Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for

Planarity and multiple components promote organic photovoltaic efficiency by improving electronic transport

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Reference	Zhao and Yu [1]	Yang *et al.* [2]	Shin *et al.* [3]	Shin *et al.* [3]	Pookpanratana and Richter [4]	Song *et al.* [5]
PTB7 UPS IP (eV)	4.9	4.93	4.93	5.01	5.04	5.07

Table I: Ultraviolet photoelectron spectroscopy ionization potentials for PTB7

Reference	Zhao and Yu [1]
PID UPS IP (eV)	5.4

Table II: Ultraviolet photoelectron spectroscopy ionization potentials for PID2

Reference	PC71BM UPS IP (eV)
Zhao and Yu [1]	5.5
Nogimura *et al.* [6]	5.51
Nogimura *et al.* [6]	5.55
Nakanishi *et al.* [7]	5.55
Ratcliff *et al.* [8]	5.8
Ratcliff *et al.* [8]	5.9
Subbiah *et al.* [9]	6.0
Yang *et al.* [2]	6.02
Yun *et al.* [10]	6.22
Yun *et al.* [10]	6.31

Table III: Ultraviolet photoelectron spectroscopy ionization potentials for PC71BM

Reference	Ratcliff *et al.* [8]	Nakanishi *et al.* [7]	Ratcliff *et al.* [8]	Nogimura *et al.* [6]	Yoshida [11]	Nogimura *et al.* [6]	Subbiah *et al.* [9]
PC71BM IPS EA (eV)	3.6	3.7	3.7	3.74	3.81	3.88	4.3

Table IV: Inverse photoemission spectroscopy electron affinities for PC71BM

Configuration	E_g (Methyl)	E_g (Hydrogen)
cis-trans	2.28	2.32
cis-cis	1.86	1.82
trans-cis	2.39	2.35
trans-trans	1.95	1.83

Table V: Comparison of B3LYP fundamental gap E_g/eV for PTB7 with different side-chain terminations.

Configuration	E_g (Methyl)	E_g (Hydrogen)
cis-trans	2.51	2.27
cis-cis	2.13	1.93
trans-cis	2.49	2.42
trans-trans	2.02	2.05

Table VI: Comparison of B3LYP fundamental gap E_g/eV for PID2 with different side-chain terminations.

