

[Supporting Information]

## Effective modulation of conjugated aryl acetylenic molecular system based on dithienyldiketopyrrolopyrrole for organic solar cells

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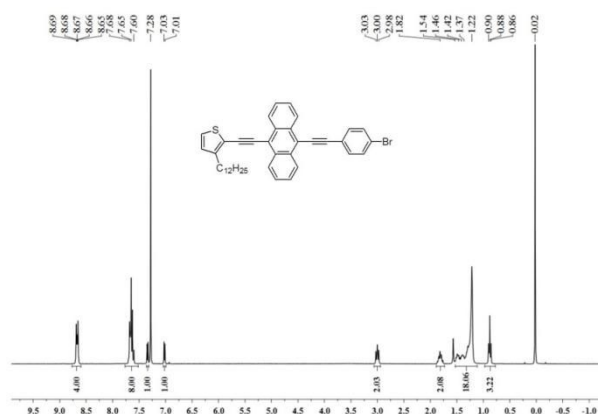
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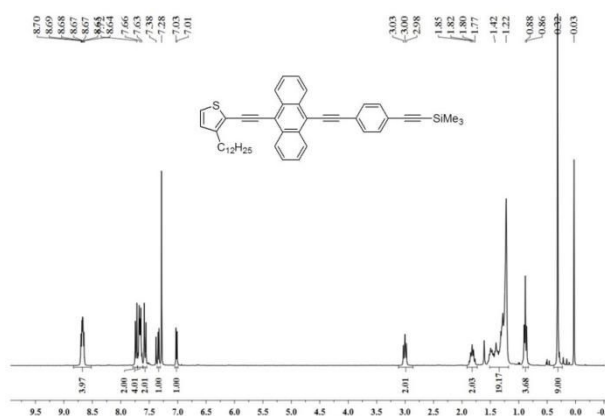
This electronic supplementary information contains the following data:

1. <sup>1</sup>H NMR spectra of **An-1** and **An-2** as well as the reaction intermediates
2. Mass spectra and microanalysis data of **An-1** and **An-2**
3. **Table S1**. The optimized geometry of **An-1** and **An-2** involving various dihedral angles
4. Thermogravimetric diagrams of **An-1** and **An-2**
5. The *J-V* characteristics of the photovoltaic devices based on different weight ratios of **An-1** or **An-2** with PC<sub>61</sub>BM
6. Topographic atomic force microscopy (AFM) images (5 μm × 5 μm) of the as-cast (a, c, e, g) and thermally annealed thin films (b, d, f, h) of **An-1**, **An-2** and their blends with PC<sub>61</sub>BM on ITO/PEDOT:PSS.

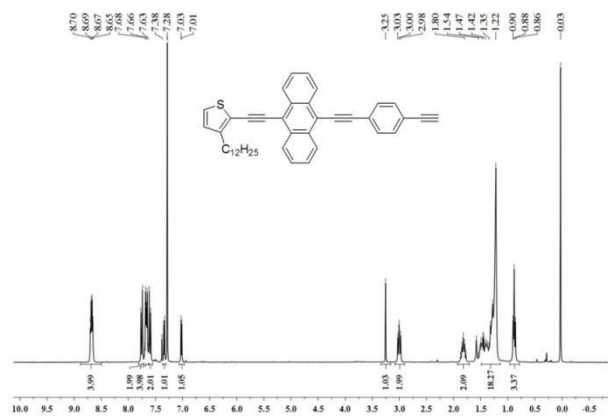
**Fig. S1**  $^1\text{H}$  NMR spectrum of compound **2**



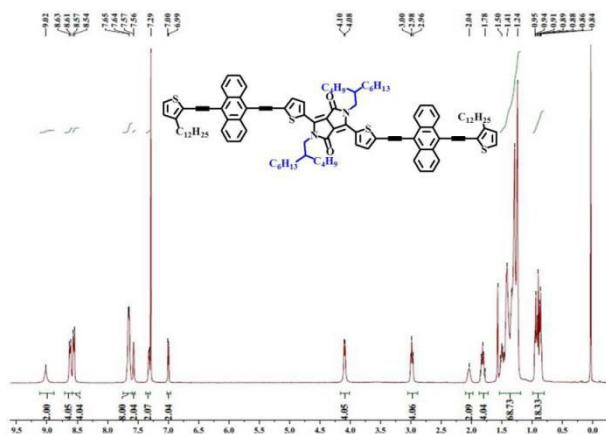
**Fig. S2**  $^1\text{H}$  NMR spectrum of compound **3**



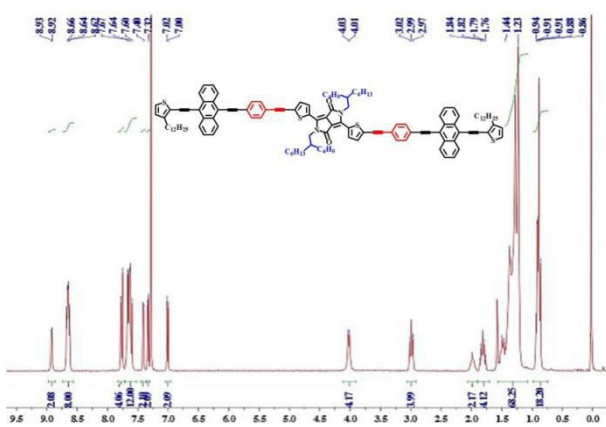
**Fig. S3**  $^1\text{H}$  NMR spectrum of compound **4**



