SUPPORTING INFORMATION

Poly(triphenyl ethene) and poly(tetraphenyl ethene): Synthesis, aggregation-induced emission property and application as paper sensors for effective nitro-compounds detection†

Hui Zhou,[a] Xiaobai Wang,[a] Ting Ting Lin,[a] Jing Song,[a] Ben Zhong Tang*[b] and Jianwei Xu*[ac]

*[a]Institute of Materials Research and Engineering, Agency for Science, Technology and Research (A*STAR), 2 Fusionopolis Way, Innovis, #08-03, Singapore 138634.*
[b]Department of Chemistry, The Hong Kong University of Science & Technology, Clear Water Bay, Kowloon, Hong Kong, China.
[c]Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore 117543.

* Corresponding author: Jianwei Xu
Email address: jw-xu@imre.a-star.edu.sg
Mailing address: 2 Fusionopolis Way, Innovis, #08-03, Singapore 138634
Tel: 65-6872-7543
Fax: 65-6872-7528

Table content

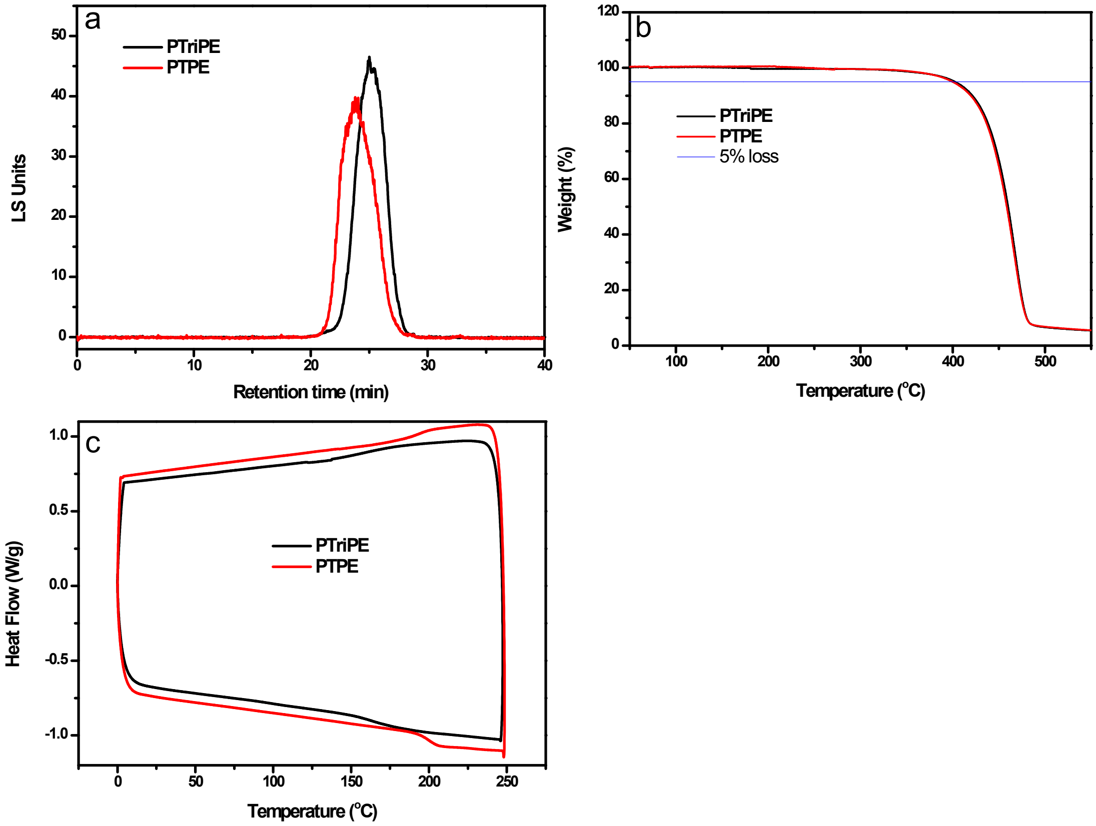

Fig. S1 (a) GPC spectrum of polymers **PTriPE** and **PTPE** in THF. (b) TGA thermograms of polymers **PTriPE** and **PTPE** under nitrogen at a heating rate of 20 °C·min^{-1}. (c) DSC thermograms of polymers **PTriPE** and **PTPE** under nitrogen at a heating rate of 20 °C·min^{-1}.

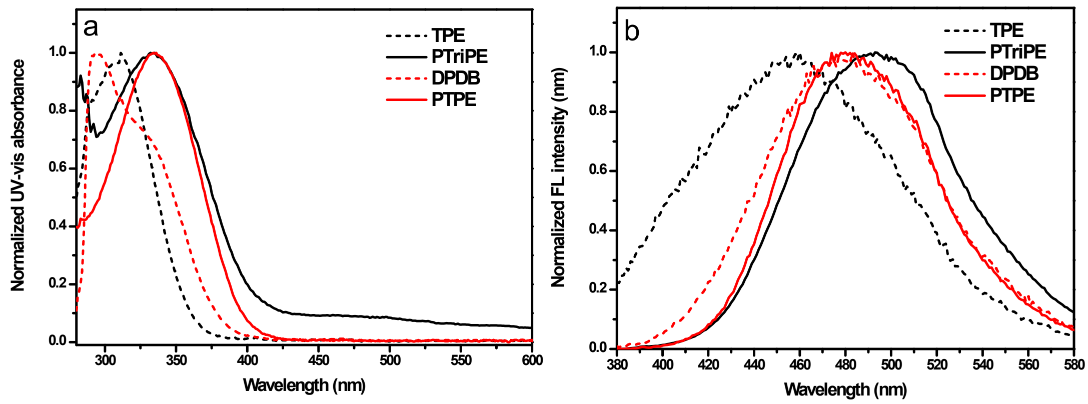

Fig. S2 UV-Vis (a) and fluorescence spectra (b) of **TPE**, **DPDB**, **PTriPE** and **PTPE** in THF, THF/H_2O (1:9 v/v) mixture.

