Synthesis, characterization and use of a POSS-Arylamine Based Push-Pull Octamer

Pablo Simón Marqués,[a] José María Andrés Castán,[a] Amir Hossein Habibi,[a] Sylvie Dabos-Seignon,[a] Sébastien Richeter,[b] Ahmad Mehdi,[b] Sébastien Clément,[b*] Philippe Blanchard,[a*] and Clément Cabanetos [a*]

[a] CNRS UMR 6200, MOLTECH-Anjou, University of Angers, 2 Bd Lavoisier, 49045 Angers, France;
[b] ICGM, Univ Montpellier, CNRS, ENSCM, 34095 Montpellier, France

Table of contents

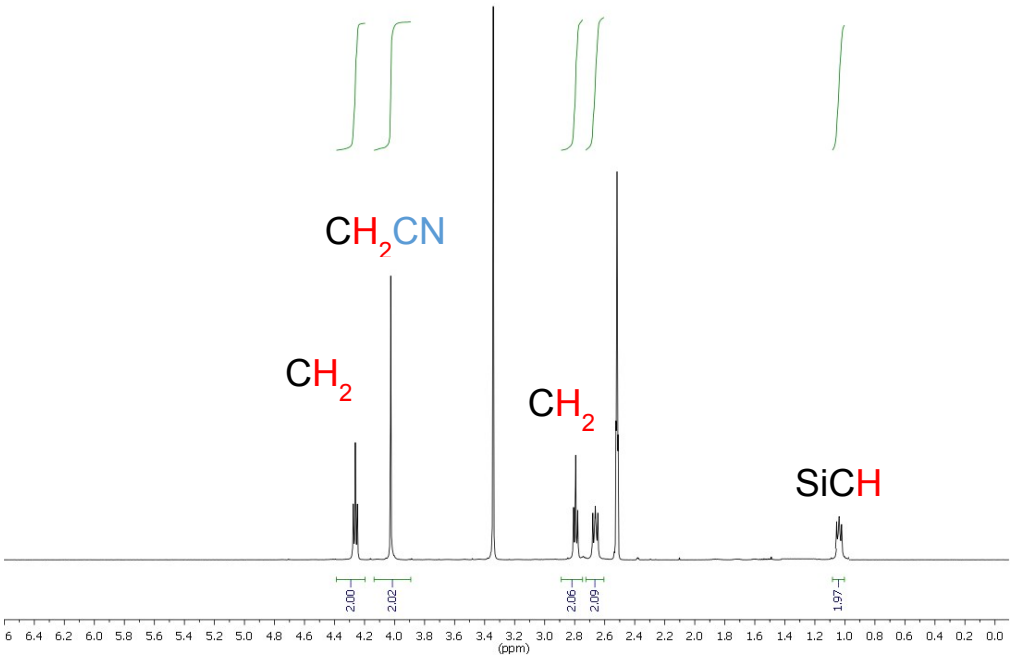


Figure S1. ^{1}H-NMR (DMSO-d_6, 500 MHz) spectrum of compound **3** recorded at 20 °C.

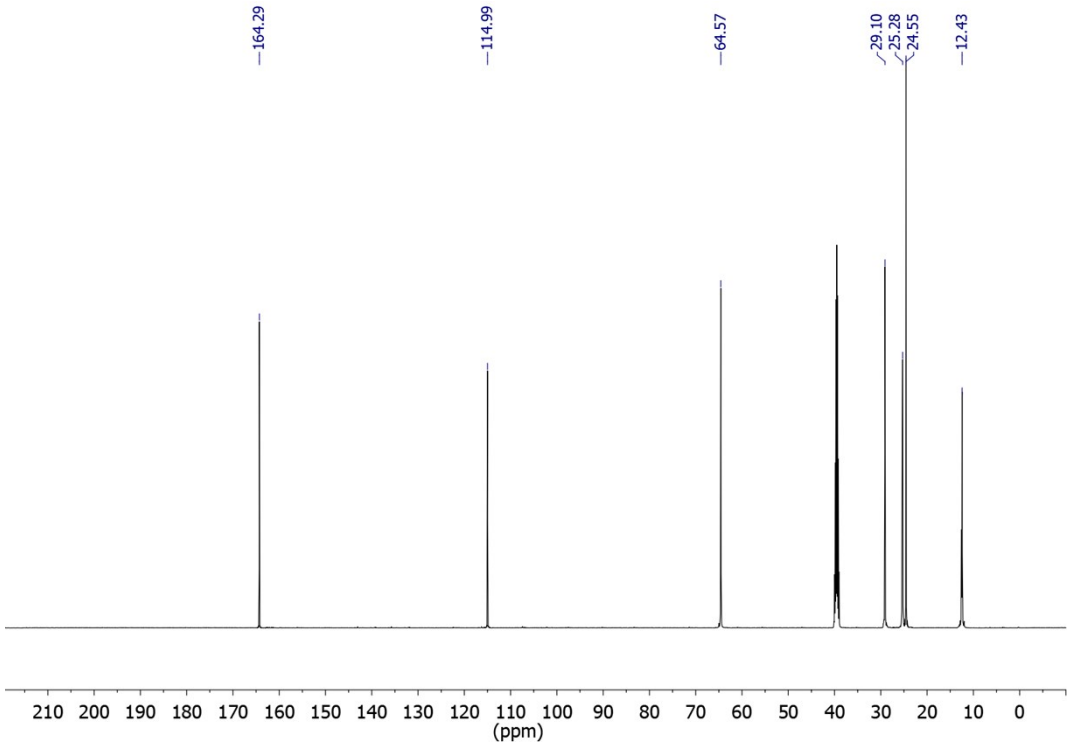


Figure S2. ^{13}C{^{1}H}-NMR (DMSO-d_6, 125 MHz) spectrum of compound **3** recorded at 20 °C.

