

Polymorphism and benzene solvent controlled stimuli responsive reversible fluorescence switching in triphenylphosphoniumfluorenylide crystals

P. S. Hariharan,^a M. Baby Mariyatra,^b E. M. Mothi,^{c*} Antonia Neels,^d Georgina Rosair^e and Savarimuthu Philip Anthony^{a*}

^a)Department of Chemistry, School of Chemical & Biotechnology, SASTRA University, Thanjavur-613401, Tamil Nadu, India. E-mail: philip@biotech.sastra.edu.

^b)Department of Chemistry, St. Xavier's College, Palayamkottai-627002, India

^c)Centre for Scientific and Applied Research, PSN College of Engineering and Technology, Melathediyoore, Tirunelveli-627152, India. E-mail: mothichem@gmail.com

^d)Center for X-ray Analytics, Empa - Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland

^e)Institute of Chemical Sciences, School of Engineering & Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, United Kingdom.

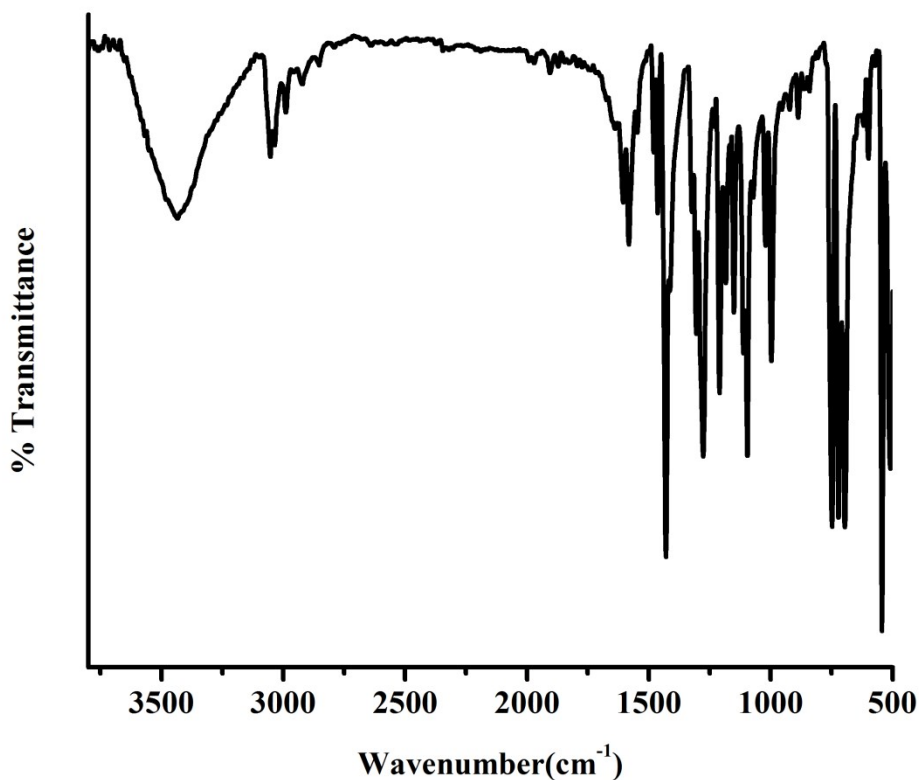


Figure S1. FTIR of TPPFY.