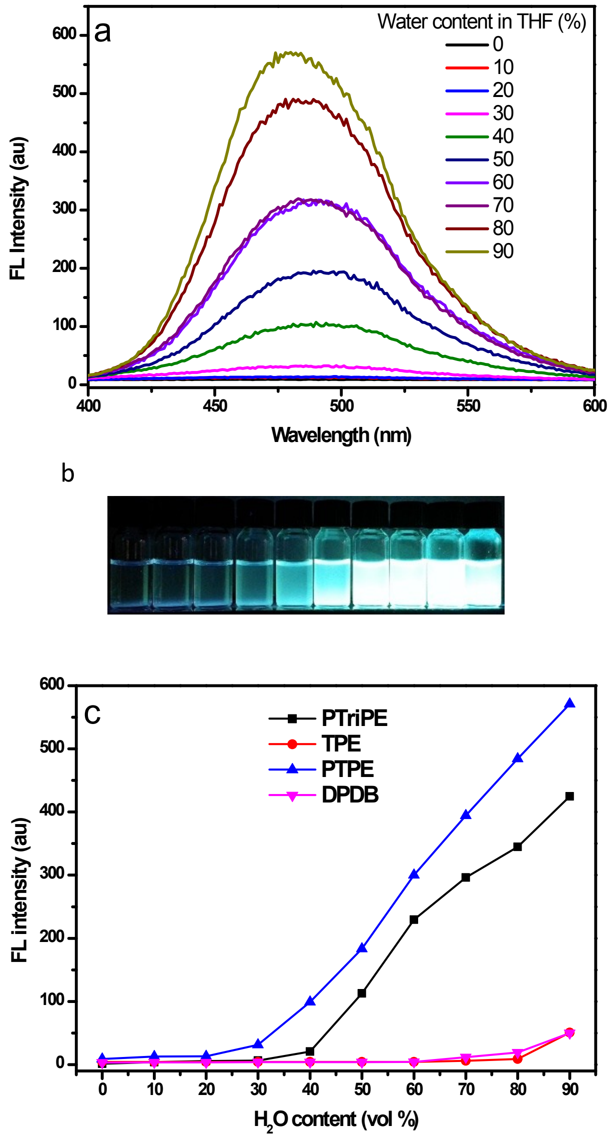

Fig. S3 (a) Fluorescence spectra of polymer **PTPE** in THF/H_2O mixtures with different H_2O contents (λ_{ex} = 334 nm, [**PTPE**] = 100.0 μg·mL^{-1}). (b) The photographs of **PTPE** solutions taken under UV illumination (λ_{ex} = 365 nm)). (c) Fluorescence intensity maximum of **TPE**, **DPDB**, **PTriPE** and **PTPE** with the same weight percentage in THF/H_2O mixtures ([C] = 100.0 μg·mL^{-1}).

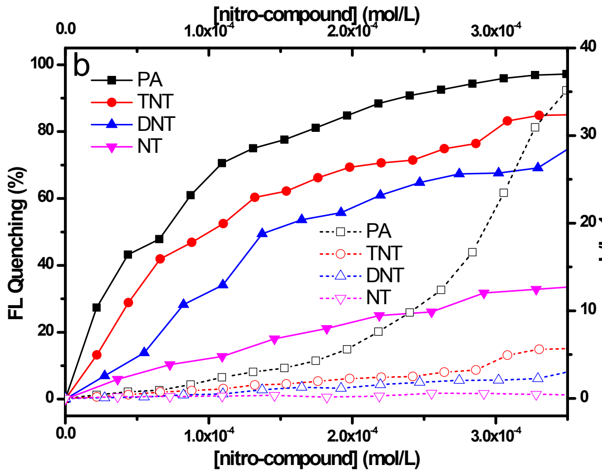

Fig. S4 Concentration-dependent fluorescence quenching of **PTPE** by nitro compounds. [**PTPE**] = 100.0 μg·mL^{-1} in THF/H_2O (1:9 v/v) mixture.

Table S1. Processing parameters for drop coating (F1) and spin coating preparation (F2), and electrohydrodynamic preparation (F3-F4).

Unit	Concentration (wt%)	Voltage (kV)	Flow rate (mL/h)	Distance (cm)	Time (h)
F1 (**PTriPE**)	2.0	Drop coating			
F2 (**PTriPE**)	2.0	Spin coating			
F3 (**PTriPE**)	2.0	9.7	4.0	10.0	1.0
F4 (**PTPE**)	2.0	9.7	4.0	10.0	1.0

[a] Experiments were performed in duplicate and mean values were taken.

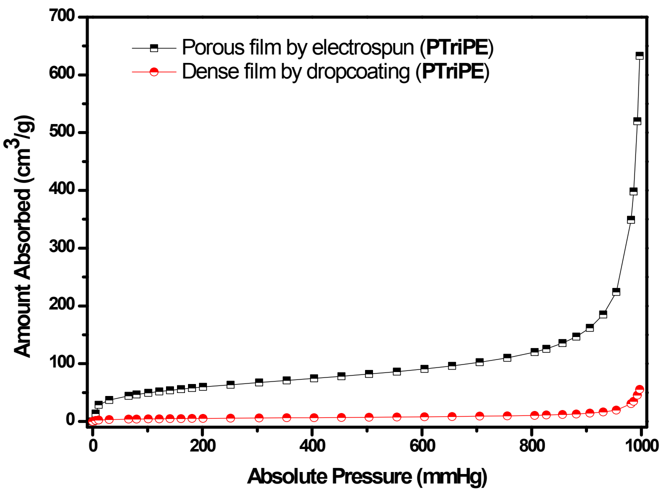

Fig. S5 N_2 absorption isotherms at -196 ^oC for **PTriPE** porous film by electrospun and **PTriPE** dense film by drop coating.

