Fiber-optic detection of nitroaromatic explosives with solution-processable triazatruxene-based hyperbranched conjugated polymer nanoparticles

Yuxiang Xu,[ab] Xiaofu Wu,[a] Yonghong Chen,[ab] Hao Hang,[ab] Hui Tong[a]* and Lixiang Wang[a]*

[a]*State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China.*

[b]*University of Chinese Academy of Sciences, Beijing 100049, P. R. China.*

E-mail: chemtonghui@ciac.ac.cn; lixiang@ciac.ac.cn.

Supporting Information

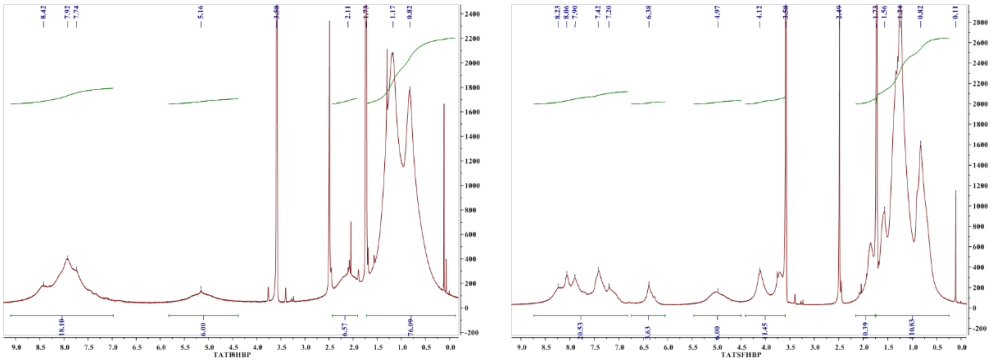

Fig. S1.^{1}H NMR spectra of **TATF8HBP** (left) and **TATSFHBP** (right) in THF-d8.

Table S1. Elemental content of **TATF8HBP** and **TATSFHBP**.

Polymer		C	H	N	O
TATF8HBP	Calc.	87.19%	9.24%	3.57%	-
	Anal.	84.55%	9.37%	3.61%	-
TATSFHBP	Calc.	83.42%	9.06%	2.29%	5.23%
	Anal.	82.72%	9.55%	2.33%	n.d.

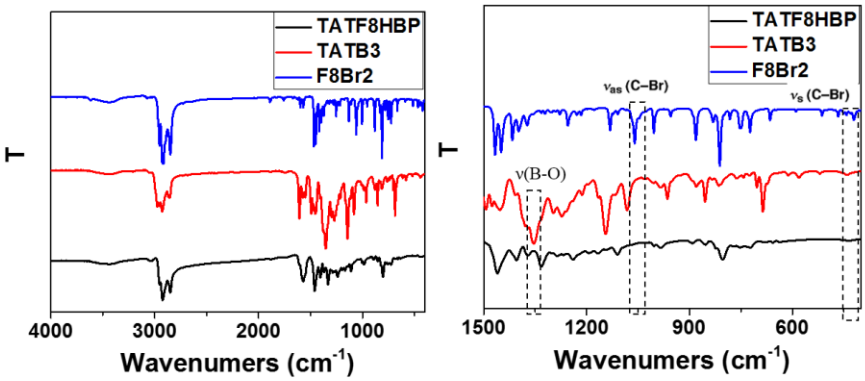

Fig. S2. FT-IR spectra of **TATF8HBP**, **TATB3** and **F8Br2**.

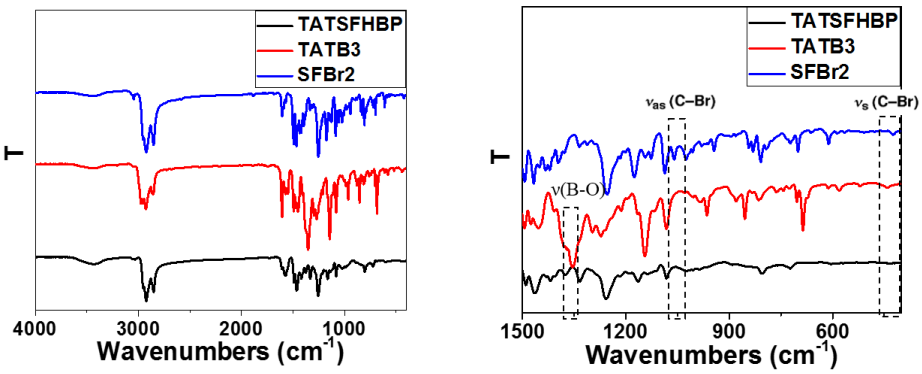

Fig. S3. FT-IR spectra of **TATSFHBP**, **TATB3** and **SFBr2**.