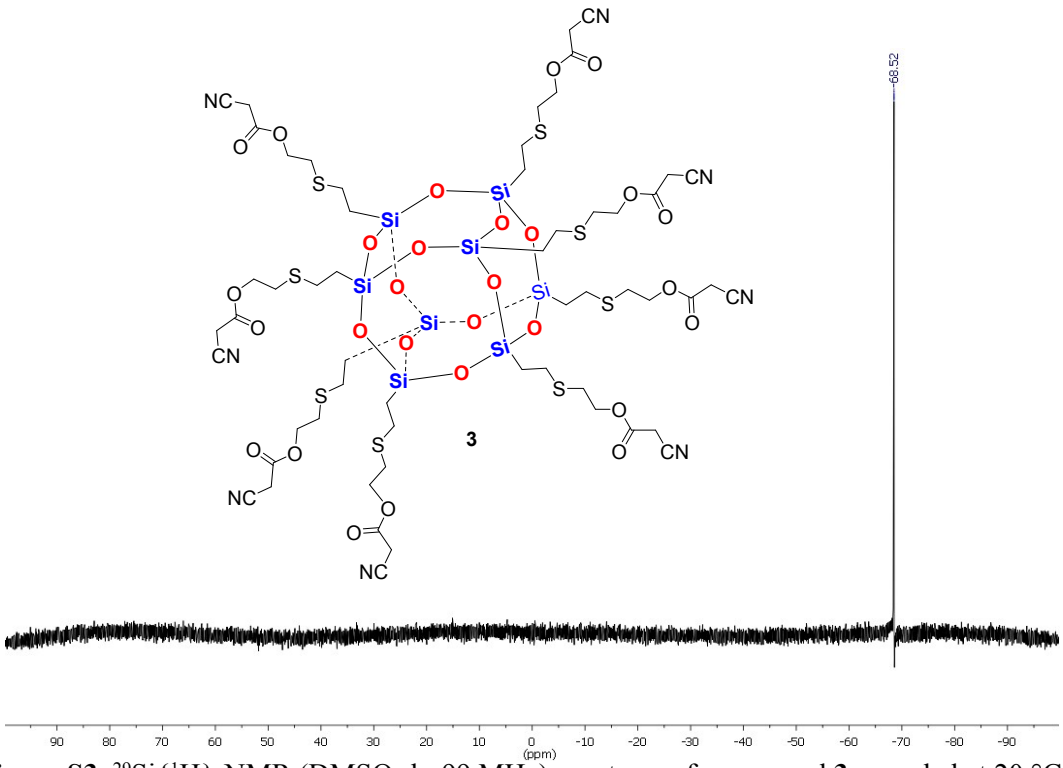


Figure S3. $^{29}Si\{^{1}H\}$-NMR (DMSO-d_6, 99 MHz) spectrum of compound **3** recorded at 20 °C.

