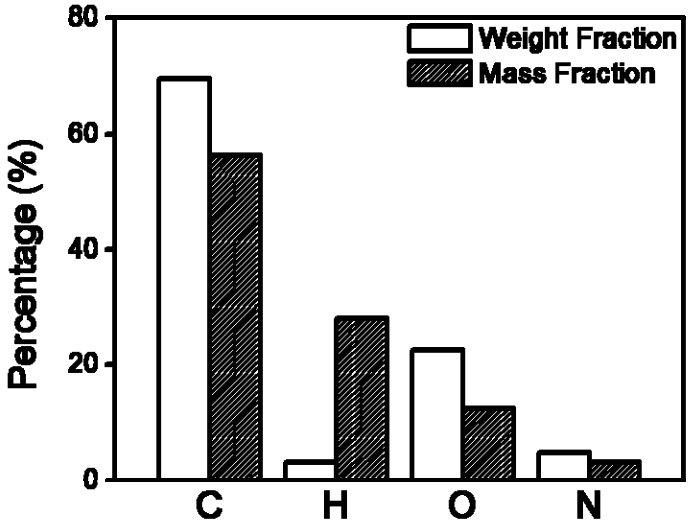


**Fig. S1**. Elemental analysis result of the acid sonicated sample shows that the ratio of the mass fraction is C:H:O:N=18:9:4:1

## 2. Energy calculation results of probable structures

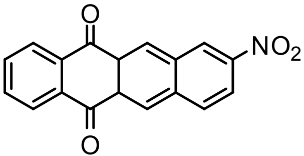
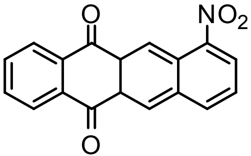
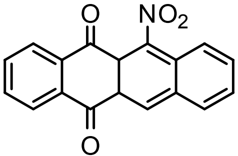
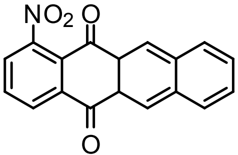
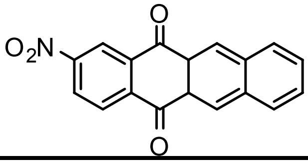
| Structure | Heat of Formation (kcal mol$^{-1}$) |
|---|---|
|  | 17.6956 |
|  | 28.4942 |
|  | 36.8294 |
|  | 34.1377 |
|  | 25.7652 |

**Table S1**. Energy calculation results of probable structures corresponding to m/z= 303 peak in the MALDI-TOF MS spectrum of the sonicated product. It is shown that 8-nitrotetracene-5,12-dione possesses the lowest energy, thus it should be the most probable product.