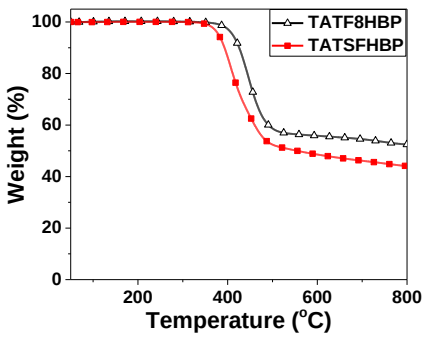

Fig. S4. TGA curves of **TATF8HBP** and **TATSFHBP** recorded under N_2 atmosphere.

Table S2. Physical properties of **TATF8HBP** and **TATSFHBP**.

Polymer	λ_{abs}[nm]		λ_{em}[nm]		QY		T_d	E_g^{opt}	E_{HOMO}[c]	E_{LUMO}[d]
	sol.	film	sol.	film	sol.[a]	film[b]	[°C]	[eV]	[eV]	[eV]
TATF8HBP	385	385	443	470	34.2%	5.3%	411	2.85	-5.12	-2.27
TATSFHBP	392	392	445	462	58.3%	14.7%	380	2.80	-5.12	-2.32

[a]In dilute THF, using 9,10-Diphenylanthracene in cyclohexene as standard. [b]Measured by the integrating sphere. [c]$E_{HOMO}=-(E_{ox}-E_{ox,Fc})-4.8$ eV. [d]$E_{LUMO}=E_g^{opt}+E_{HOMO}$.

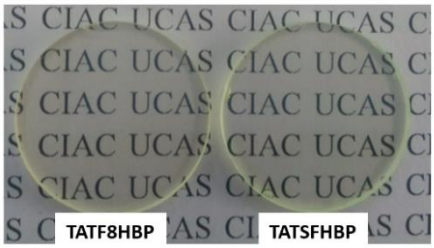

Fig. S5. Images of **TATF8HBP** and **TATSFHBP** films coated on quartz plates.

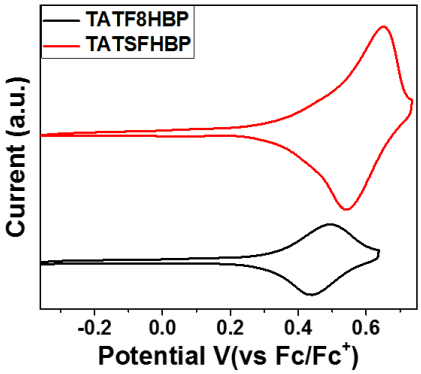

Fig. S6. Cyclic voltammograms of **TATF8HBP** and **TATSFHBP** in thin films measured in acetonitrile with TBAPF6 as supporting electrolyte.

