Electronic Supplementary Information (ESI)

Photochemical Stability of High Efficiency PTB7:PC70BM Solar Cell Blends

Joseph Razzell-Hollis,[a] Jessica Wade,[a] Wing Chung Tsoi,[a] Ying Soon,[b] James Durrant,[b] and Ji-Seon Kim[a,*]

[a] *Department of Physics and Centre for Plastic Electronics, Imperial College London, London SW7 2AZ, United Kingdom*

[b] *Department of Chemistry and Centre for Plastic Electronics, Imperial College London, London SW7 2AZ, United Kingdom*

**E-mail: ji-seon.kim@imperial.ac.uk*

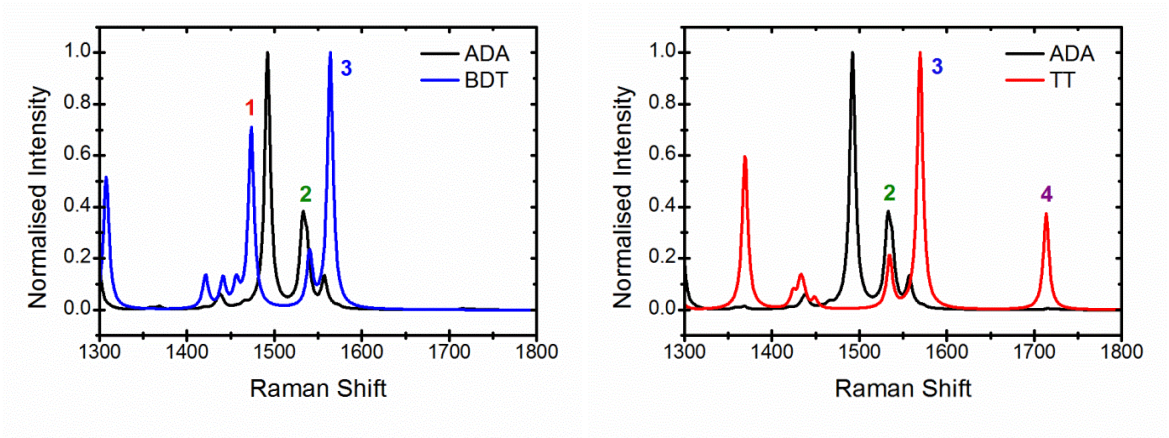


Figure S1: Theoretical Raman spectra of an ADA oligomer of PTB7 and of isolated TT (A) and BDT (D) units, simulated by Density Functional Theory in order to assign vibrational modes to specific bonds on PTB7

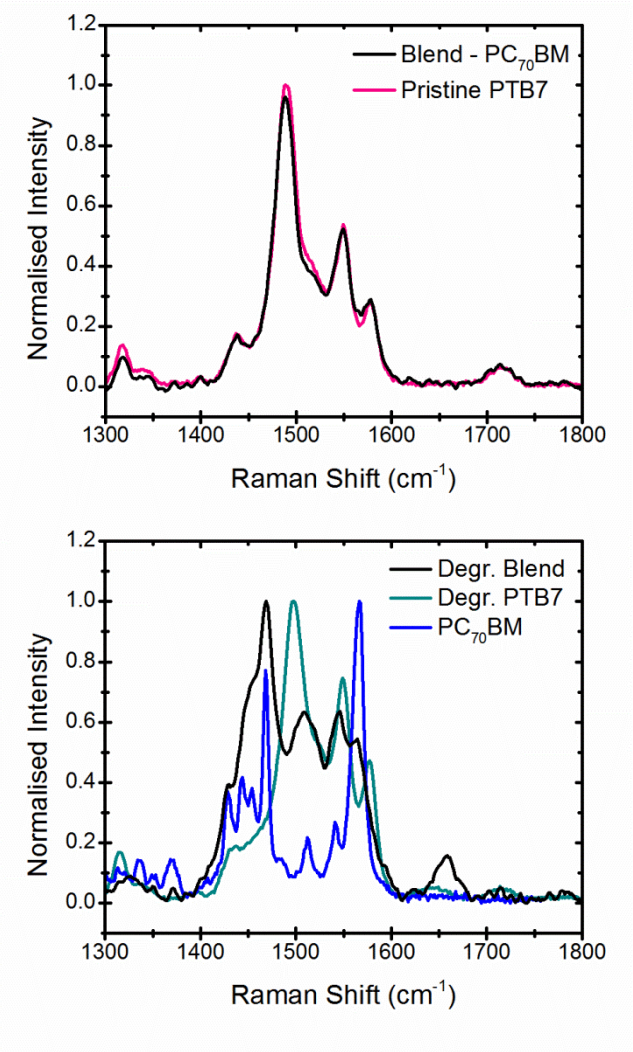


Figure S2: a) Normalised Raman spectrum of the PTB7:$PC_{70}BM$ blend film, before and after subtraction of the neat $PC_{70}BM$ spectrum, which restores Peaks 1-3 of the original neat PTB7 spectrum (also shown). b) Normalised Raman spectrum of the degraded blend compared to neat films of $PC_{70}BM$ and degraded PTB7.