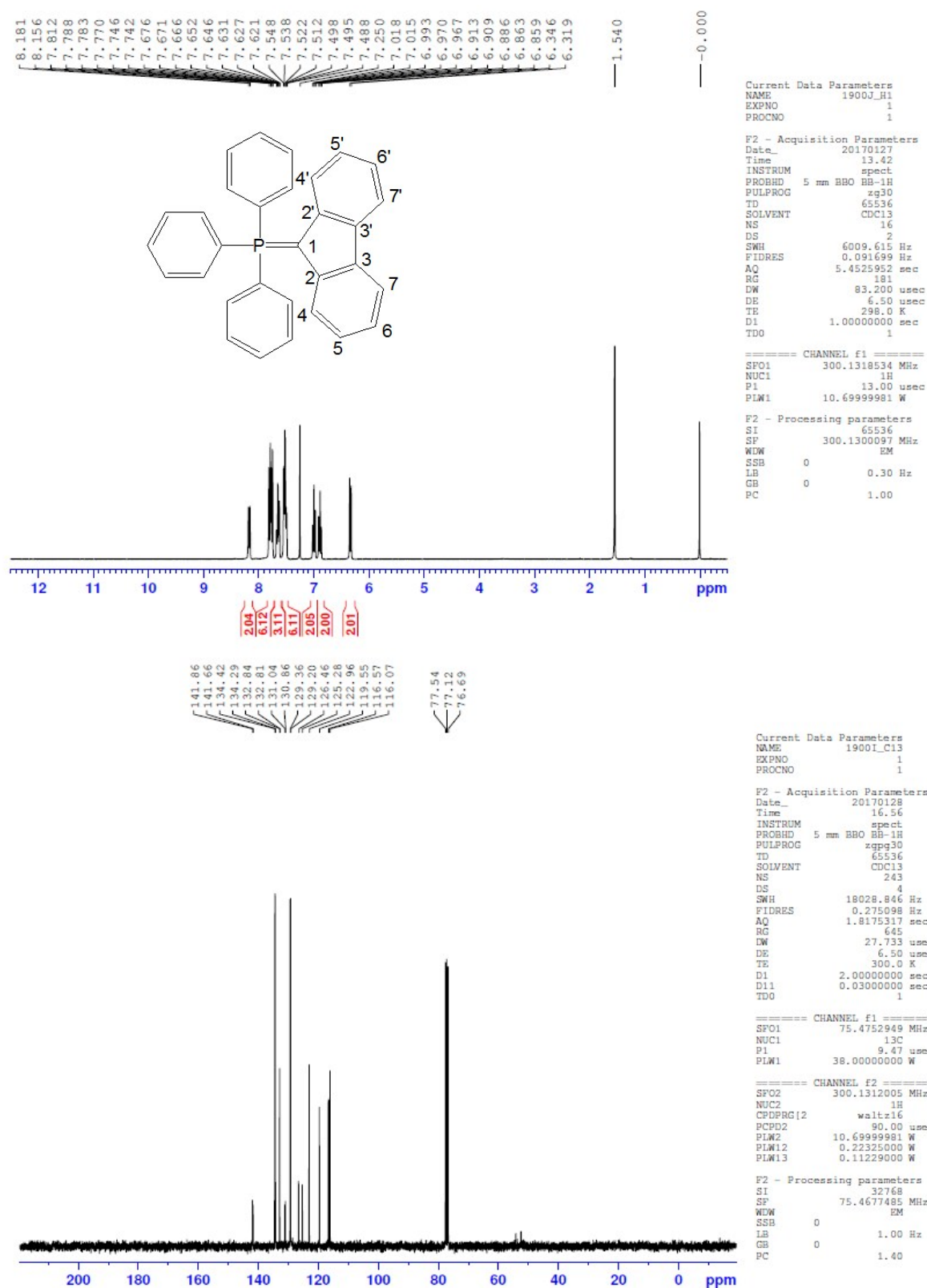


Fig. S2. ¹H and ¹³C-NMR spectra of TPPFY.