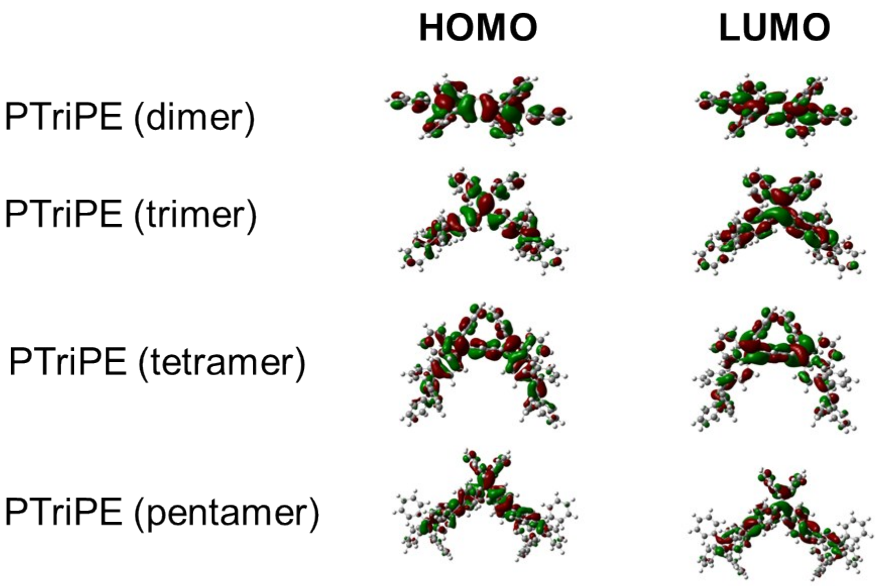

Fig. S6 Optimized molecular structures and molecular orbital amplitude plots of HOMO and LUMO energy levels of the **PTriPE** calculated using the B3LYP/6-31G(d,p) basis set.

Table S2. DFT (G09 [reference 1]: B3LYP/6-31G(d,p)) calculated energy level of **PTriPE** oligomers.

Unit	HOMO (eV)	LUMO (eV)	E_g (eV)
Monomer	-5.328	-1.218	4.111
Dimer	-5.109	-1.437	3.672
Trimer	-5.043	-1.484	3.559
Tetramer	-4.987	-1.543	3.444
Pentamer	-4.969	-1.545	3.424
Hexamer	-4.940	-1.576	3.365

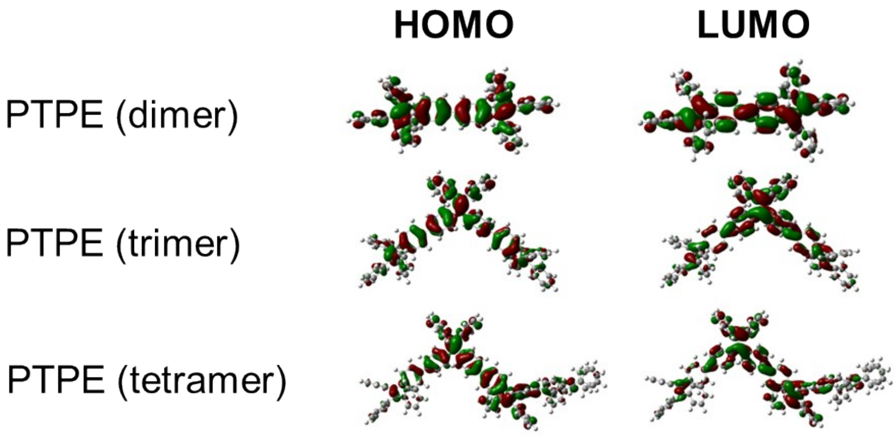

Fig. S7 Optimized molecular structures and molecular orbital amplitude plots of HOMO and LUMO energy levels of the **PTPE** calculated using the B3LYP/6-31G(d,p) basis set.

Table S3. DFT (G09 [reference 1]: B3LYP/6-31G(d,p)) calculated energy level of **PTPE** oligomers.

Unit	HOMO (eV)	LUMO (eV)	E_g (eV)
Monomer	-5.223	-1.412	3.811
Dimer	-5.144	-1.448	3.696
Trimer	-5.083	-1.513	3.570
Tetramer	-5.060	-1.527	3.533
Hexamer	-5.039	-1.551	3.487

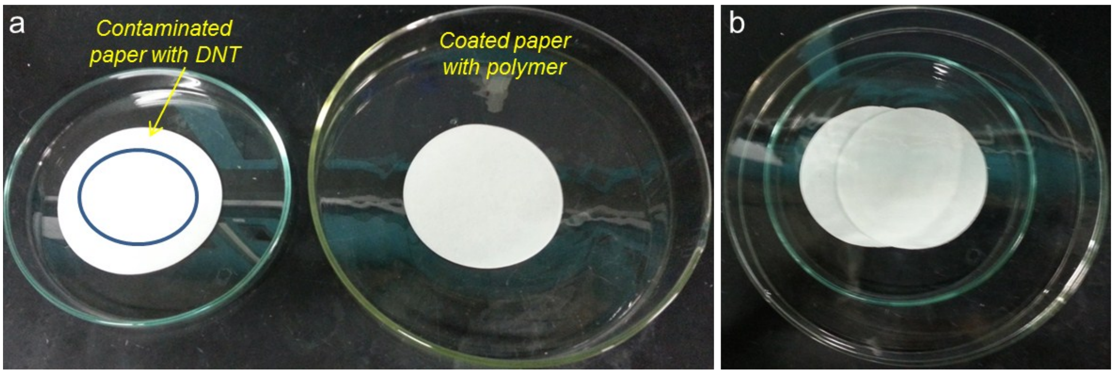

Fig. S8 The demonstration for nitro compound vapors detection. (a) The bright image of filter paper contaminated by nitro compound (left). The right one is the substrate fabricated by spray coating polymer nanoparticles of **PTriPE** in THF/H_2O (1:9 v/v) mixture onto filter paper, amounting to approximately concentration as 1.0 μg/cm^2. (b) The demonstration for DNT vapor detection.

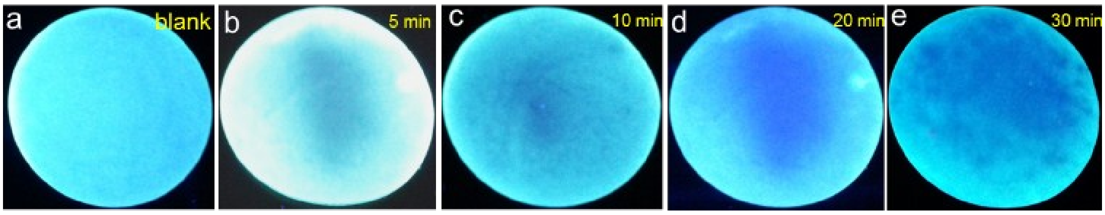

Fig. S9 The fluorescence quenching of substrate on exposure to DNT saturated vapor for different time: (a) 0 min, (b) 5 min, (c) 10 min, (d) 20 min, (e) 30 min. The images of substrate are under UV light illumination (365 nm).

