

Electronic Supplementary Information

A dimeric fullerene derivative for efficient inverted planar perovskite solar cells with improved stability

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General Methodology

All chemicals were reagent grade, purchased from Sigma Aldrich. Silica gel (Redisep silica, 40-60 μ , 60 Å) was used to separate the products from the pristine fullerene. MALDI-TOF mass spectrometric measurements were obtained on a Bruker Microflex LRF mass spectrometer on reflector positive mode. The NMR spectra were recorded using a Bruker 400 MHz spectrometer. The UV/Vis-NIR spectra were taken using a Cary 5000 UV/Vis-NIR spectrophotometer using toluene solutions. Cyclic voltammetry (CV) experiments were carried out under an Argon atmosphere at room temperature using a CH Instrument Potentiostat. Scan rate for CV experiments was 100 mV/s. A one compartment cell with a standard three-electrode set up was used, consisting of a 1 mm diameter glassy carbon disk as the working electrode, a platinum wire as the counter electrode and a silver wire as the pseudo-reference electrode, in a solution of anhydrous *o*-DCB containing 0.05 M *n*-Bu₄NPF₆. Ferrocene was added to the solution at the end of each experiment as an internal standard.

Characterization of D-C₆₀

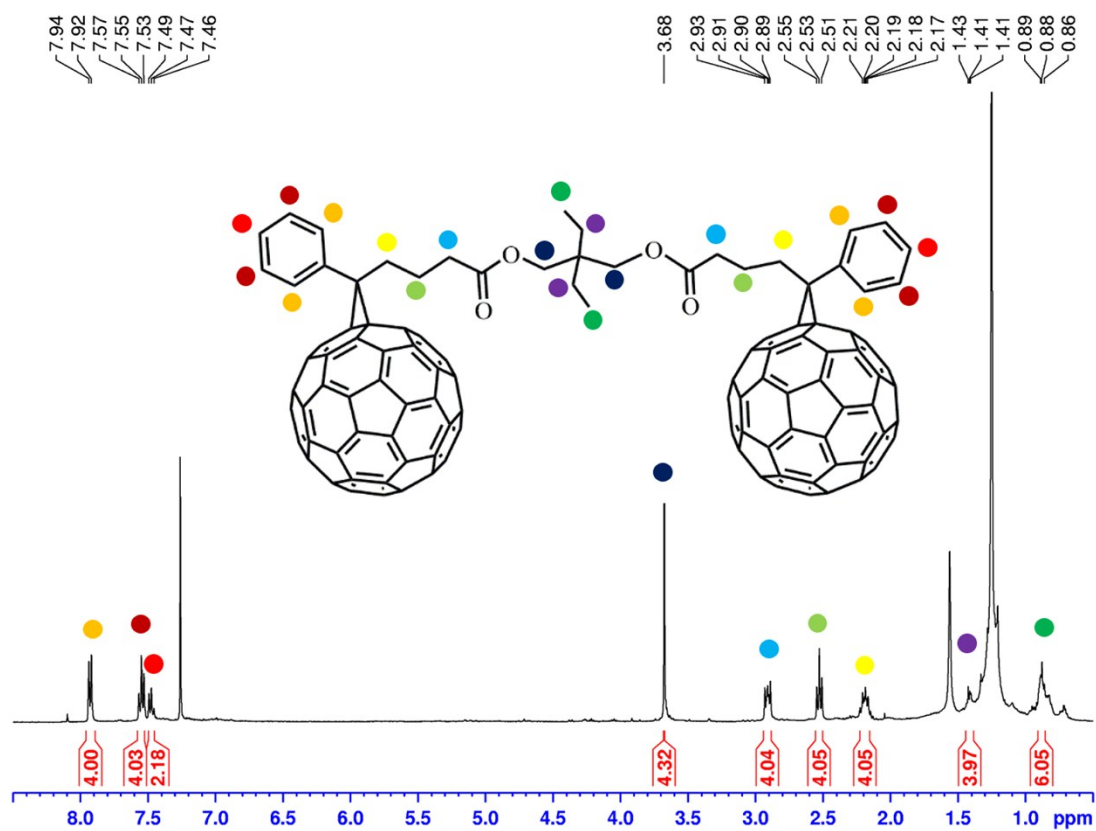


Figure S1. ¹H-NMR (400 MHz; CDCl₃, 298 K) of D-C₆₀.