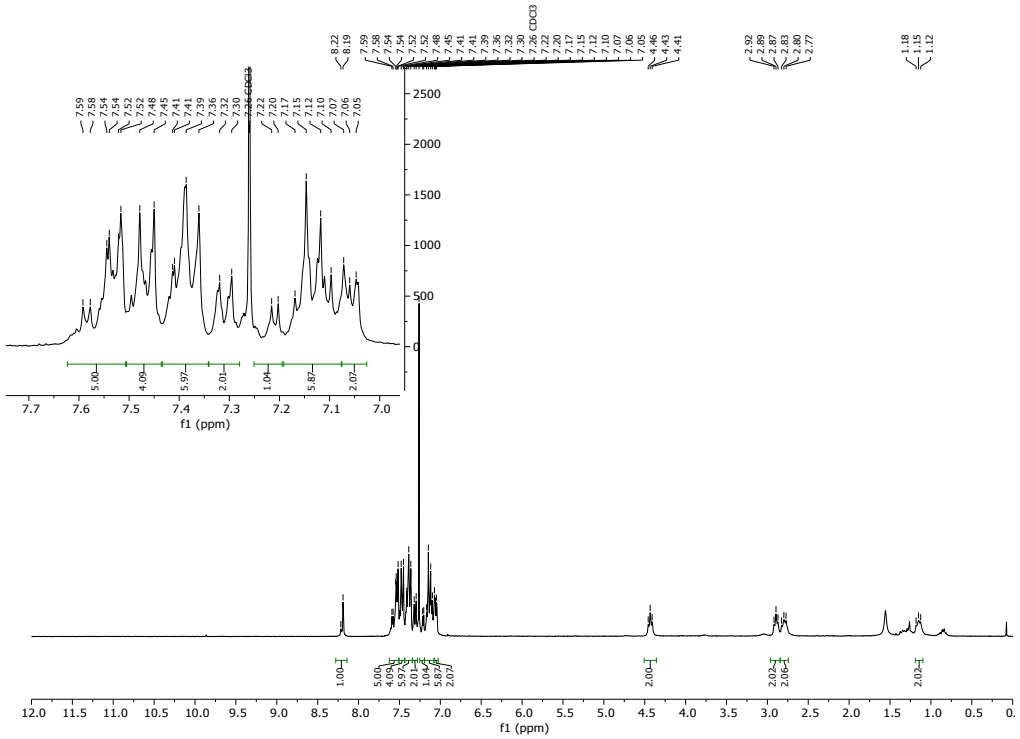


Figure S4. ^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **EA-POSS** recorded at 20 °C.

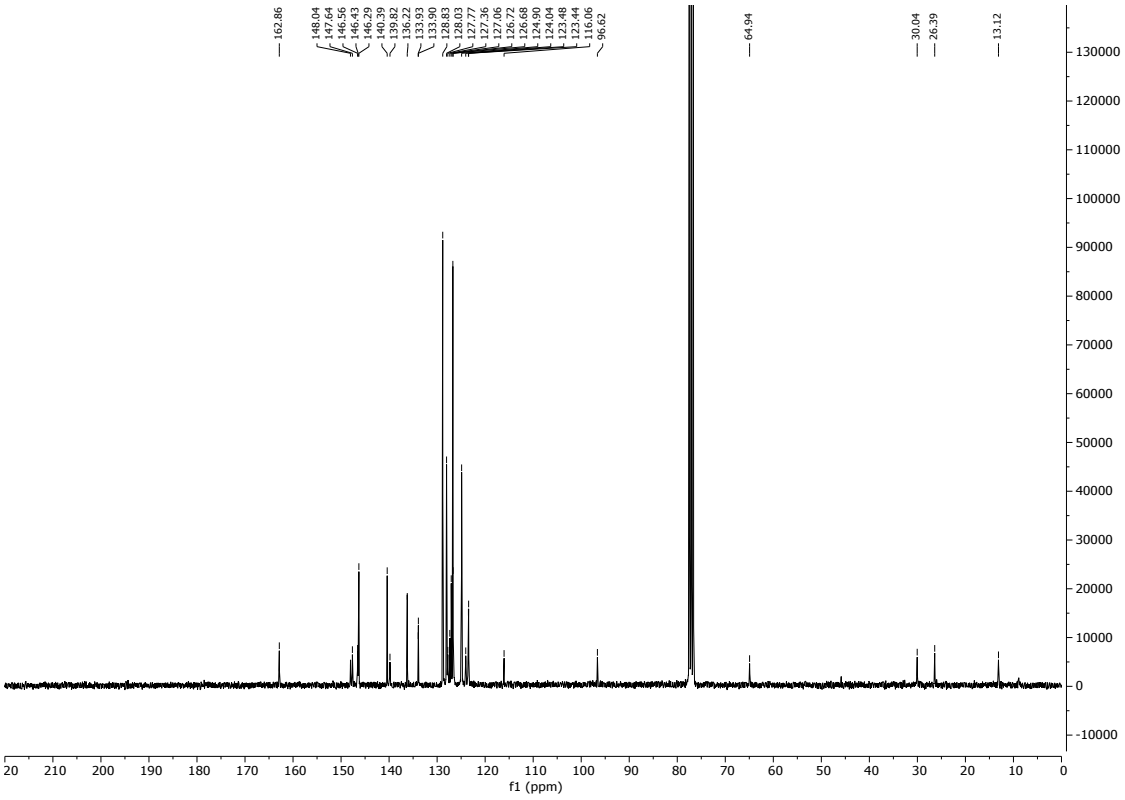


Figure S5. ^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **EA-POSS** recorded at 20 °C.