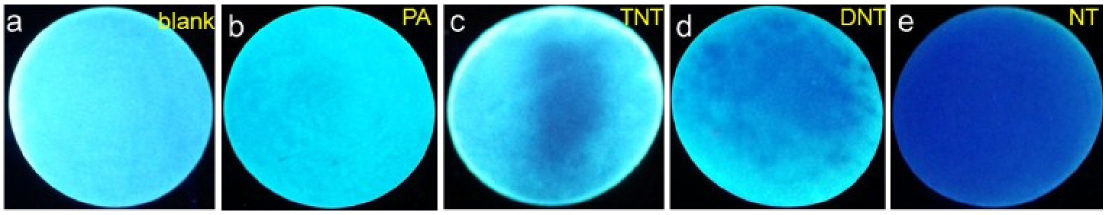

Fig. S10 The fluorescence quenching of substrate on exposure to nitro compounds vapor, the fluorescent images of substrates are check by neck eyes after 30 min. (a) The image of substrate under UV light illumination (365 nm) without nitro compound. Figure b, c, d and e are the images of substrate under UV light illumination (365 nm) after contacting for PA, TNT, DNT and NT, respectively.

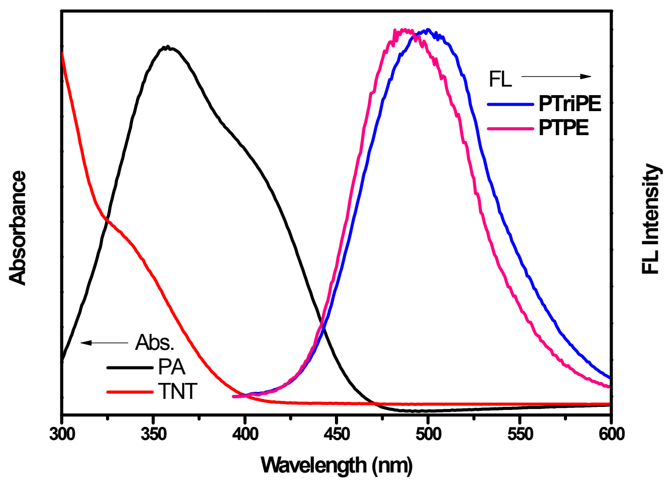

Fig. S11 The normalized UV-vis absorption of PA and TNT, and normalized fluorescence of **PTriPE** and **PTPE** in THF/H_2O (1:9 v/v).

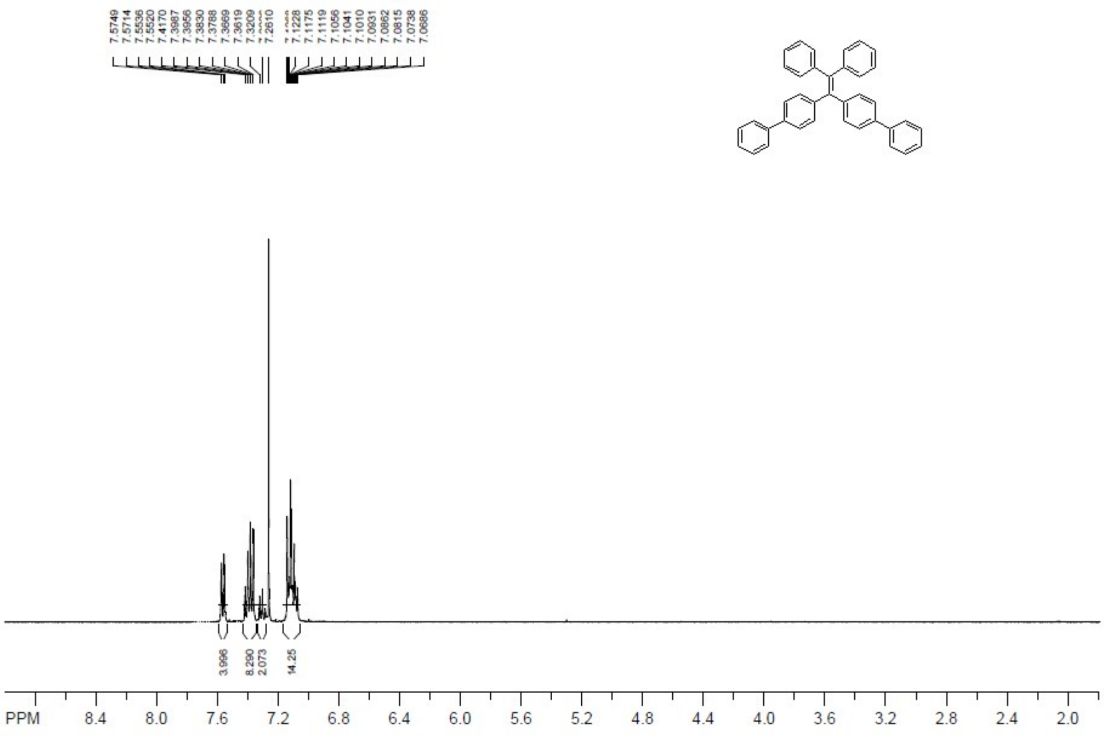

Fig. S12 ^{1}H NMR spectrum of **DPDB** in $CDCl_3$.