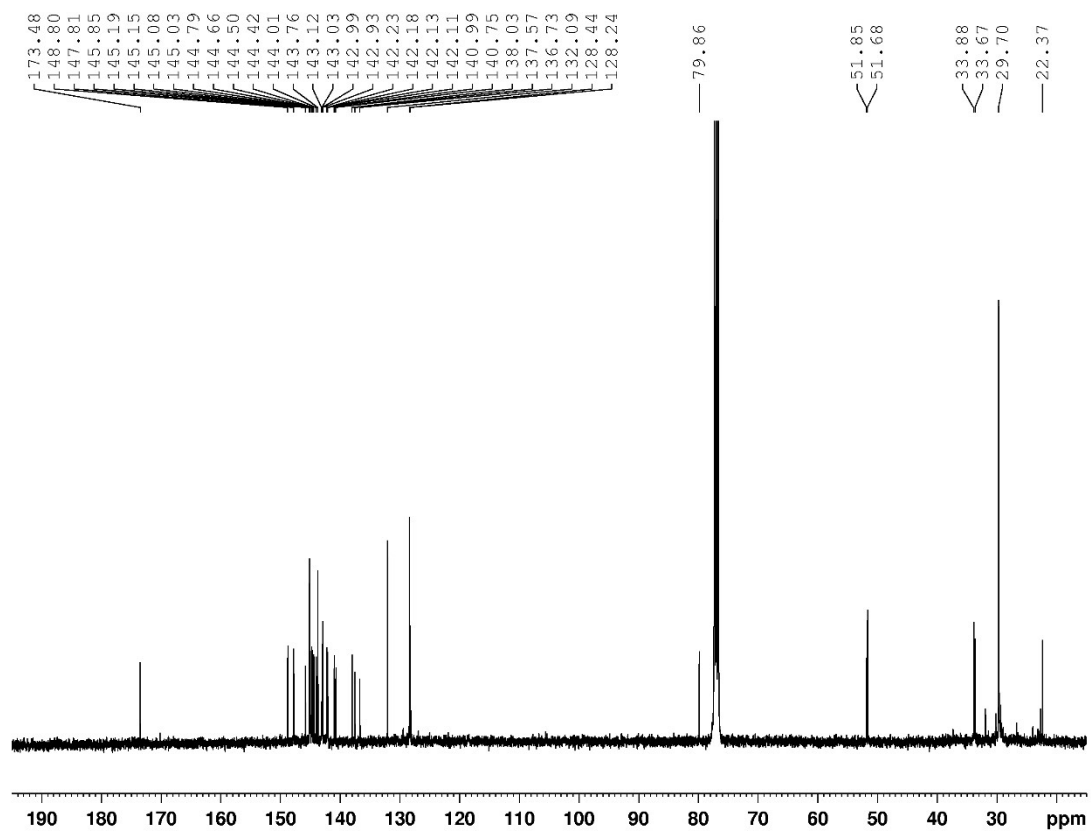


Figure S2. ^{13}C -NMR (100 MHz; CDCl_3 , 298 K) of D-C_{60} .

Electrochemical Properties.

The electrochemical properties of PC₆₁BM and D-C₆₀ were measured by cyclic voltammetry (CV) on a glassy carbon electrode with *o*-dichlorobenzene (*o*-DCB) as solvent and *n*-Bu₄NPF₆ as supporting electrolyte. The reduction potentials are shown in **Table 1**. The reduction potentials of PC₆₁BM and D-C₆₀ are similar.

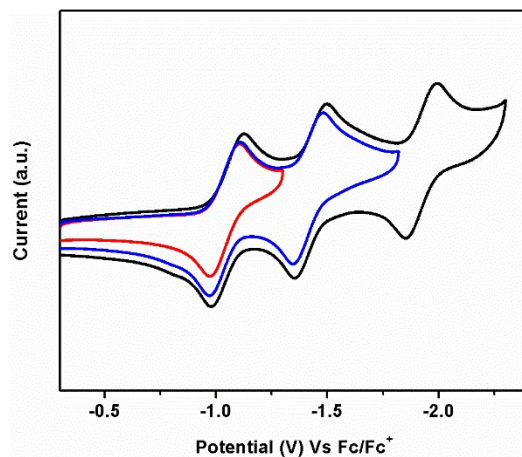


Figure S3. Cyclic voltammetric curves of D-C₆₀ at a scan rate of 100 mV/s.

Table S1. Redox Potentials of PC₆₁BM and D-C₆₀.