**Fig. S4**  $^1\text{H}$  NMR spectrum of An-1

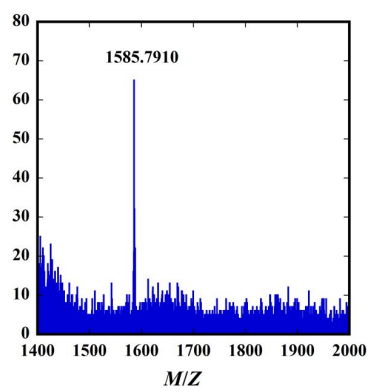


**Fig. S5**  $^1\text{H}$  NMR spectrum of An-2

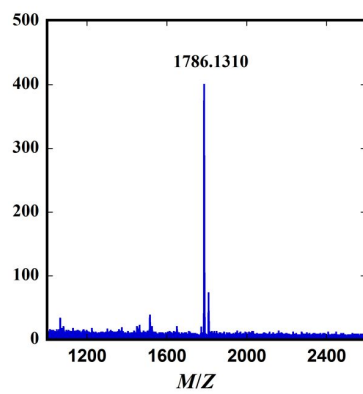


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**Fig. S6** Mass spectrum of **An-1**



**Fig. S7** Mass spectrum of **An-2**



**Fig. S8** Microanalysis data of An-1

Document: 20141120 CHNS test (varioELcube) from: 2014-11-21 10:35:05

CHNS元素含量测定  
vario EL cube 元素分析仪

Text report

| No. | Name | Weight [mg] | C [%] | H [%] | N [%] | S [%] | C/N ratio | C/H ratio | Date       | Time  |
|-----|------|-------------|-------|-------|-------|-------|-----------|-----------|------------|-------|
| 39  | BoAn | 1.6630      | 80.05 | 7.701 | 1.69  | 8.116 | 47.4631   | 10.3956   | 20.11.2014 | 14:31 |
| 40  | BoAn | 1.7860      | 79.91 | 7.969 | 1.68  | 8.112 | 47.6904   | 10.0279   | 20.11.2014 | 14:40 |

**Fig. S9** Microanalysis data of An-2

Document: 20151027 CHNS test (varioELcube) from: 2015-10-28 8:45:19

CHNS元素含量测定  
vario EL cube 元素分析仪

151009 张春晖

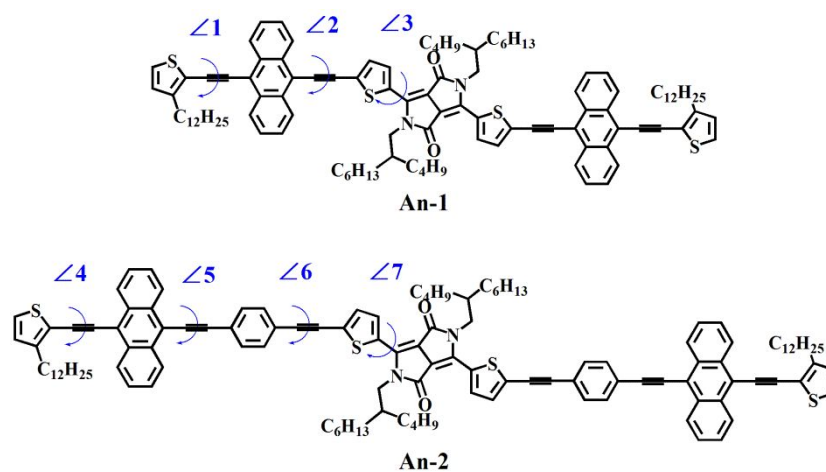
Text report

| No. | Name           | Weight [mg] | C [%] | H [%] | N [%] | S [%] | C/N ratio | C/H ratio | Date       | Time  |
|-----|----------------|-------------|-------|-------|-------|-------|-----------|-----------|------------|-------|
| 45  | C122H132N2O2S4 | 1.8140      | 82.13 | 7.484 | 1.40  | 7.102 | 58.5738   | 10.9750   | 27.10.2015 | 17:56 |

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<sup>1</sup> The microanalysis data provided by the Instrumental Analysis & Research Center, Sun Yat-Sen University, Guangzhou, China

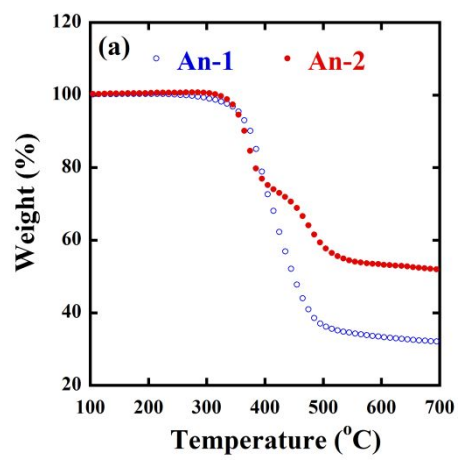
**Table S1.** The optimized geometry of **An-1** and **An-2** involving various dihedral angles