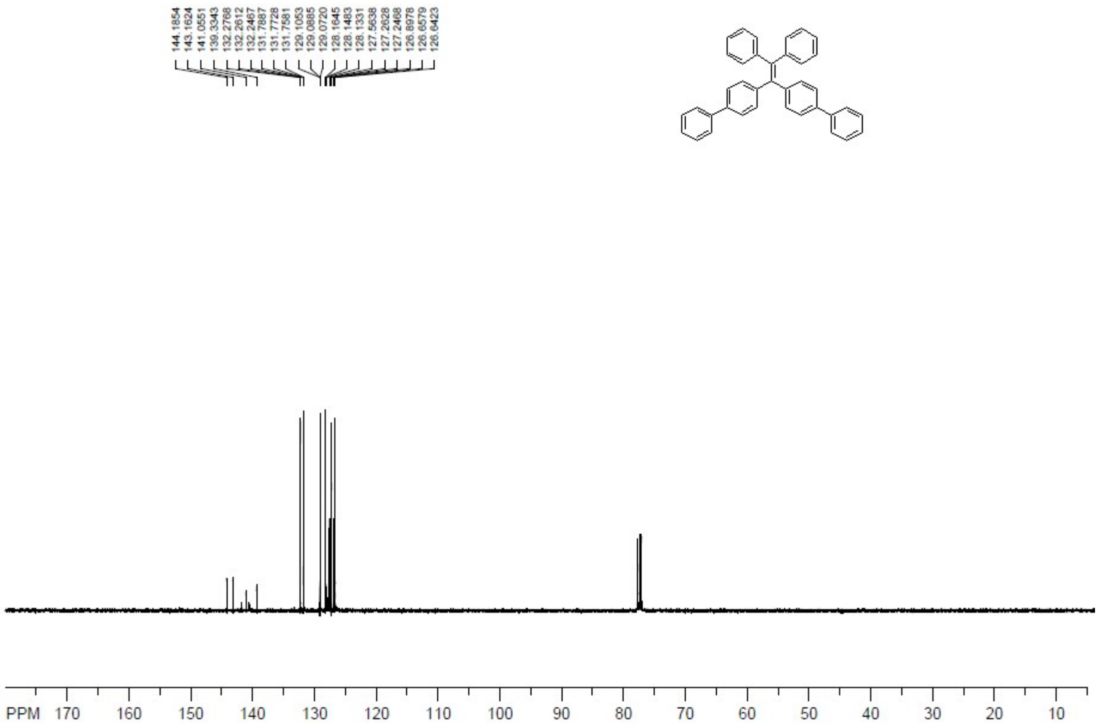

Fig. S13 ^{13}C NMR spectrum of **DPDB** in $CDCl_3$.

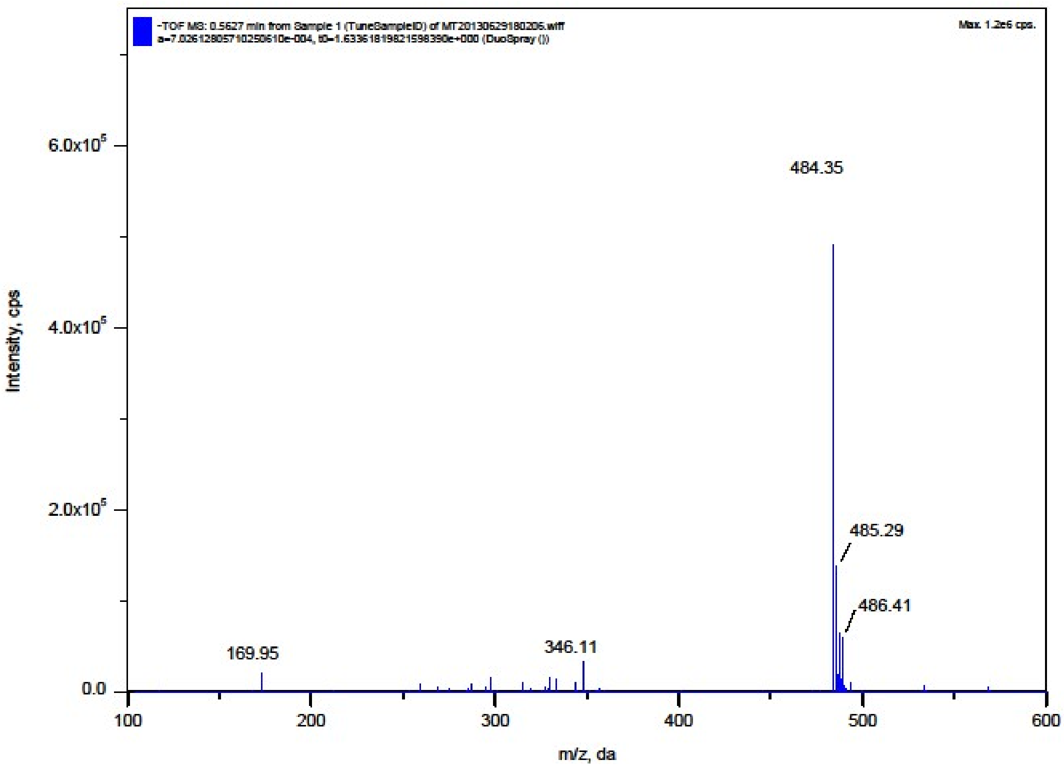

Fig. S14 MALDI-TOF of **DPDB**.