Compound	E ^{0/-}	E ^{-/-2}	E ^{-2/-3}
PC ₆₁ BM	-1.03	-1.41	-1.90
D-C ₆₀	-1.05	-1.44	-1.92

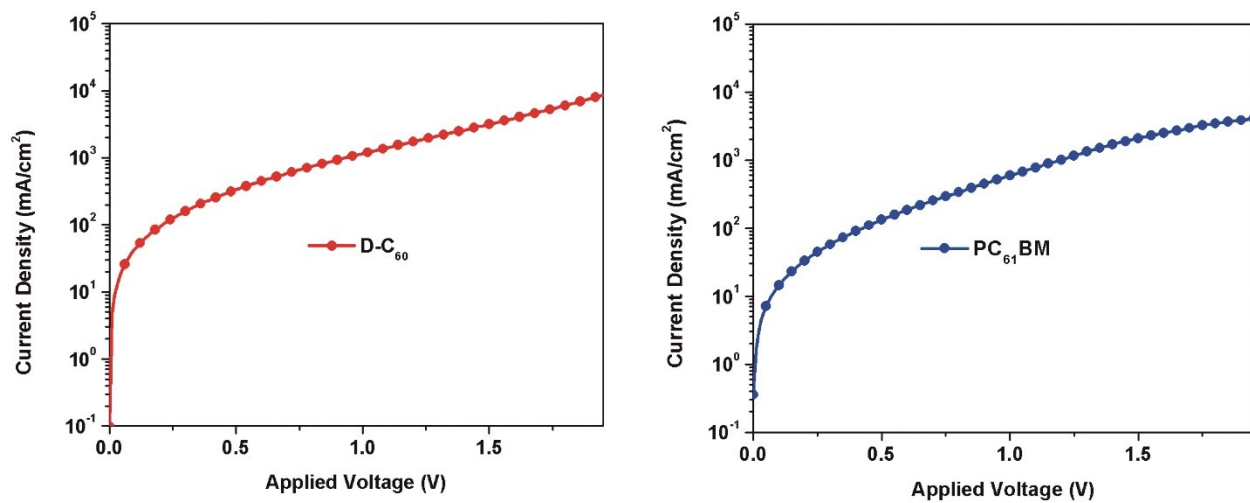


Figure S4. Measured space-charge limited J – V characteristics of the PC_{61}BM and D-C_{60} for electron-only devices. The devices with a structure of $\text{ITO}/\text{Cs}_2\text{CO}_3/\text{D-C}_{60}$ (PC_{61}BM)/ Ca/Al were fabricated.

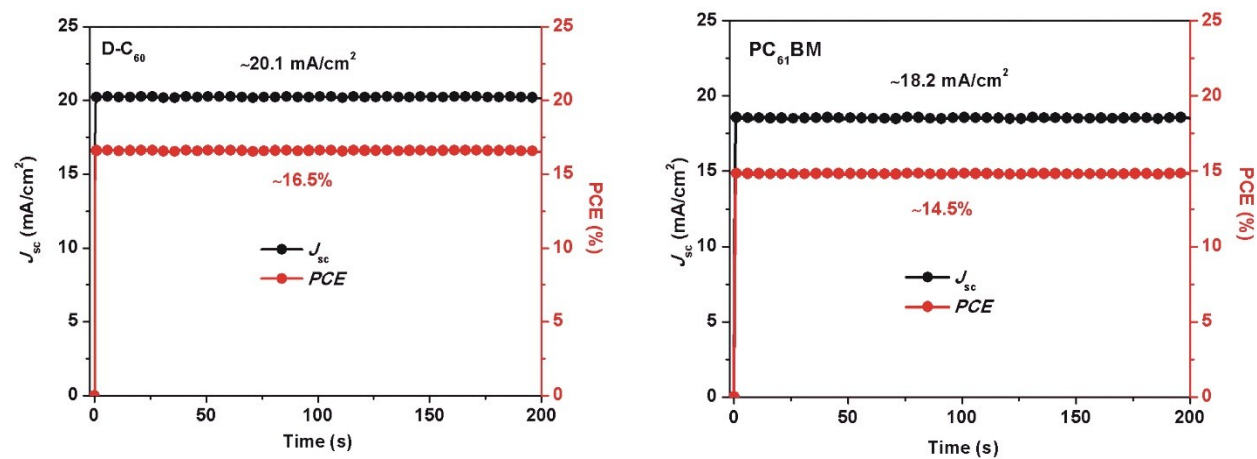


Figure S5. Maximal steady-state photocurrent output at the maximum power point (for PC₆₁BM based device at 0.80 V, and D-C₆₀ based device at 0.82 V) and their corresponding power output.