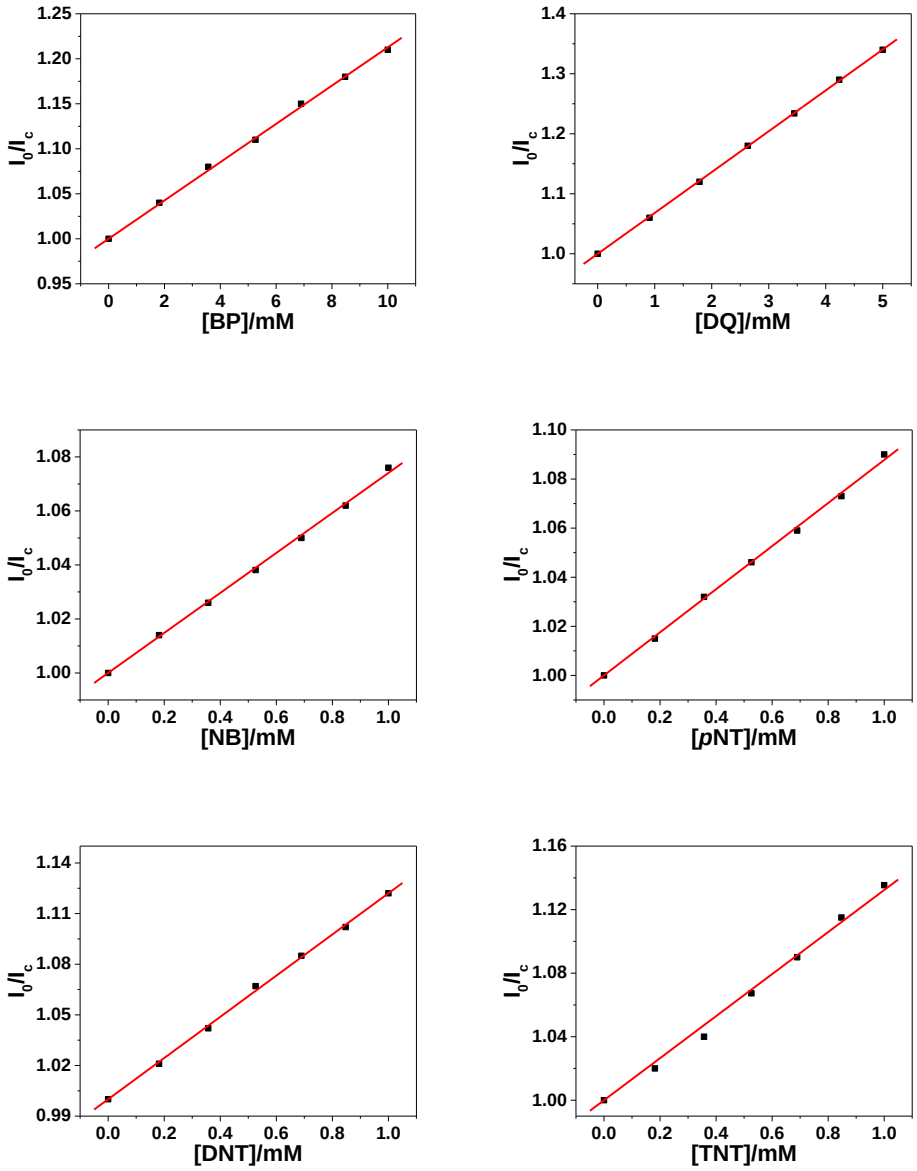

Fig. S7. Stern-Volmer plots and fits for **TATF8HBP** with the six different analytes.