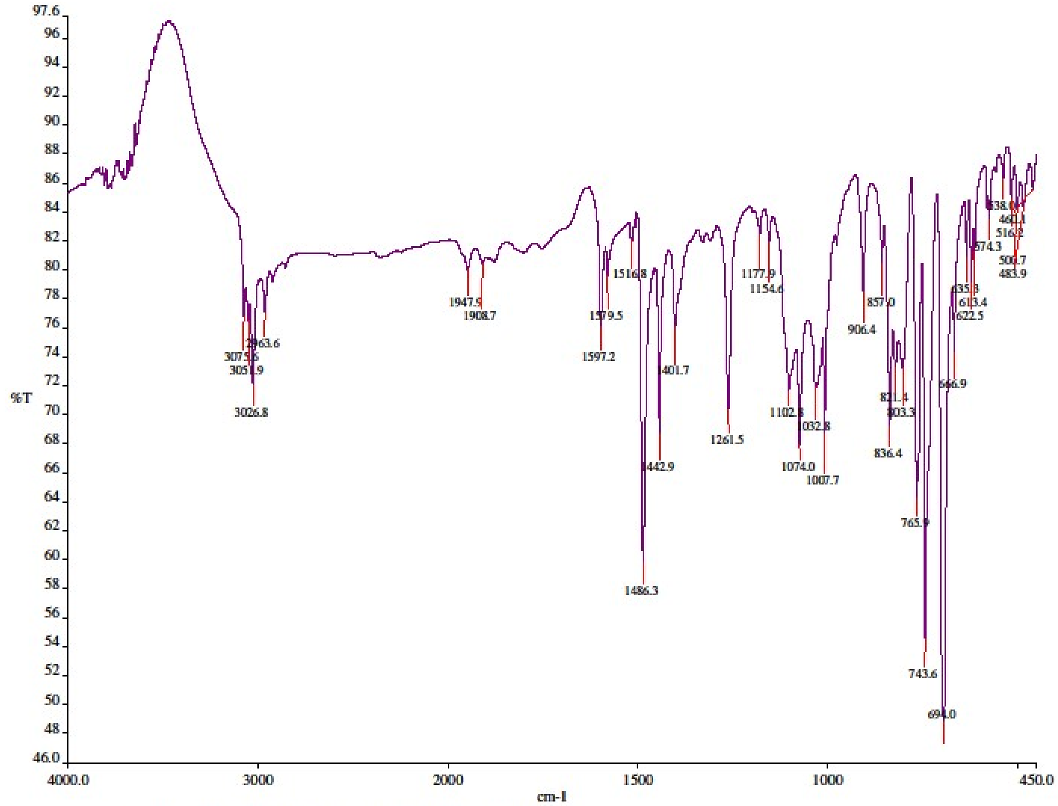

Fig. S15 FTIR of **DPDB** in KBr.

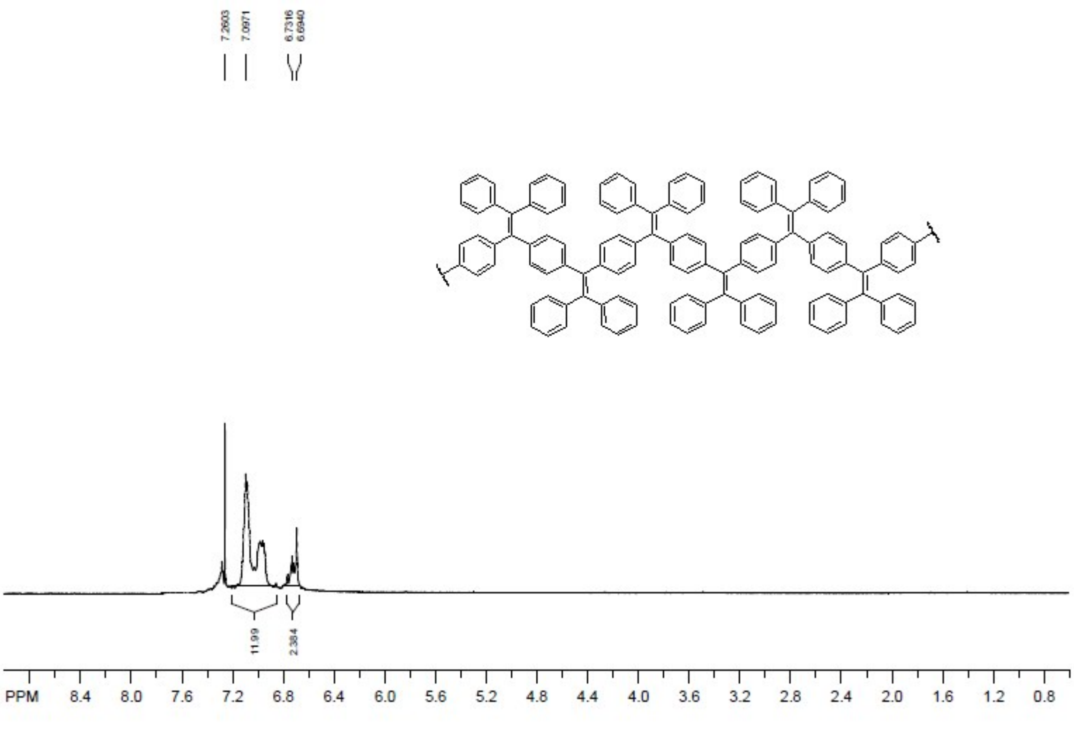

Fig. S16 ^{1}H NMR spectrum of **PTriPE** in $CDCl_3$.

