

Electronic Supporting Information

Influence of alkyl chain length in *S,N*-heteropentacenes on the performance of organic solar cells

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Differential scanning calorimetry

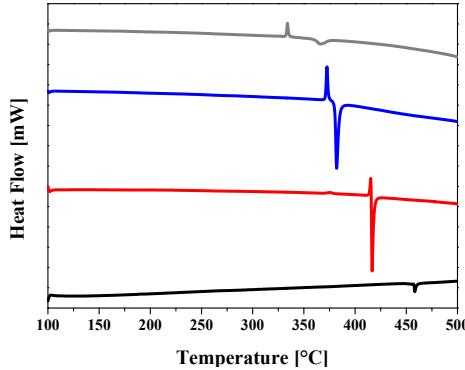


Figure S1. DSC traces of DCV-SN5 derivatives **6b** (black line), **6c** (red line), **6d** (blue line), and **6e** (grey line) measured under Ar flow at a heating rate of 10 °C min^{-1} .

Optical and redox data

Table S1: Summarized optoelectronic data of SN5-derivatives **4-6**.

	λ_{abs} (sol.) [nm]	ϵ [M $^{-1}$ cm $^{-1}$]	ΔE_{opt} (sol.) [eV]	λ_{em}	Stokes shift [cm $^{-1}$]	λ_{abs} (film ^a) [nm]	ΔE_{opt} (film ^a) [eV]	E_{ox1} [V]	E_{ox2} [V]	E_{red} [V]	E_{HOMO} [eV] ^b	E_{LUMO} [eV] ^b	ΔE_{CV} [eV]
4a	356	33,200	3.35	379	1670	-	-	0.06	-	-	-5.07	-1.72 ^c	3.35
4b	356	40,500	3.35	377	1565	-	-	0.06	-	-	-5.08	-1.73 ^c	3.35
4c	356	33,600	3.34	370	1063	-	-	0.15	-	-	-5.12	-1.78 ^c	3.34
4d	356	40,600	3.35	377	1565	-	-	0.12	-	-	-5.14	-1.79 ^c	3.35
4e	356	40,600	3.35	379	1670	-	-	0.14	-	-	-5.15	-1.79 ^c	3.35
4f	356	37,300	3.36	369	1316	-	-	0.11	-	-	-5.13	-1.76 ^c	3.36
5a	456	51,600	2.57	488	1438	-	-	0.53	1.20	-2.11	-5.54	-3.12	2.43
5b	456	72,400	2.57	490	1501	-	-	0.55	1.23	-2.09	-5.59	-3.16	2.42
5c	456	80,500	2.58	483	1226	-	-	0.56	1.26	-2.08	-5.59	-3.15	2.44
5d	456	81,400	2.57	487	1375	-	-	0.55	1.23	-1.99	-5.58	-3.18	2.40
5e	456	81,300	2.57	490	1501	-	-	0.55	1.17	-1.98	-5.58	-3.21	2.38
5f	456	80,200	2.58	483	1226	-	-	0.60	1.27	-2.12	-5.60	-3.19	2.41
6a	582	- ^d	1.94	616	948	589	1.74	0.59	-	-	-5.55	-3.65	1.89
6b	582	- ^d	2.00	620	1040	593	1.70	0.57	1.13	-1.47	-5.59	-3.85	1.74
6c	582	140,000	2.00	617	962	595	1.69	0.61	1.22	-1.43	-5.64	-3.78	1.86
6d	582	137,500	2.01	619	1014	598	1.71	0.58	1.20	-1.52	-5.60	-3.76	1.84
6e	582	152,700	2.00	619	1014	588	1.72	0.62	1.20	-1.53	-5.65	-3.80	1.85
6f	582	139,100	2.01	612	842	594	1.73	0.62	1.23	-1.50	-5.66	-3.81	1.84

^a Film, thickness 30 nm by evaporation; ^b Determined from the onset potential, referenced against Fc/Fc⁺ (5.1 eV); ^c Calculated by $E_{\text{LUMO}} = E_{\text{HOMO}} + E_{\text{g}}^{\text{opt}}$; ^d Solubility too low.