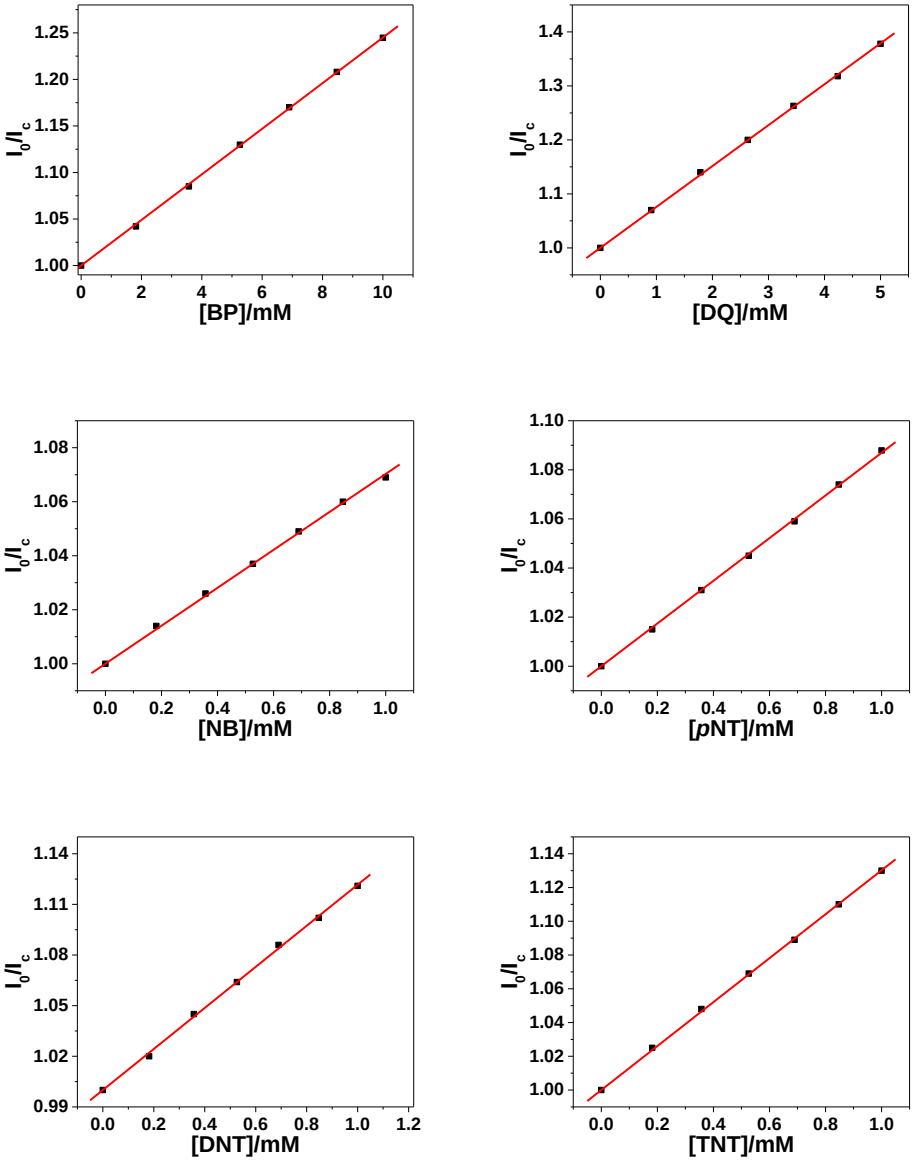

Fig. S8. Stern-Volmer plots and fits for **TATSFHBP** with the six different analytes.

Table S3. Summary of the Stern-Volmer Constants (K_{SV}) for each polymers with different analytes.

Polymer	TNT/M^{-1}	DNT/M^{-1}	*p*NT/M^{-1}	NB/M^{-1}	DQ/M^{-1}	BP/M^{-1}
TATF8HBP	132.3±2.4	122.0±1.0	87.8±0.8	74.1±0.7	68.1±0.2	21.3±0.2
TATSFHBP	130.2±0.5	121.7±0.9	86.9±0.4	70.3±0.5	75.8±0.3	24.5±0.1

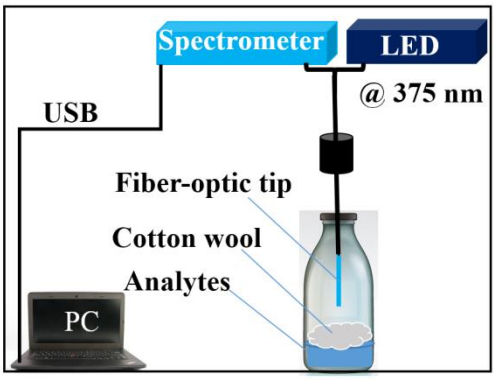

Fig. S9. A schematic drawing of an experimental setup for fiber-optic sensing of explosive vapors.

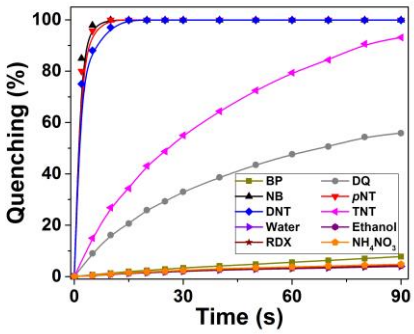

Fig. S10. Time-dependent fluorescence quenching of **TATSFHBP** films coated on fiber-optic tips upon exposure to saturated DNT, TNT, *p*NT, NB, DQ, BP, ethanol, water, RDX and NH_4NO_3 vapors.

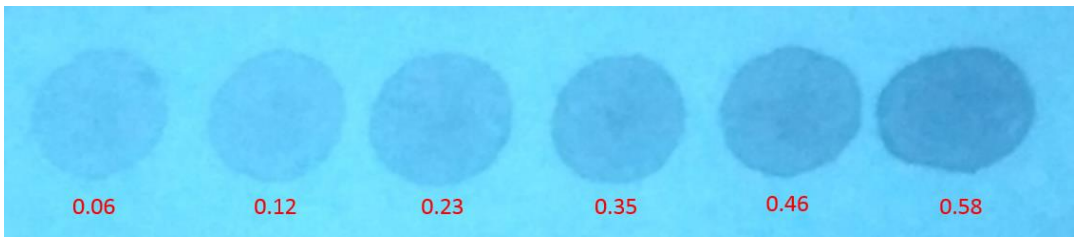

Fig. S11. Fluorescence quenching images of TNT-indicating papers quenched by TNT with various amounts (unit: $ng \cdot mm^{-2}$).