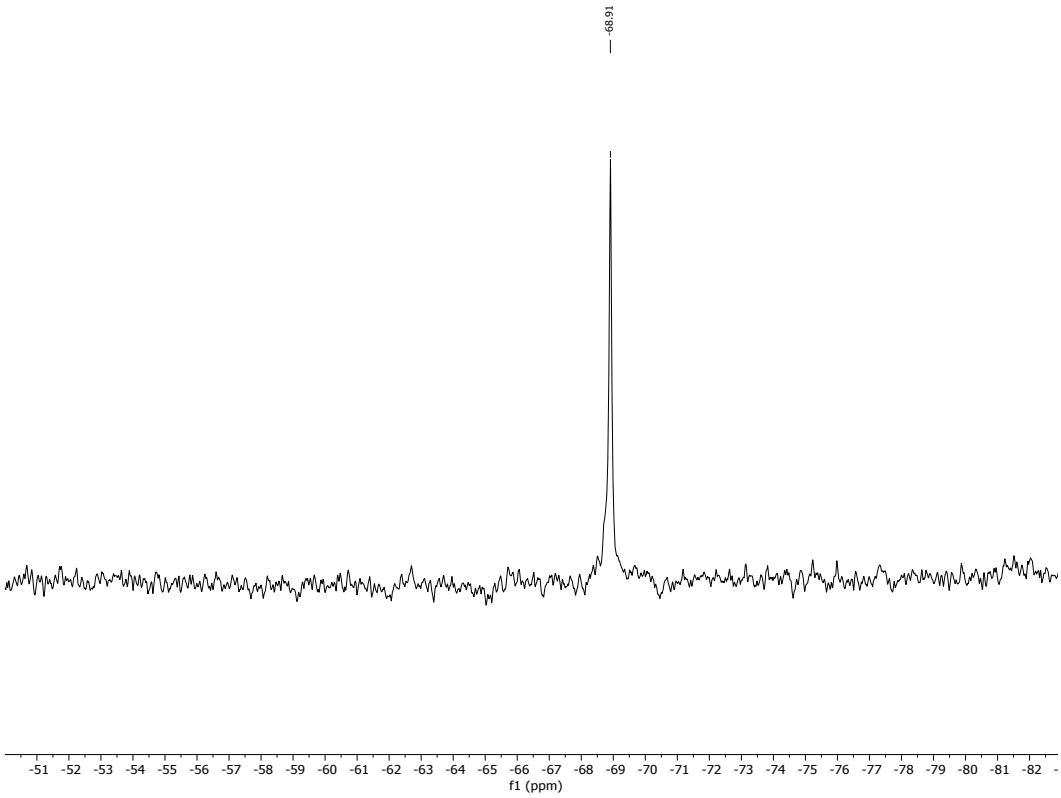


Figure S6. ^{29}Si{^{1}H}-NMR ($CDCl_3$, 59.6 MHz) spectrum of **EA-POSS** recorded at 20 °C.

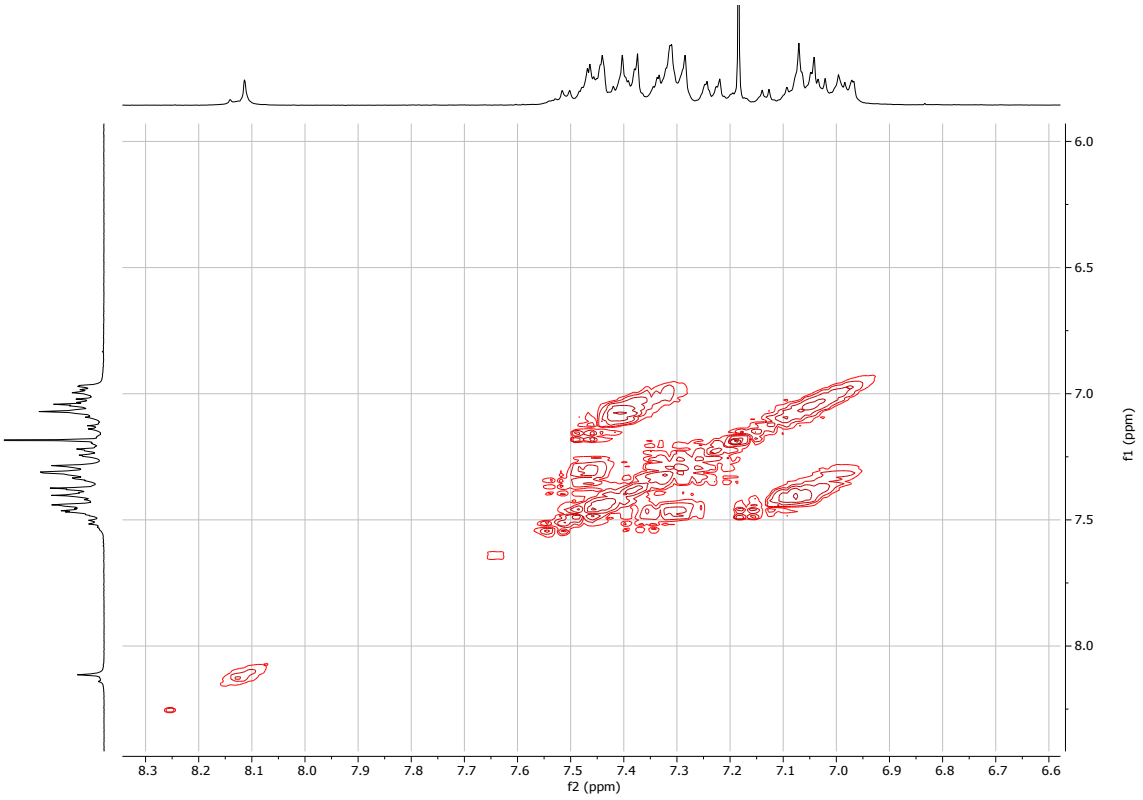


Figure S7. 2D-COSY ($CDCl_3$, 300 MHz) aromatic zoom of **EA-POSS** recorded at 20 °C.