Solar cell data

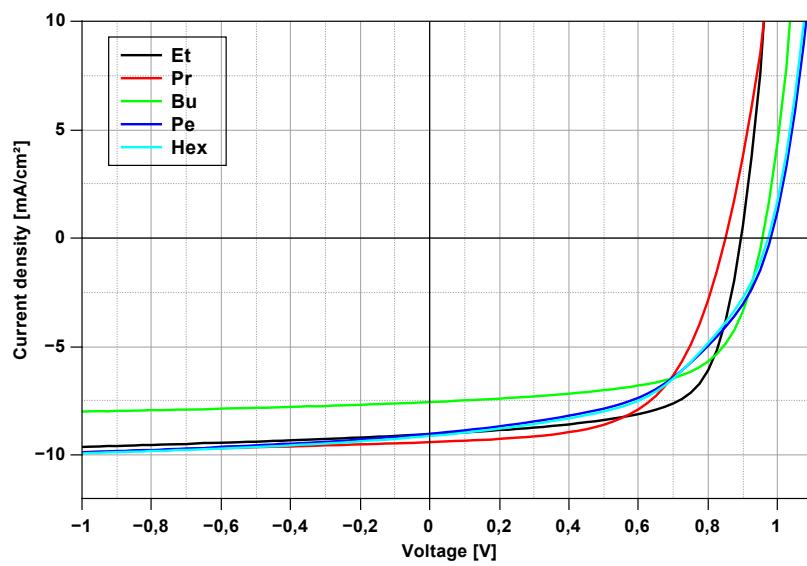


Figure S2. J-V characteristics of a series of heteropentacenes **6b-f:C₆₀** (2:1) in m-i-p bulk heterojunction solar cells with an active layer thickness of 20 nm.

AFM measurement

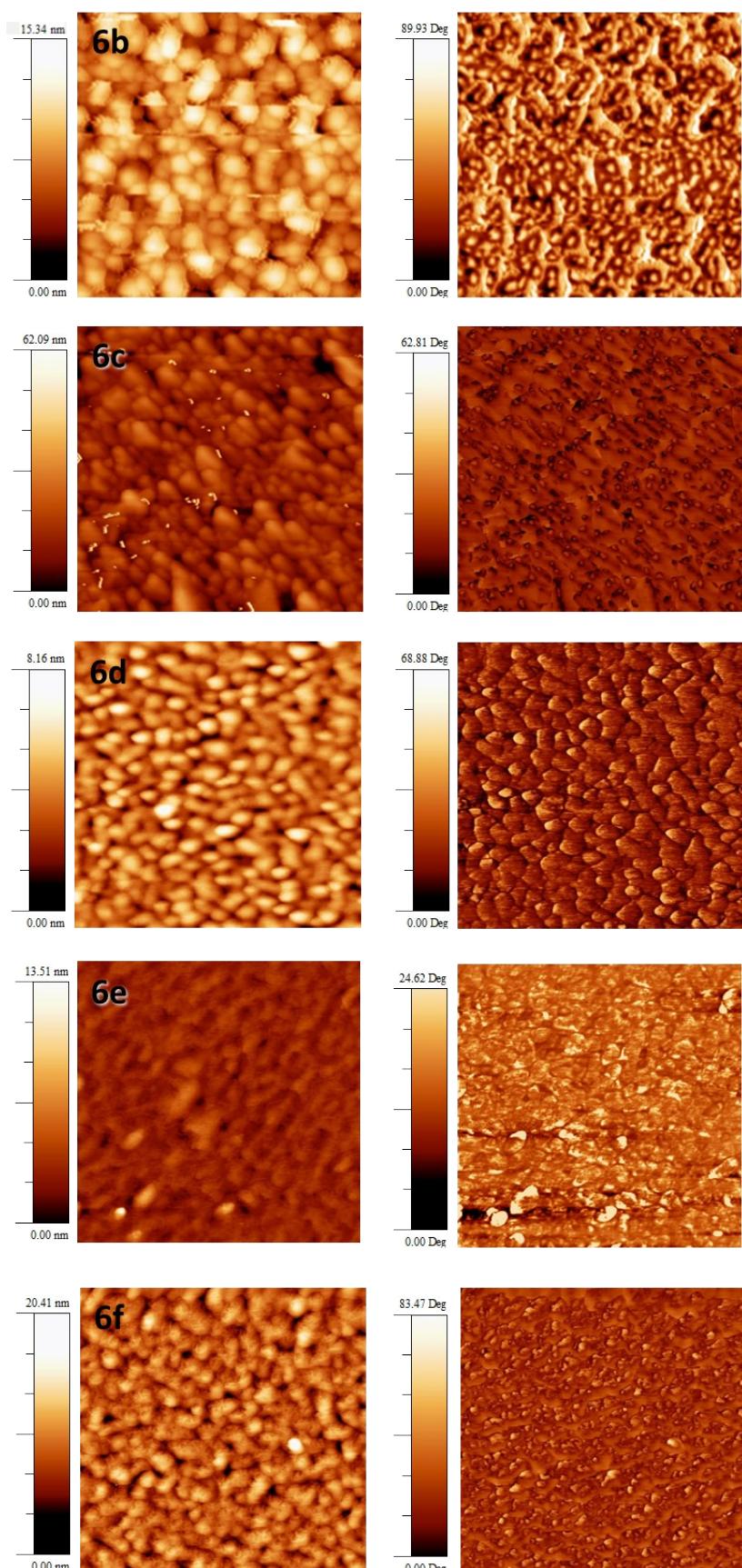


Figure S3. Tapping mode AFM topography (left) and phase (right) images of **6b-f:C₆₀** (2:1) photoactive blends ($1 \times 1 \mu\text{m}^2$).