Supplementary Materials

Figure S1. FT-IR spectra of **PBI** (dashed line) and 1-**A** (solid line).

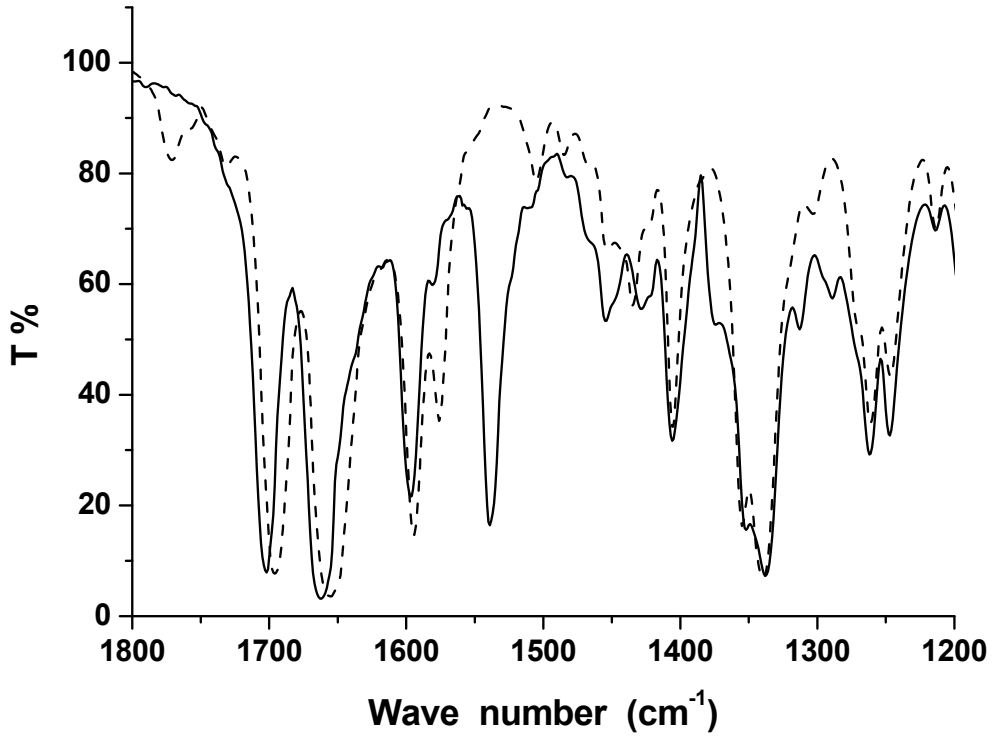

Figure S2. The ^{1}H-NMR (400 MHz, $CDCl_3$) spectra of 1-**B**.