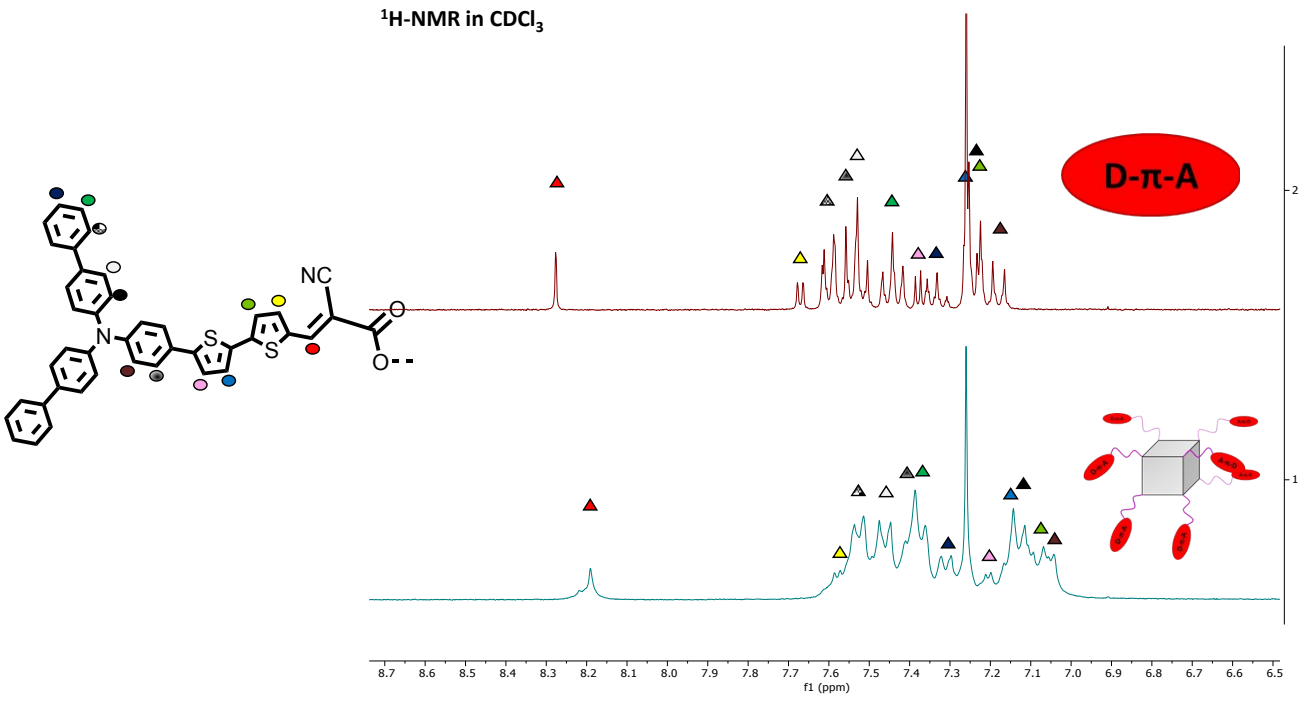


Figure S8. [1]H-NMR aromatic comparison and signal assignment of monomer **EA-M** (top) and octamer **EA-POSS** (bottom).

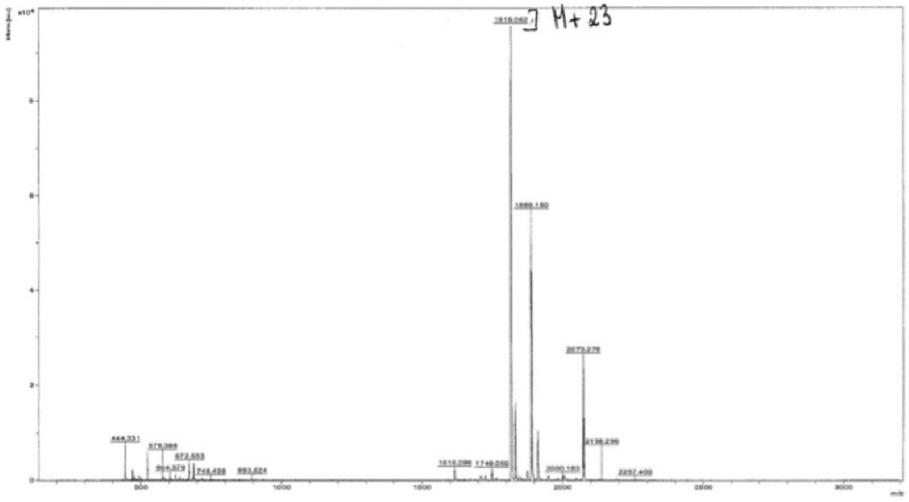
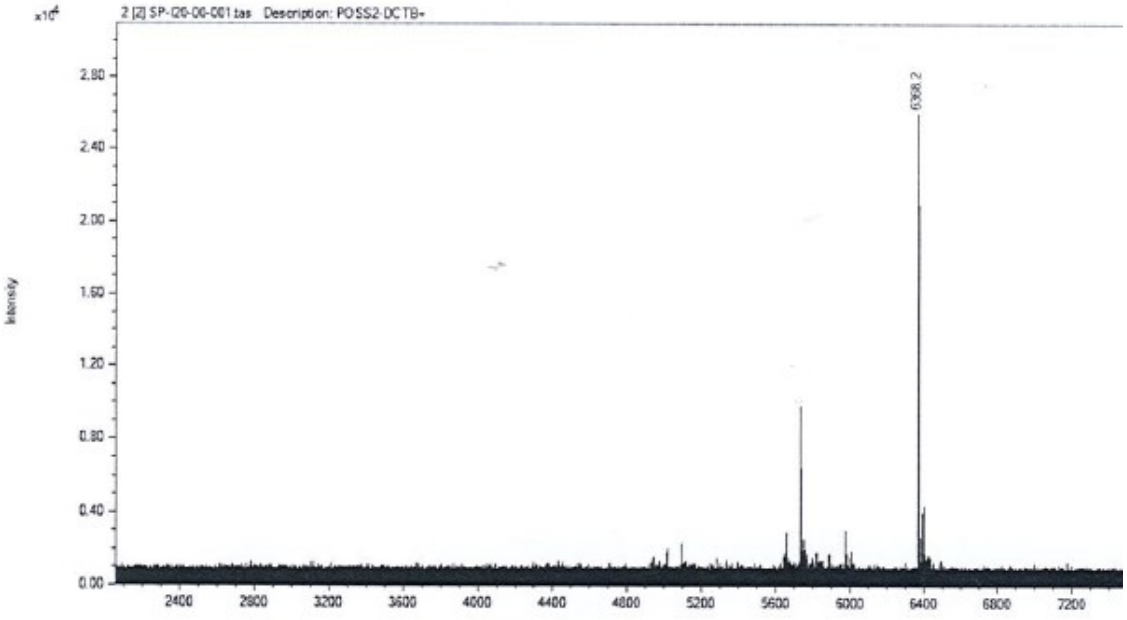