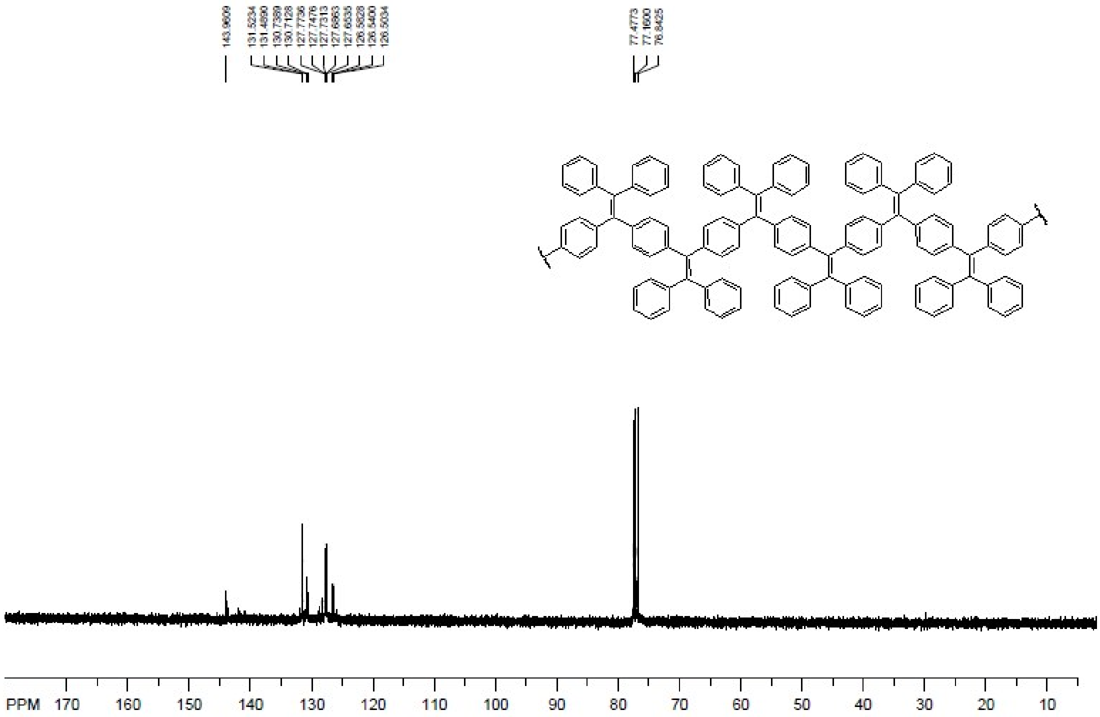

Fig. S17 ^{13}C NMR spectrum of **PTriPE** in $CDCl_3$.

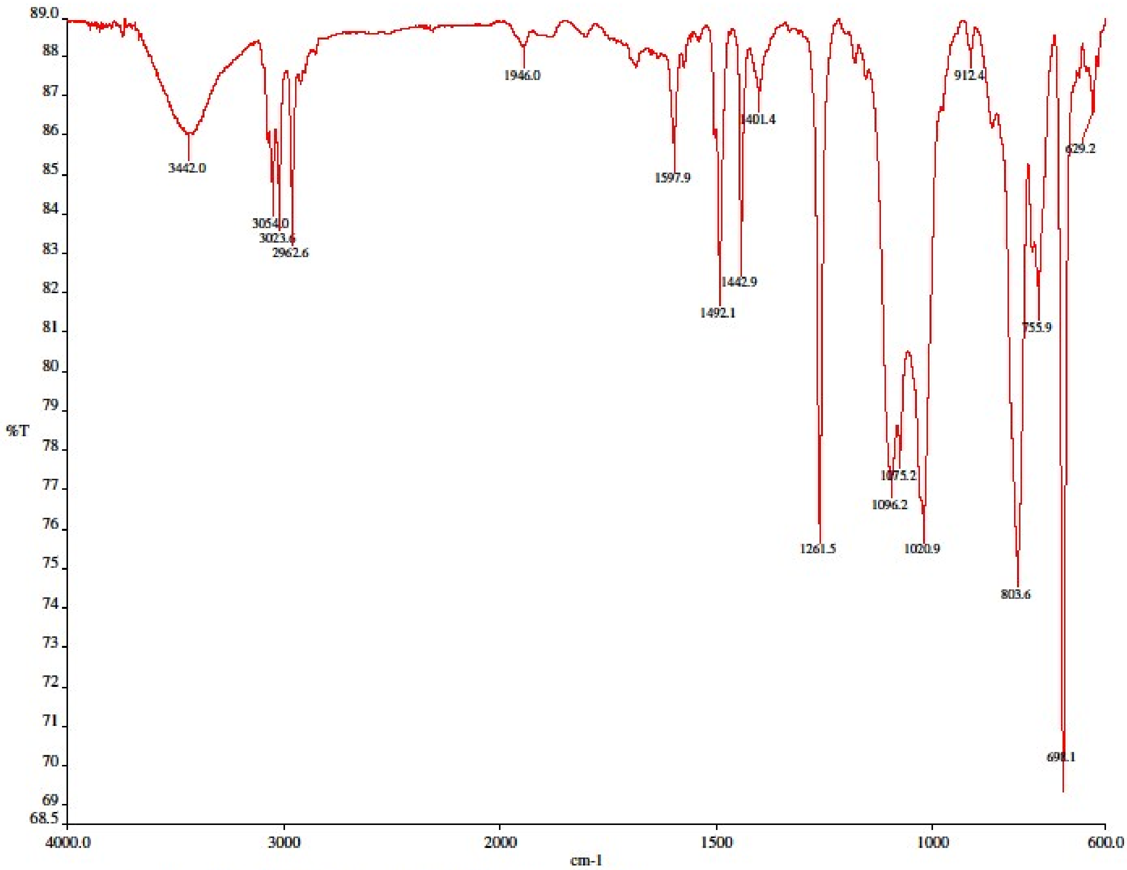

Fig. S18 FTIR of **PTriPE** in KBr.

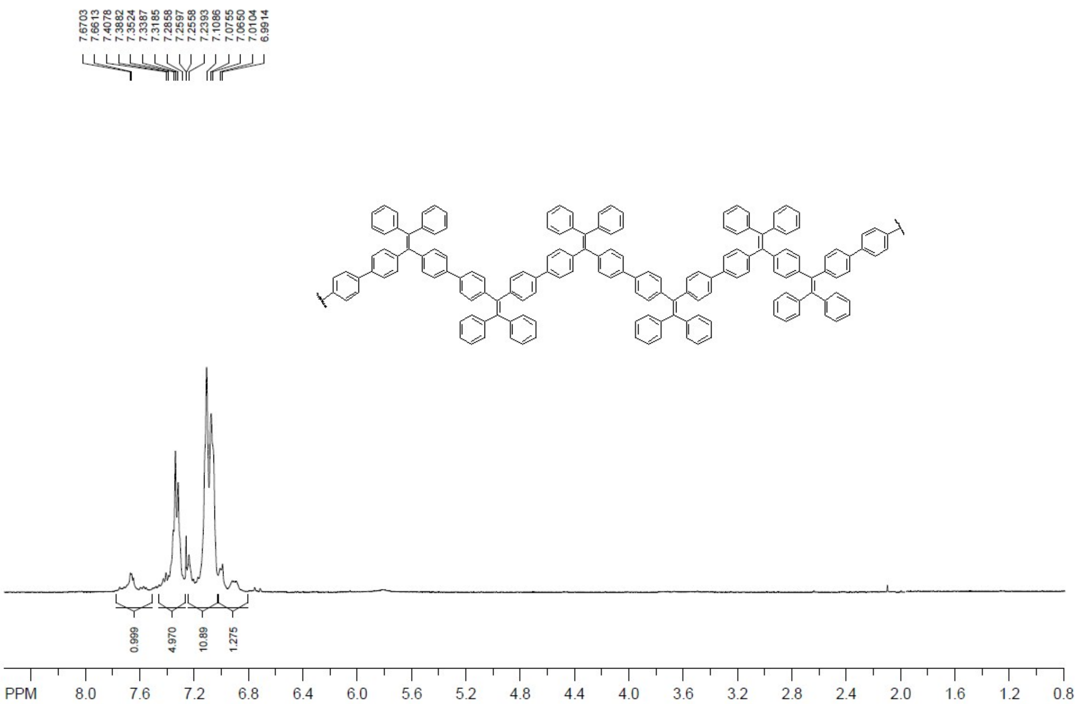

Fig. S19 ^{1}H NMR spectrum of **PTPE** in $CDCl_3$.