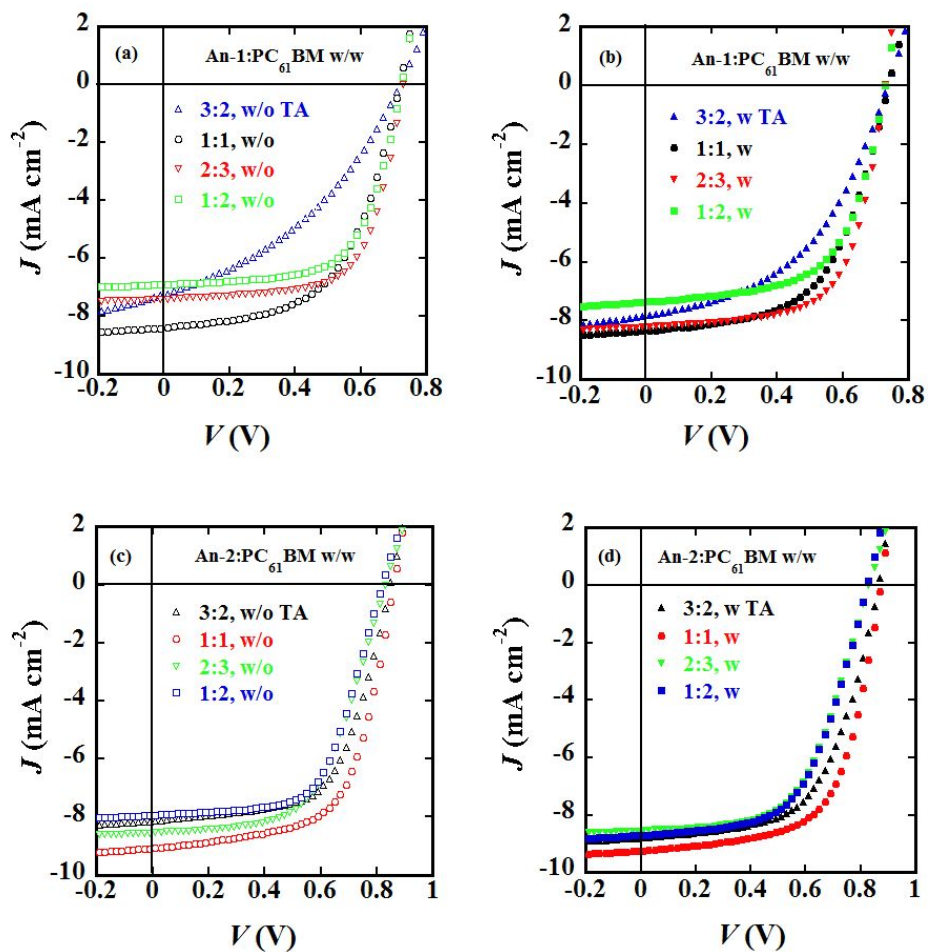
| An-1   |       |       | An-2   |       |       |       |
|--------|-------|-------|--------|-------|-------|-------|
| ∠1     | ∠2    | ∠3    | ∠4     | ∠5    | ∠6    | ∠7    |
| 11.10° | 0.59° | 0.43° | 12.64° | 0.13° | 0.11° | 0.11° |

The geometries of molecules **An-1** and **An-2** were optimized at the level of **B3LYP/6-31G(d)** via density functional theory (DFT). All the alkyl-groups were replaced by methyl group for convenience.

**Fig. S10** Thermogravimetric (TG) diagrams of **An-1** and **An-2**.



**Fig. S11**  $J$ - $V$  characteristics of photovoltaic devices (ITO/PEDOT:PSS/**An-1** or **An-2**:PC<sub>61</sub>BM/Al), under simulated AM1.5G with an illumination intensity of 100 mW cm<sup>-2</sup>. Device area: 0.16 cm<sup>2</sup>.



The active layer involving different D/A weight ratios were spin-cast from chloroform solution (total concentration, 20 mg mL<sup>-1</sup>) with (W) or without (w/o) thermal annealing (TA) at 50 °C for 10 min.



**Fig. S12** Topographic atomic force microscopy (AFM) images ( $5\ \mu\text{m} \times 5\ \mu\text{m}$ ) of the as-cast (a, c, e, g) and thermally annealed thin films (b, d, f, h) of **An-1**, **An-2** and their blends with PC<sub>61</sub>BM on ITO/PEDOT:PSS. (a, b) **An-1**. (c, d) **An-2**. (e, f) **An-1**:PC<sub>61</sub>BM = 2:3 w/w. (g, h) **An-2**:PC<sub>61</sub>BM = 1:1 w/w. Concentration: 20 mg mL<sup>-1</sup> CHCl<sub>3</sub> solution, spin speed: 3000 rpm. Thermal annealing (TA) was performed at 50 °C for 10 min.