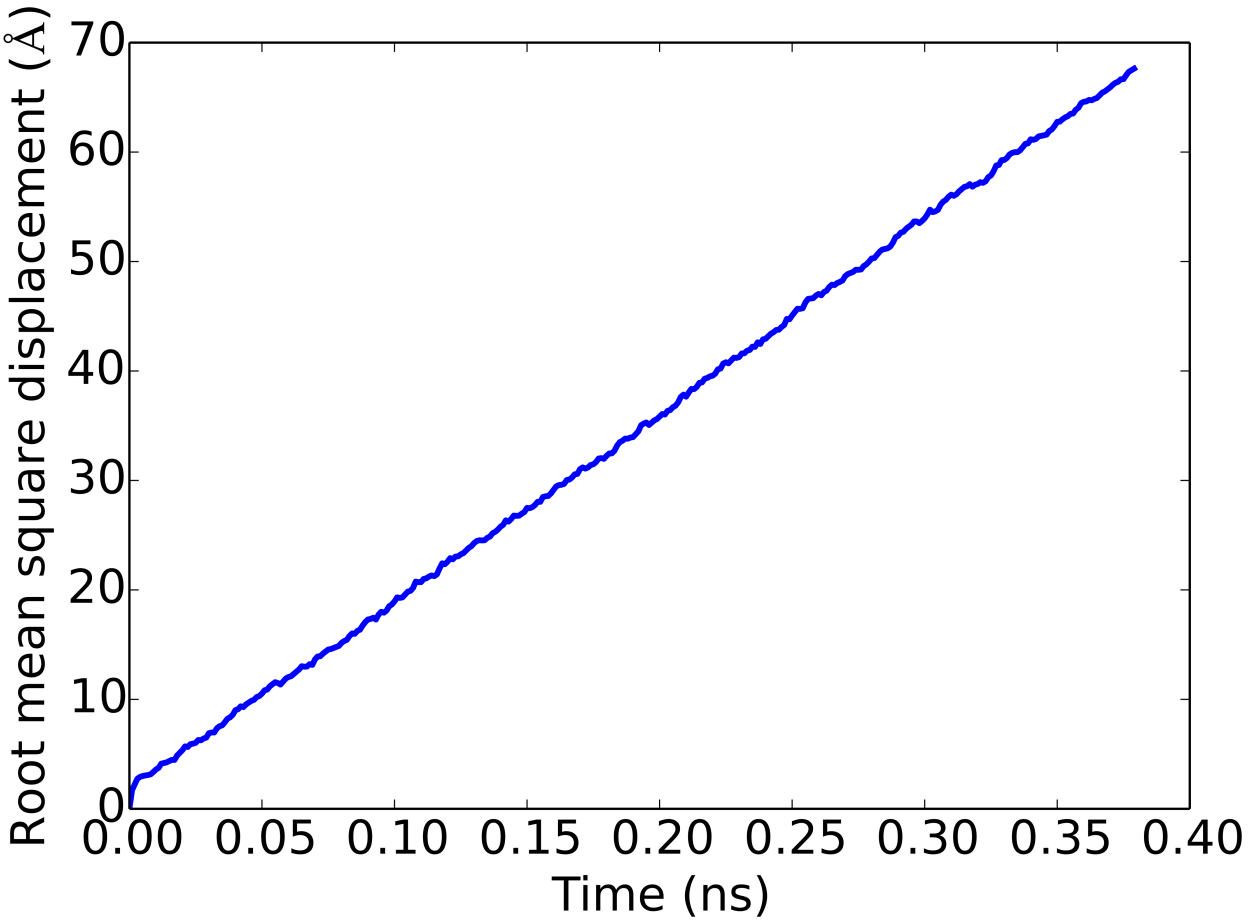

Figure 1: Root mean square displacement of 5-mer PTB7 molecules in the liquid phase at 500 K. Molecules are in the diffusive regime after 10 picoseconds.