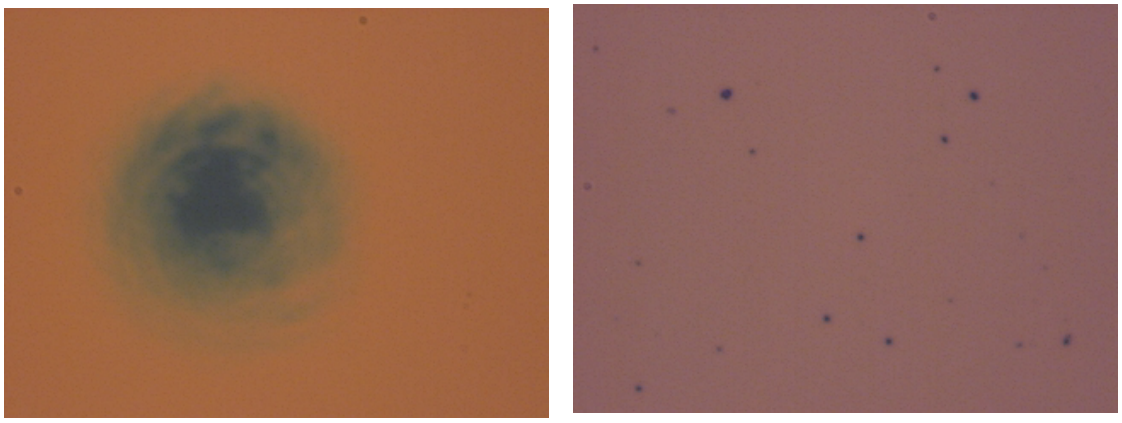
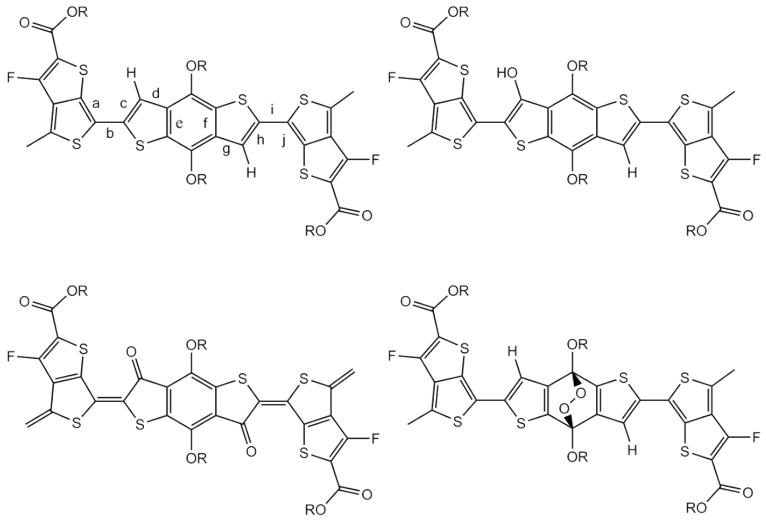


Figure S3 Optical micrographs of neat PTB7 (left) and blended PTB7:$PC_{70}BM$ (right) films exposed to the 488nm laser at ~0.9mW for 10min.



Bond	Bond Length [pm]	Length Change [pm]	
	Pristine PTB7	Hydroxy-PTB7	Dihydroxy-PTB7
a	138.21	0.29	2.51
b	144.49	-0.19	-3.13
c	137.10	0.37	9.57
d	143.22	0.72	3.39
e	142.48	-0.65	-1.13
f	142.46	0.18	-0.91
g	143.07	0.01	3.33
h	137.13	-0.12	9.77
i	144.53	-0.04	-3.99
j	138.23	0.00	1.83

Figure S4: a) Molecular structures for ADA oligomers of pristine PTB7 and three potential degradation products: hydroxyl-PTB7, diketo-PTB7, peroxy-PTB7. b) Table of major bond lengths on the conjugated backbone of pristine PTB7, with bond length changes for the hydroxy-PTB7 and diketo-PTB7 products.

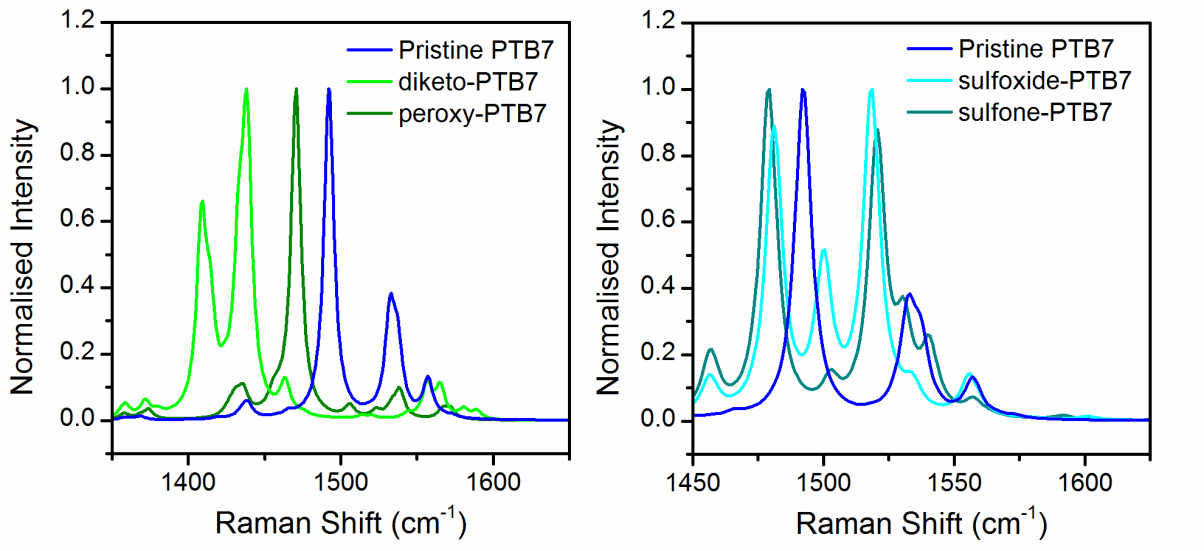


Figure S5: Theoretical Raman spectra for other oxidised products investigated, including oxidation of the BDT unit to form a diketone or an *endo*-peroxide (left) and oxidation of the TT unit to form a sulfoxide or a sulfone (right).