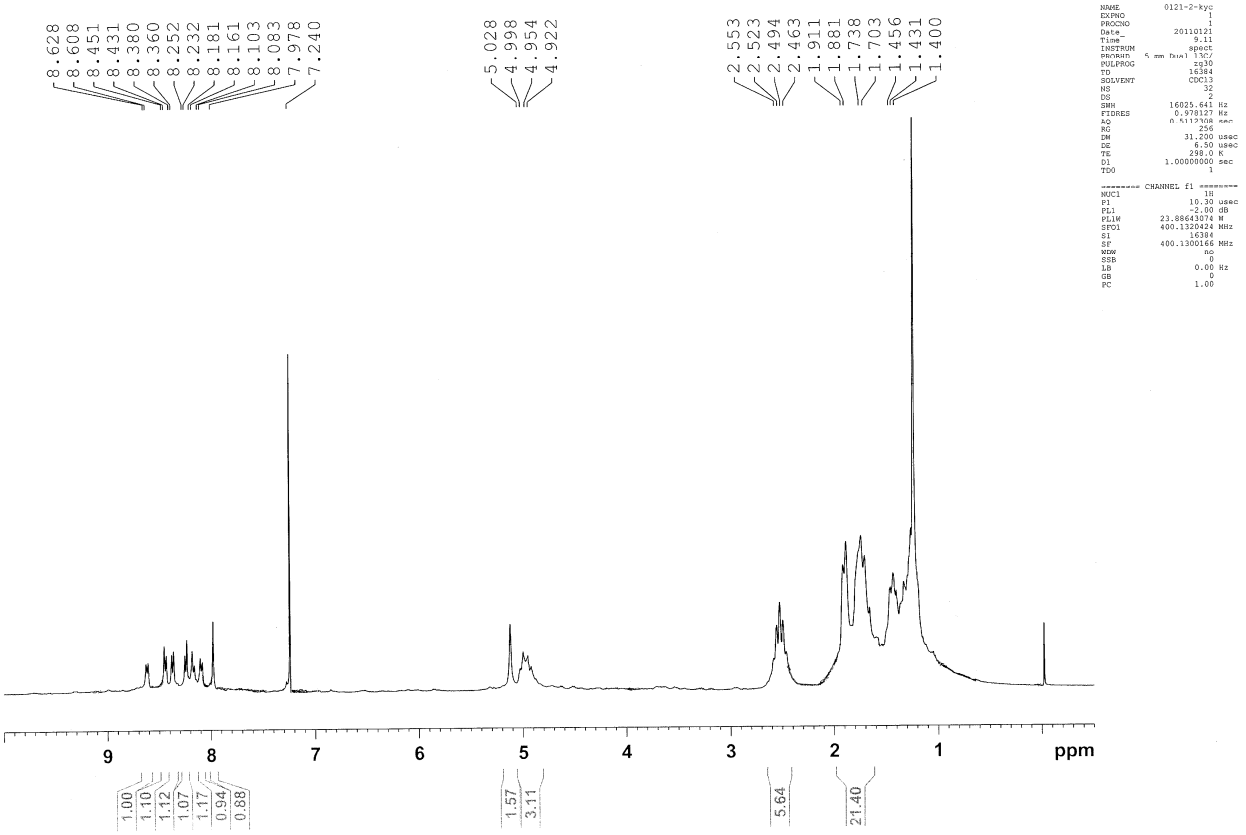

Figure S3. Computed frontier orbitals of 1,6-**A** and 1,7-**A**. The upper graphs are the LUMOs and the lower ones are the HOMOs.