## 3. ESP maps of tetracene and suggested structure

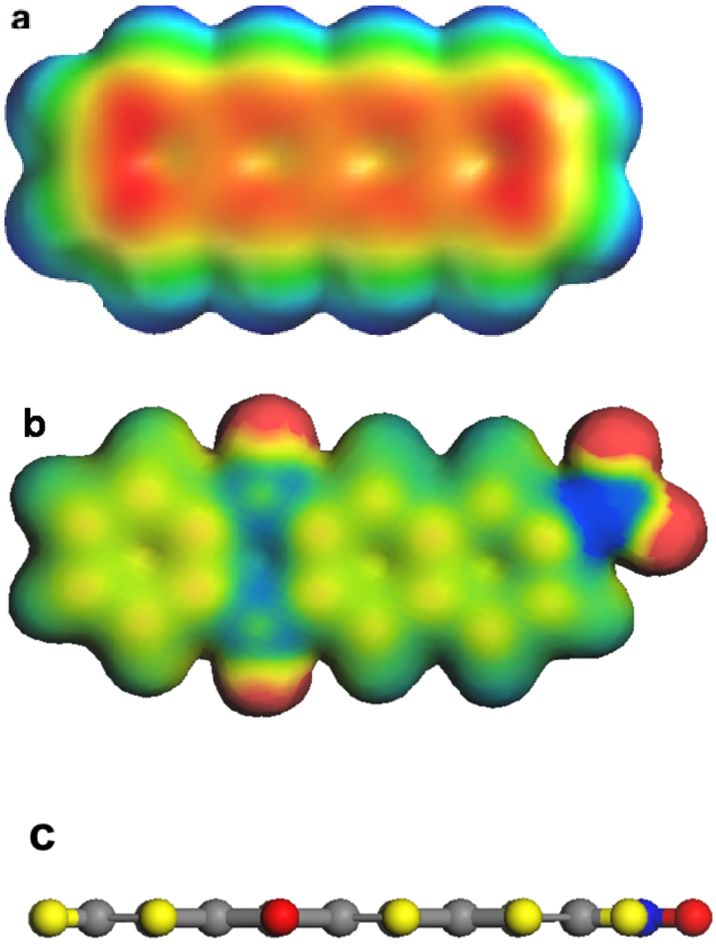


**Fig. S2.** ESP surface plot for (a) tetracene and (b) 8-nitrotetracene-5,12-dione. The ESP maps combine electrostatic potential and electron density surfaces together, in which the electron rich regions are indicated in red while the electron poor regions are indicated in blue. (C) Calculated planar structure of 8-nitrotetracene-5,12-dione.

## 4. Experimental section

### Chemicals and Materials

Tetracene (98%), 1- pyrenylboronic acid, coronene (97%) and triphenylene (98%) were obtained from Sigma-Aldrich. Fuming nitric acid (100%) was purchased from Merck. Dimethylformamide (DMF, HPLC) and Tetrahydrofuran (THF, HPLC) were obtained from RCI lab-scan. Hexane (HPLC) was purchased from Fisher Scientific and Methanol (HPLC) was obtained from Tedia.

### Synthesis of derivatized tetracene organic wires

10 mL 70 % diluted fuming $HNO_3$ was prepared by adding 3 mL deionized water to 7 mL fuming nitric acid (100%) in a 500 mL glass bottle, and 10 mg tetracene was added subsequently. A yellow transparent solution of the mixture was generated and the bottle was full of reddish-brown vapors. The mixture was sonicated at 60 °C for 30 minutes. After the reaction, about 400 ml water was added to the bottle to dilute the solution. A yellow cotton-like product appeared immediately and was kept standing for 12 hours to allow it to grow and precipitate. The solution containing the wires was centrifuged at 8000 rpm for 15 minutes to remove the acid solution. It was then repeatedly centrifuged and washed by water and decanted until the supernatant is neutral. The supernatant was removed and the product was dried in the vacuum box.

## 5. Characterization section

**Scanning electron microscopy (SEM)** images were recorded using the JEOL 6701 FESEM at 30 kV.

**Fourier transform infrared spectroscopy (FTIR)** was recorded at room temperature on the Varian 3100 FTIR spectrometer. The samples were ground with KBr and then pressed into disks.

**Matrix-assisted laser desorption/ionization-Time-of-Flight Mass Spectometry (MALDI-TOF MS)** spectra were obtained using Bruker Daltonics Autoflex II ion extraction linear time-of-flight mass spectrometer with solution-dispersible graphene (G) as the matrix.[1] To prepare the MALDI-TOF MS sample, graphene (1 mg/mL) in deionized water and derivatized tetracene (0.5 mg/mL) in DMF were sonicated to obtain a homogeneous dispersion. 250 μL graphene/$H_2O$ solution and 400 μL derivatized tetracene/DMF solution were mixed and vortexed together in a shaker for 3 hours to ensure equilibration, after which the mixture was centrifuged (10000rpm, 15mins) and the supernatant was collected. The derivatized tetracene could be absorbed sufficiently by graphene.

**X-ray diffraction (XRD)** was carried out using a Siemens D5005 X-ray diffractometer with CuKa (*l* = 1.54060 A°) as the incident beam. The sample powder was ground and then loaded into a plastic baby holder and leveled with a glass slide before mounting it on the sample chamber. The step size was 0.02° in two-theta angles and the step time was set to 1 s. The specimens were scanned at 1.4-60°.

**Transmission electron microscopy (TEM)** analysis was performed with JEOL JEM-3010 microscope at an acceleration voltage of 300 kV.

**UV-vis** spectroscopic data was collected using the UV-2450 Shimadzu UV-vis Spectrometer with THF as the solvent and scan range from 800-200 nm. **Thermogravimetric analysis (TGA)** was performed using TA Instruments – SDT 2960 Simultaneous DSC-TGA with the temperature increasing from room temperature to 1000 °C at the rate of 10 °C/min.

## Reference

1. Tang, L. A. L.; Wang, J. Z.; Loh, K. P., Graphene-Based SELDI Probe with Ultrahigh Extraction and Sensitivity for DNA Oligomer. *J Am Chem Soc* 2010, **132** , 10976-10977.