Figure S9. MALDI-TOF MS (DCTB+) of **3**.



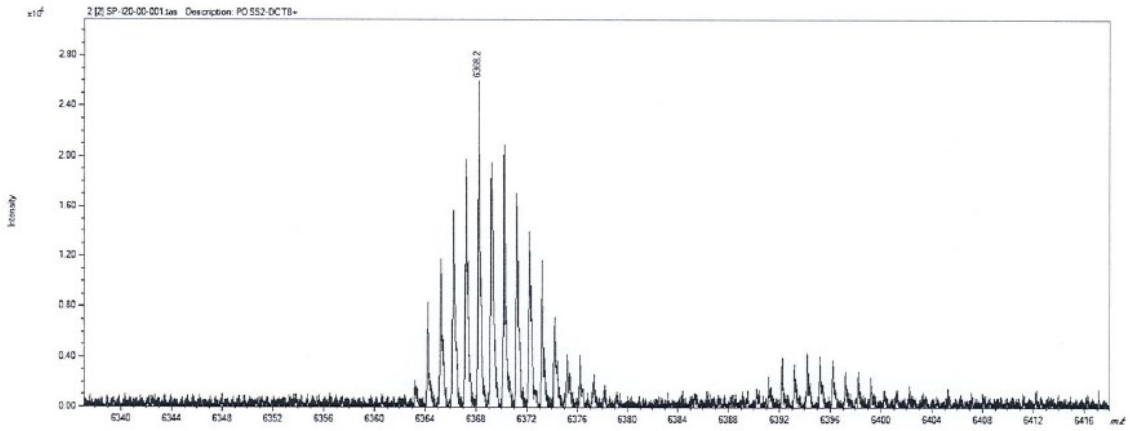


Figure S10. MALDI-TOF MS (DCTB+) of **EA-POSS**.

IR spectra

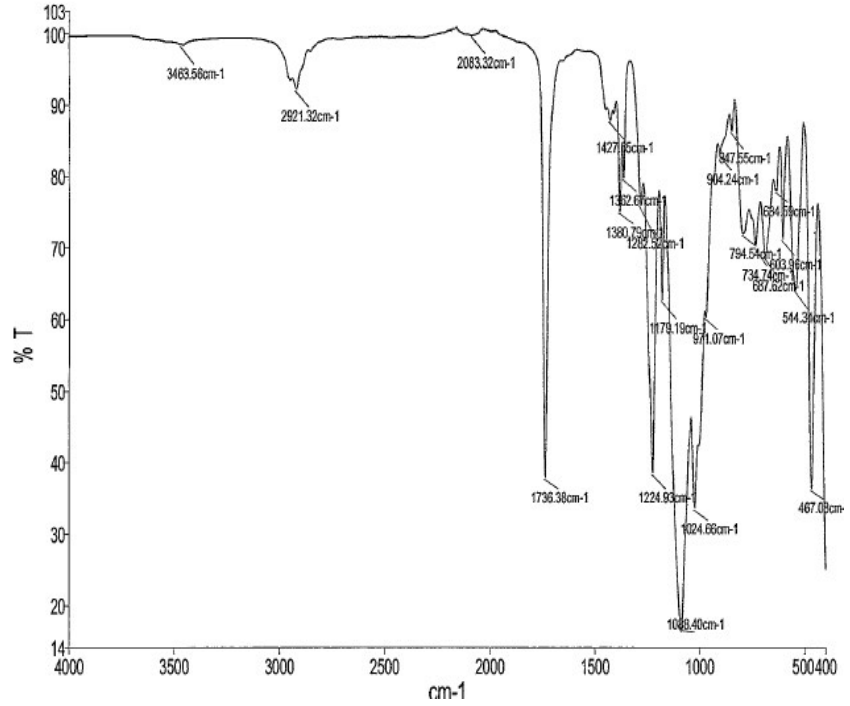


Figure S11. IR spectrum of **3**.