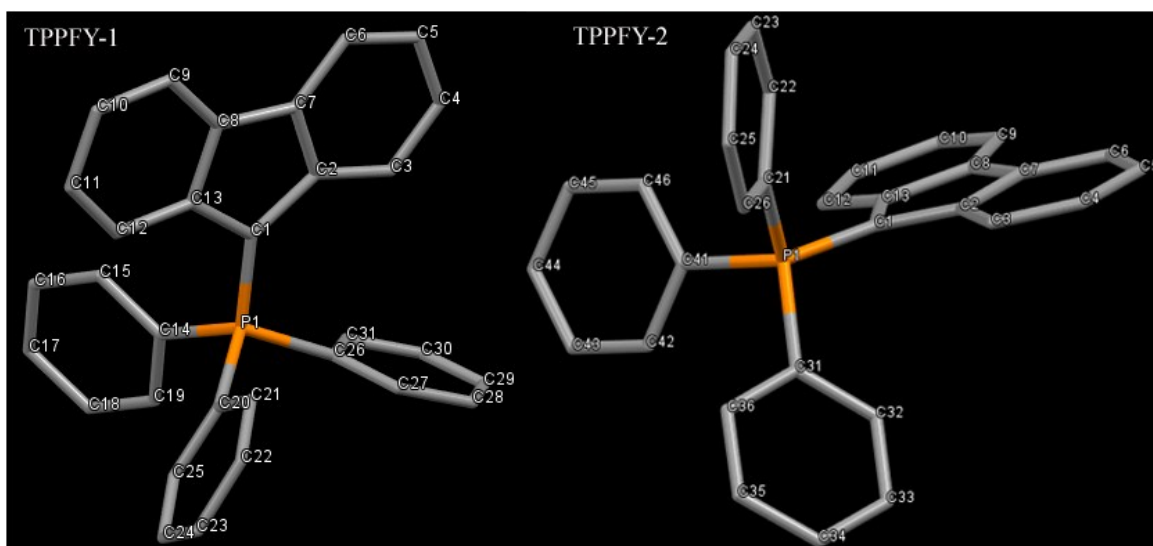
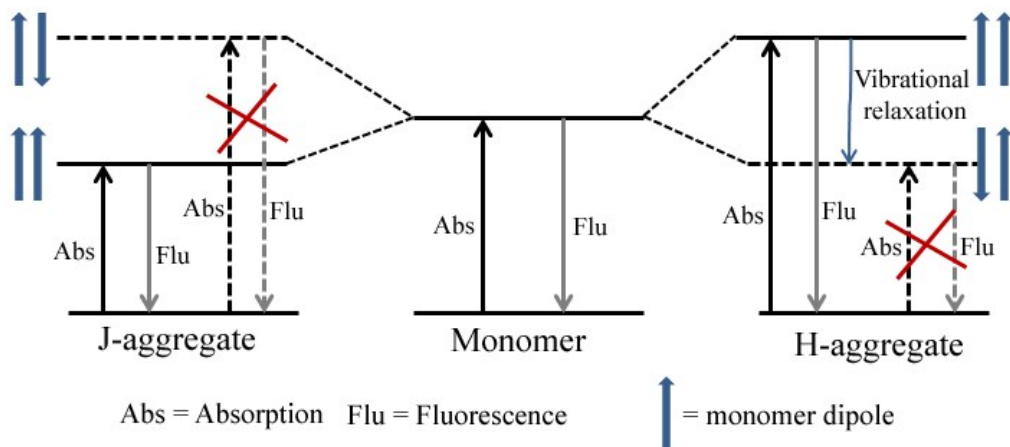


Fig. S3. Molecular structure of TPPFY in TPPFY-1 and TPPFY-2 crystal lattice. C (grey), P (orange). H-atoms are omitted for clarity.

Table S1. Geometric parameters around P atom for TPPFY-1 and TPPFY-2.

Bond distances (Å)	TPPFY-1	Bond distances (Å)	TPPFY-2
P1-C1	1.7160(19)	P1-C1	1.7237(15)
P1-C14	1.810(2)	P1-C21	1.8233(15)
P1-C20	1.8175(18)	P1-C31	1.8096(15)
P1-C26	1.797(2)	P1-C41	1.8065(16)
Bond angles (deg)		Bond angles (deg)	
C1-P1-C14	115.74(9)	C1-P1-C21	109.67(7)
C1-P1-C20	110.78(9)	C1-P1-C31	113.78(7)
C1-P1-C26	110.33(9)	C1-P1-C41	111.33(7)
C14-P1-C20	105.36(8)	C21-P1-C31	106.97(7)
C14-P1-C26	106.94(9)	C21-P1-C41	108.14(7)
C20-P1-C26	107.26(9)	C31-P1-C41	106.71(7)



Scheme S1. Exciton splitting in H- and J-aggregate (forbidden transition is indicated by red cross).