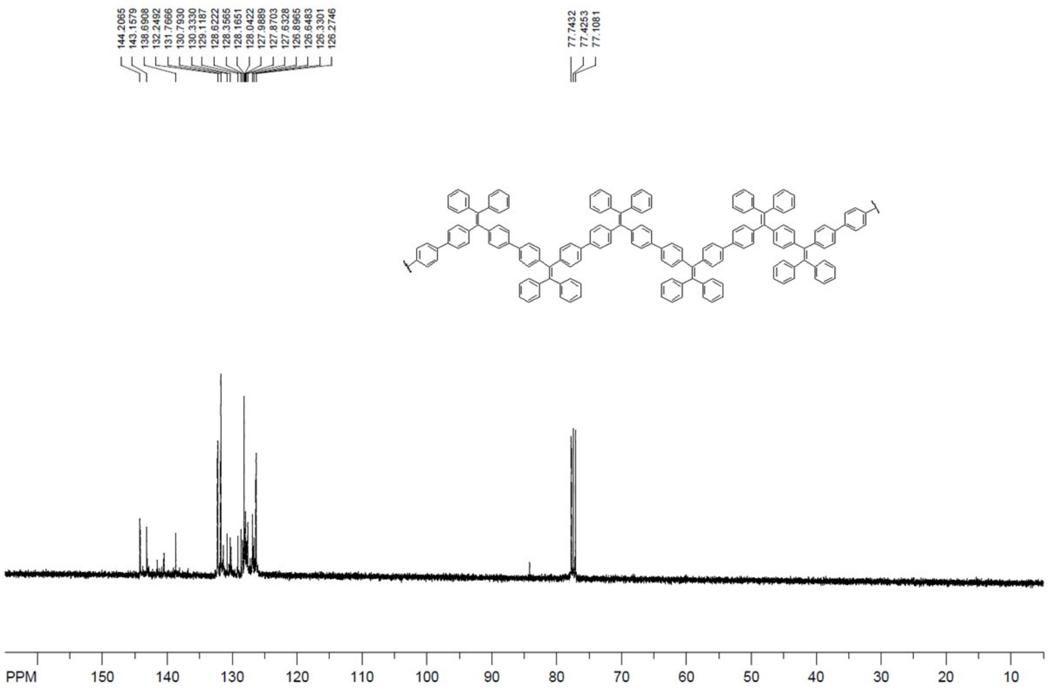

Fig. S20 ^{13}C NMR spectrum of **PTPE** in $CDCl_3$.

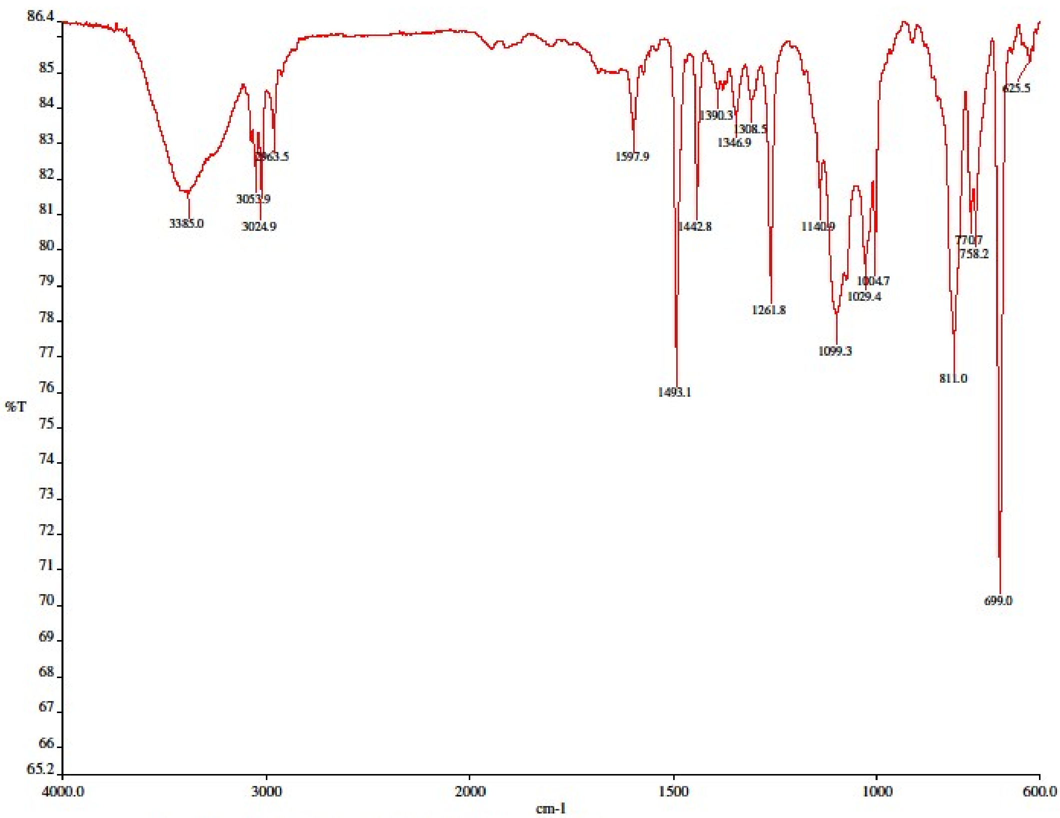

Fig. S21 FTIR of **PTPE** in KBr.