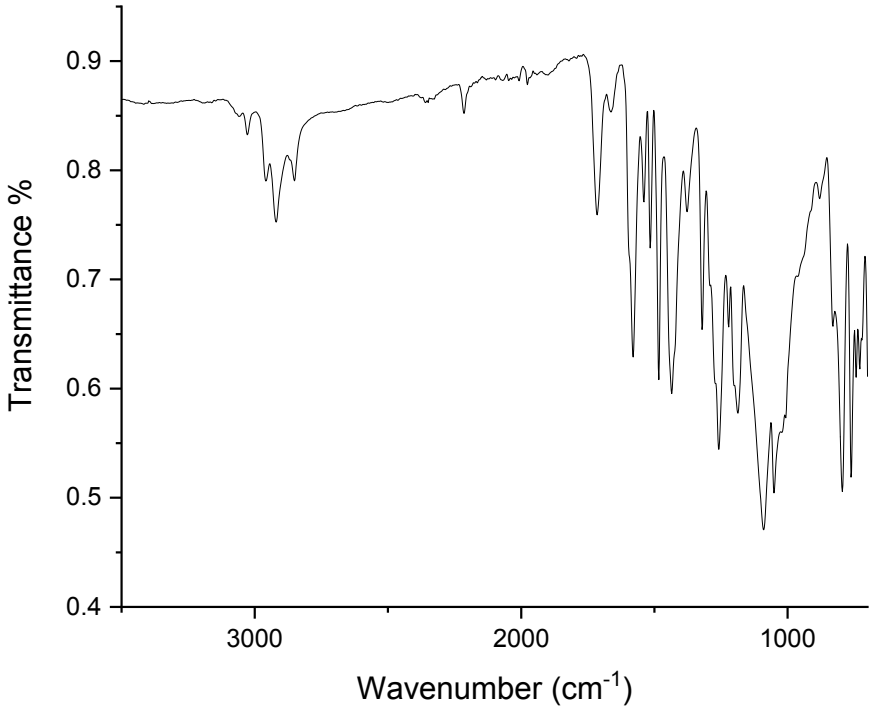
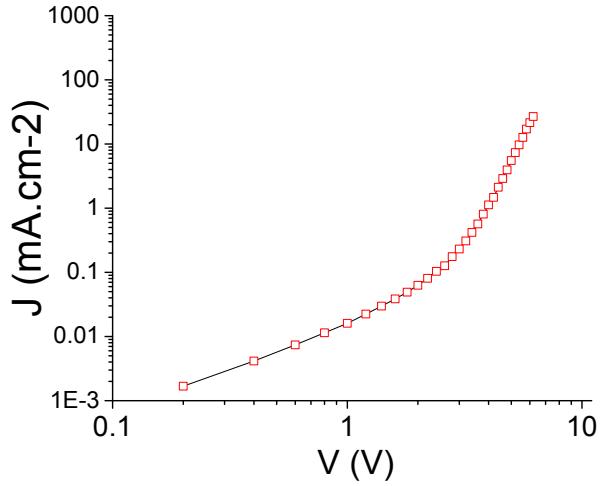


Figure S12. IR spectrum of neat **EA-POSS**.

Table S1. Photovoltaic characteristics of the BHJ cells based on $PC_{61}BM$ blended with **EA-POSS**. Measurements performed under an AM. 1.5 simulated solar illumination (100 $mW.cm^{-2}$). Averages values and standard deviation collected on 6 devices in parentheses.

Compound	D:A Ratio (w:w)	Voc (V)	Jsc (mA cm-2)	FF (%)	PCE (%)
$PC_{61}BM$	1:1	0.92 (0.91±0.02)	3.70 (3.62±0.21)	35.63 (35.89±0.84)	1.21 (1.17±0.04)
	1:2	0.95 (0.93±0.03)	4.11 (417±0.13)	36.67 (35.86±1.46)	1.44 (1.38±0.04)
	1:3	0.88 (0.86±0.05)	3.50 (3.34±0.20)	36.54 (36.60±1.20)	1.13 (1.05±0.06)
$PC_{71}BM$	1:1	0.93 (0.94±0.02)	5.34 (5.24±0.11)	36.21 (35.35±0.95)	1.80 (1.73±0.07)
	1:2	0.96 (0.95±0.01)	7.21 (7.09±0.12)	36.05 (35.45±0.51)	2.50 (2.39±0.07)
	1:3	0.95 (0.95±0.01)	5.01 (4.70±0.31)	36.01 (35.10±0.76)	1.71 (1.56±0.13)