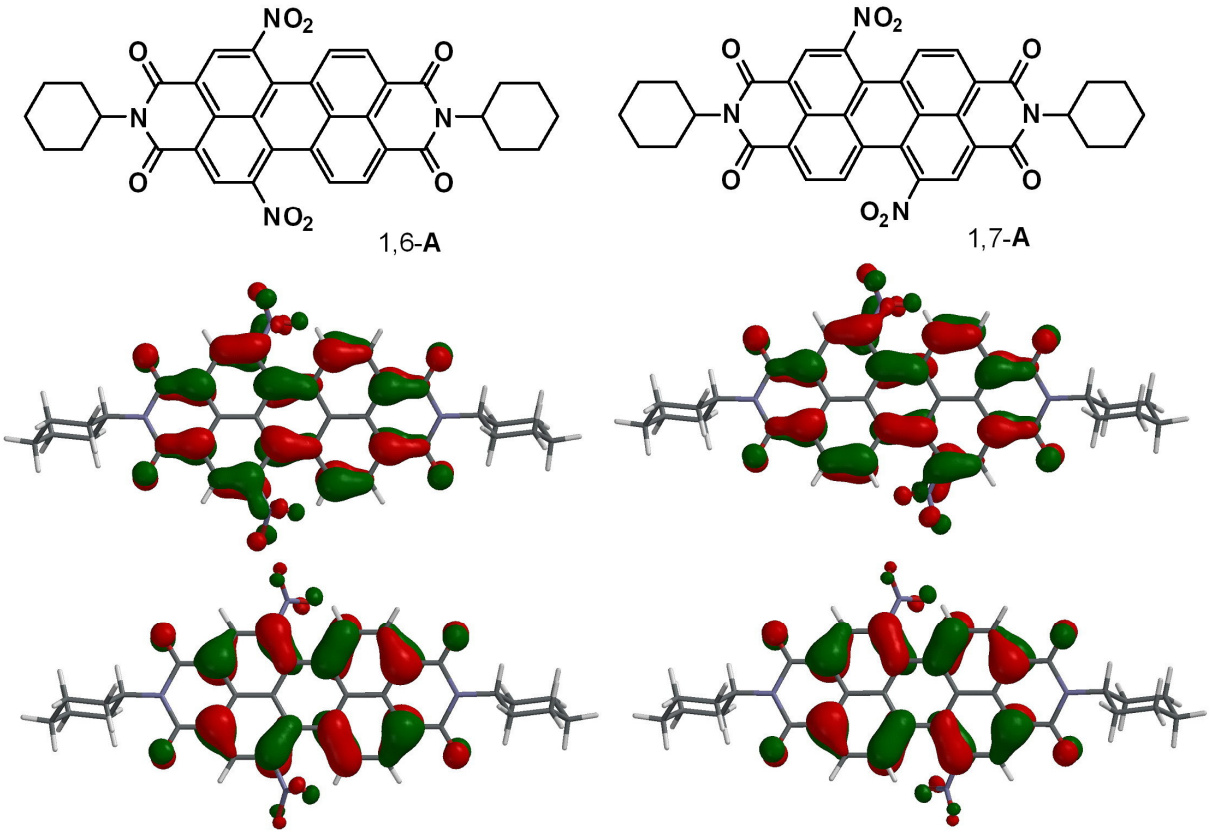

Figure S4. DFT (B3LYP/6-31G**) geometry-optimized structures of 1,6-**B** (left) and 1,7-**B** (right) shown with view along the long axis. For computational purposes, methyl groups replace the cyclohexyl groups at the imide positions.

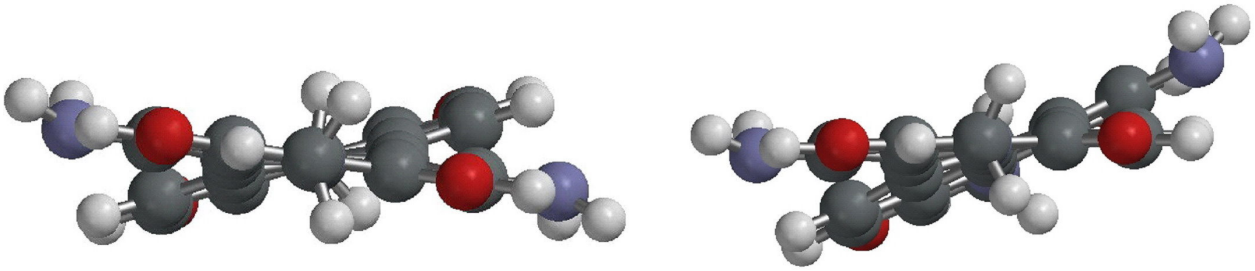

Table S1. Selected electronic excitation energies and corresponding oscillator strengths (*f*), main configurations, and CI coefficients of the low-lying electronically excited states of **B** and **C** [a].

Compound	Singlet	Electronic transition	Energy	*f*	Composition [b]	CI [c]
1,6-C	UV–Vis	$S_0 \rightarrow S_1$	2.17 eV/571 nm	0.4161	H→L	0.70363
					H-1→L	0.18917
		$S_0 \rightarrow S_2$	2.97 eV/417 nm	0.1133	H→L+1	0.66735
1,7-C	UV–Vis	$S_0 \rightarrow S_1$	2.16 eV/573 nm	0.4947	H→L	0.70363
					H-1→L	0.64469
		$S_0 \rightarrow S_2$	2.97 eV/418 nm	0.0304	H→L+1	0.24965
1,6-B	UV–Vis	$S_0 \rightarrow S_1$	2.22 eV/558 nm	0.5806	H→L	0.70663
					H-1→L	0.69227
		$S_0 \rightarrow S_2$	2.74 eV/452 nm	0.0692	H→L+4	0.11954
1,7-B	UV–Vis	$S_0 \rightarrow S_1$	2.14 eV/579 nm	0.5645	H→L	0.70753
					H-1→L	0.68128
		$S_0 \rightarrow S_2$	2.95 eV/420 nm	0.0036	H→L+1	0.12636
1-B	UV–Vis	$S_0 \rightarrow S_1$	2.26 eV/547 nm	0.6165	H→L	0.70581
		$S_0 \rightarrow S_2$	3.11 eV/399 nm	0.1002	H-1→L	0.68061

[a] Calculated by TDDFT/B3LYP/6-31G**; [b] H stands for HOMO and L stands for LUMO. Only the main configurations are presented; [c] CI coefficients are in absolute values.