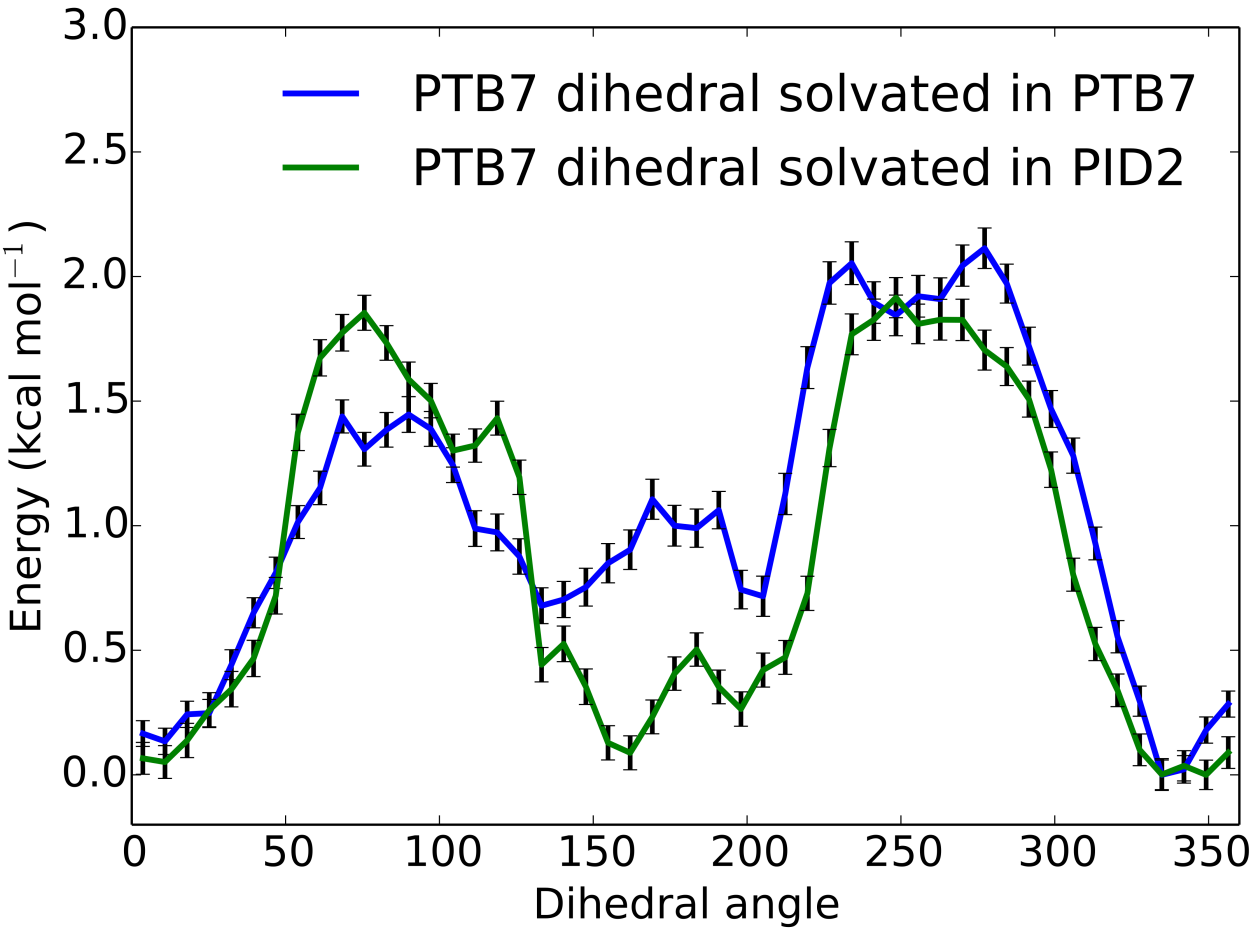

Figure 2: Free energies (kcal mol^{-1}) of rotation for a central PTB7 β dihedral (see Figure 1 of the main text) in two different solvents (PTB7 and PID2) at 400 K.

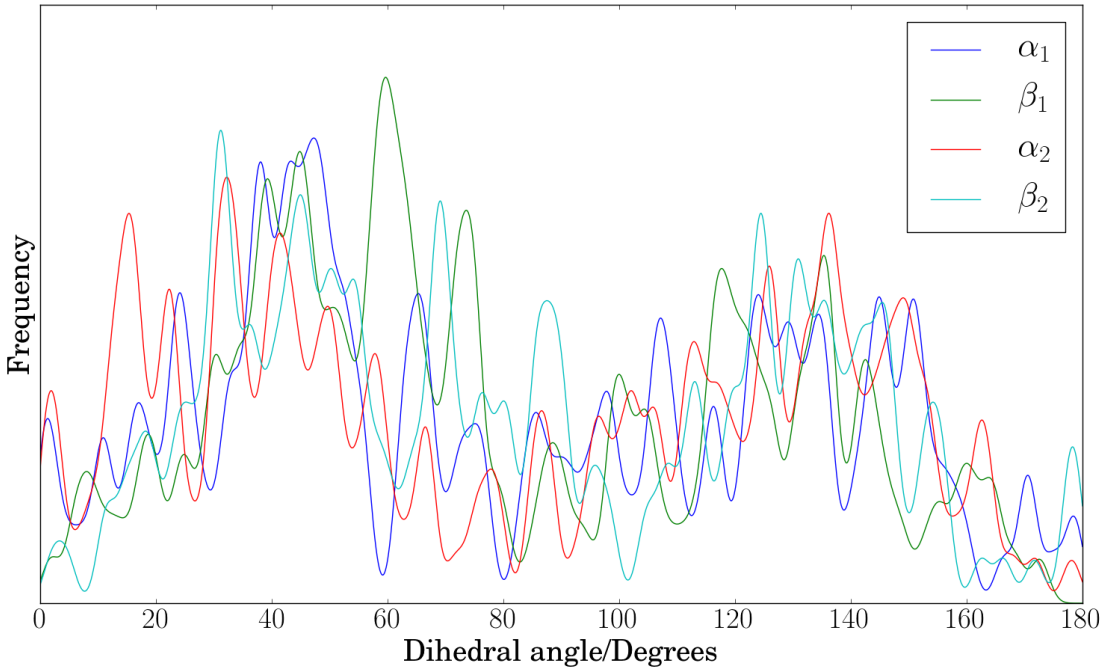

Figure 3: Histogram of α and β dihedrals (absolute values) of the 200 PTB7 configurations used in Section 3.3.

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