Device Fabrication and Characterization



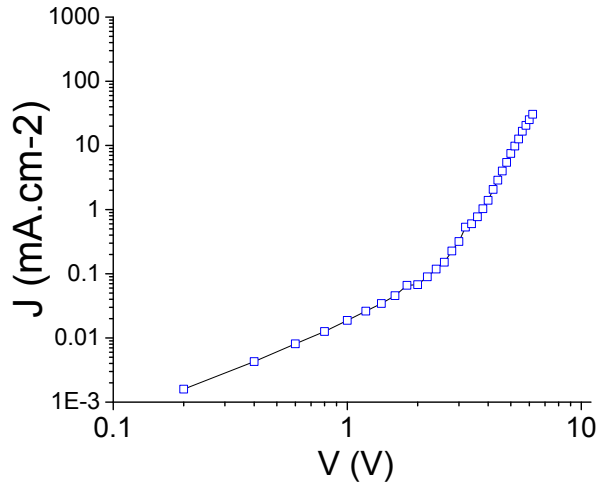


Figure S13. J–V characteristics of hole only devices ITO/PEDOT:PSS/ EA-POSS:$PC_{61}BM$ (red) or EA-POSS:$PC_{71}BM$ (blue)/Au.

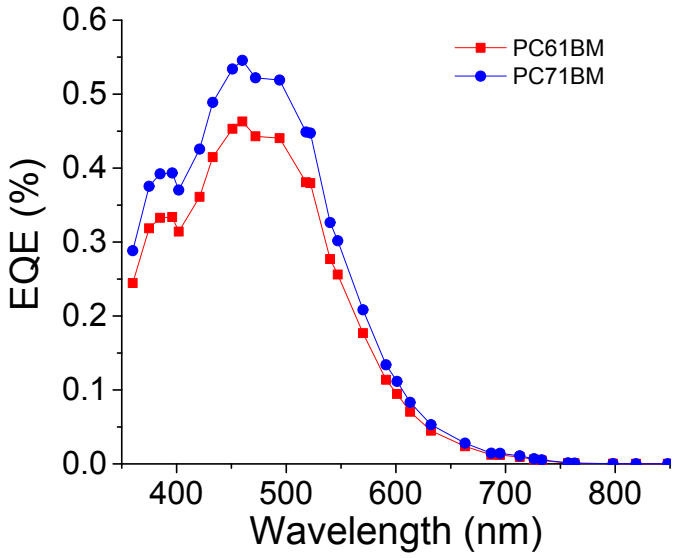


Figure S14 External quatum efficiency spectra of the best working solar cells (1:2 D:A ratio)

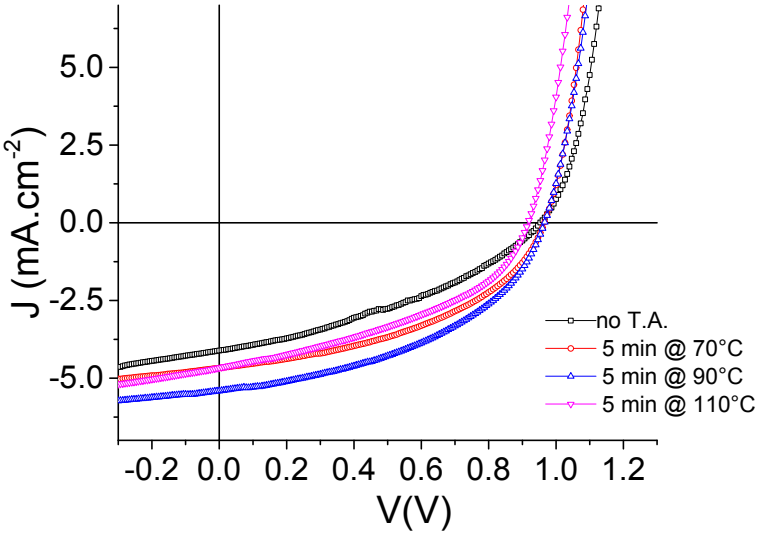


Figure S15. Effect of a thermal treatment on a **$PC_{61}BM$** based solar cell (D:A = 1:2)

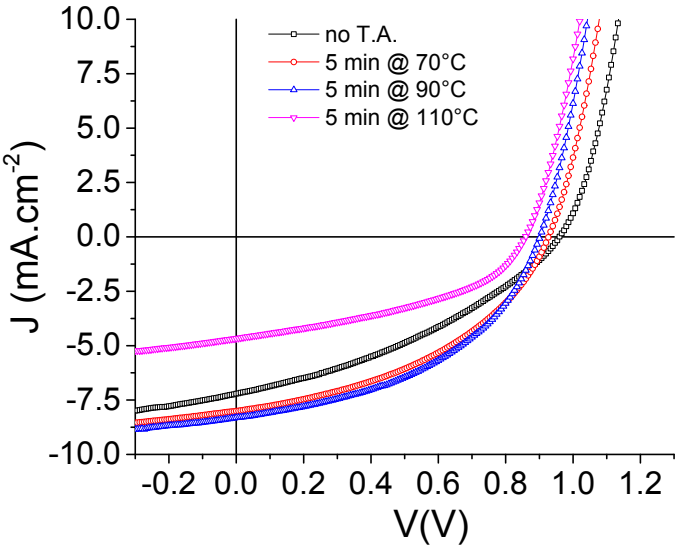


Figure S16. Effect of a thermal treatment on a **$PC_{71}BM$** based solar cell (D:A = 1:2)