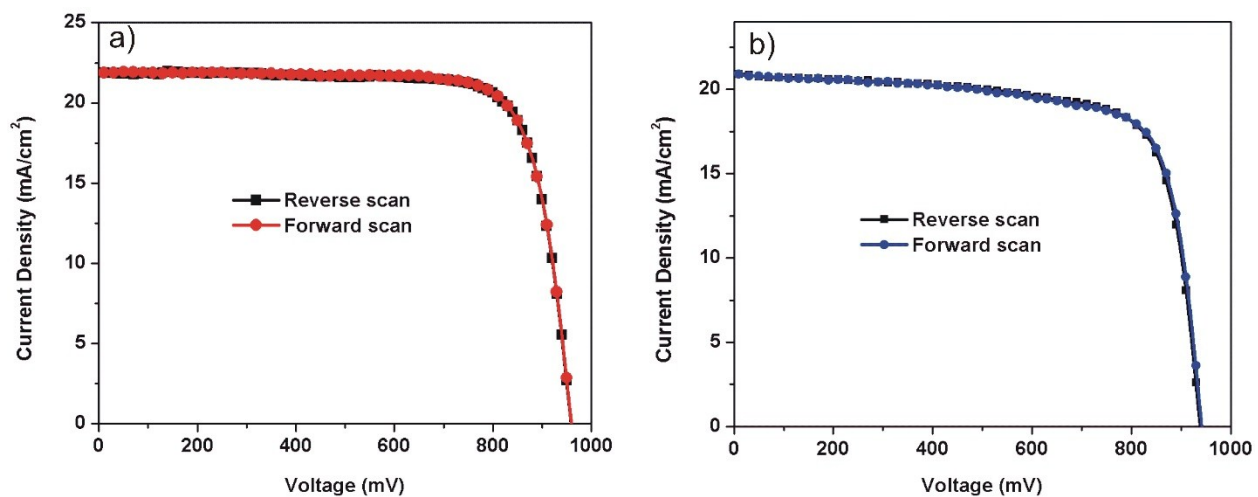


Figure S6. J - V curves of the inverted planar perovskite solar cells based on D- C_{60} and PC_{61}BM with respect to forward and reverse scan directions (The scanning rate was 100 mV/s).

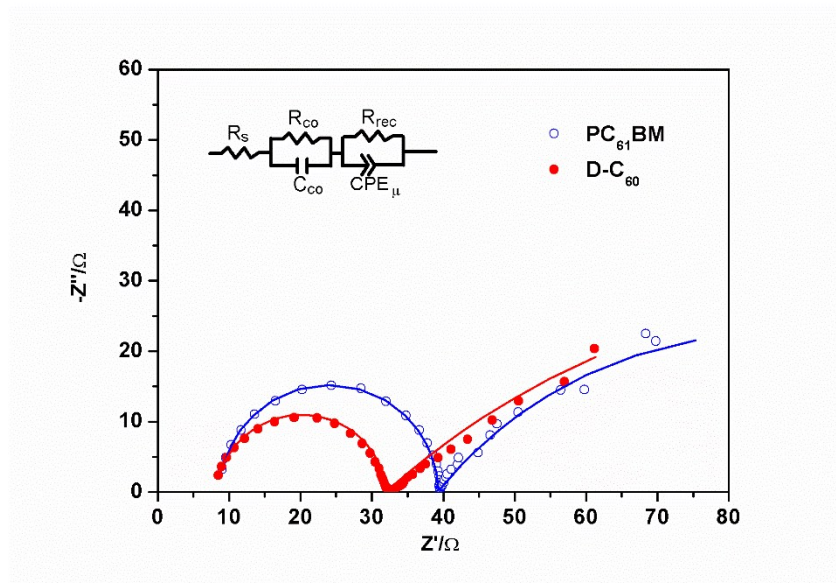


Figure S7. Nyquist plots of the perovskite solar cells based on PC₆₁BM and D-C₆₀.

Table S2. Fitting parameters for EIS data under 1 sun illumination.

Device	$R_s(\Omega)$	$R_{co}(\Omega)$	$C_{co}(F)$	$R_{rec}(\Omega)$	$CPE_{\mu-T}(F)$	$CPE_{\mu-p}(F)$
PC ₆₁ BM	8.80	30.43	1.959E-8	92.85	0.02028	0.5734
D-C ₆₀	8.26	23.68	5.353E-8	146.7	0.02879	0.9543