## **Supporting Information**

## **Regioselective 1,2,3-Bisazfulleroid: Doubly N-Bridged Bisimino-PCBMs for Polymer Solar Cells**

Boram Kim<sup>a,+</sup>, Junghoon Lee<sup>a,+</sup>, Jung Hwa Seo<sup>d</sup>, Fred Wudl<sup>c</sup>, Sung Heum Park<sup>\*,b</sup>, and Changduk Yang<sup>\*,a</sup>

<sup>[a]</sup> Interdisciplinary School of Green Energy and KIER-UNIST Advanced Center for Energy,

Low Dimensional Carbon Materials Center, Ulsan National Institute of Science and Technology (UNIST), Ulsan 689-798 (Korea).

<sup>[b]</sup> Department of Physics, Pukyong National University, Busan 608-737, (Korea).

<sup>[c]</sup> Center for Energy Efficient Materials, University of California Santa Barbara, CA 93106,

USA,

<sup>[d]</sup> Department of Materials Physics, Dong-A University, Busan 604-714, (Korea).

\*E-mail: yang@unist.ac.kr, and spark@pknu.ac.kr,

<sup>§</sup>These authors contributed equally.

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Figure S1. MALDI-MS spectrum of bisimino-PCBM.



Figure S2. <sup>13</sup>C NMR spectrum for bisimino-PCBM in 3:1 CS<sub>2</sub>/acetone- $d_6$ .



Figure S3. HOMOs and LUMOs isosurfaces of bisimino-PCBM.



Figure S4. Electrostatic charge distributions of bisimino-PCBM. This structure exhibits the broken symmetric geometry.



Figure S5. Current density versus voltage characteristics of P3HT:PCBM device.