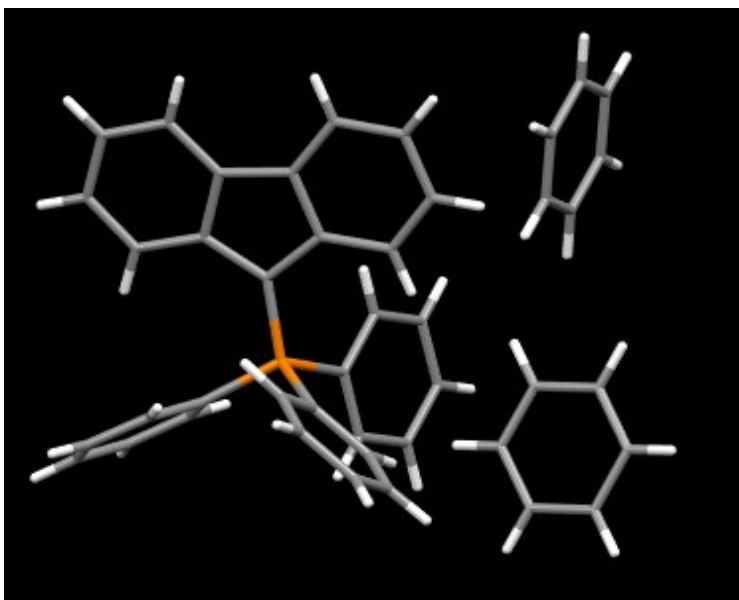


Fig. S4. Molecular structure of TPPFY-2 with benzene molecules included in the crystal lattice. C (grey), P (orange), H (white).

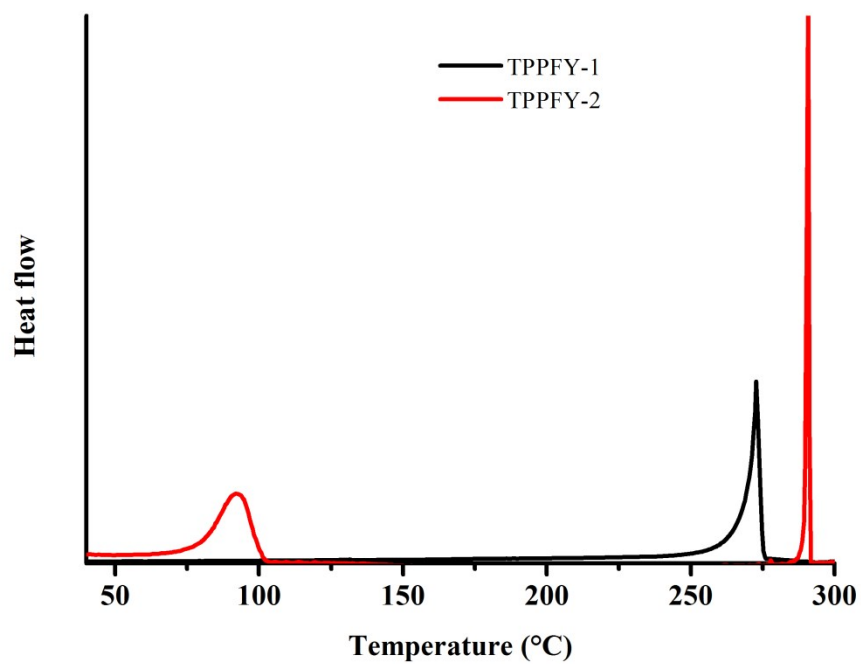


Figure S5. DSC spectrum of TPPFY-1 and TPPFY-2.

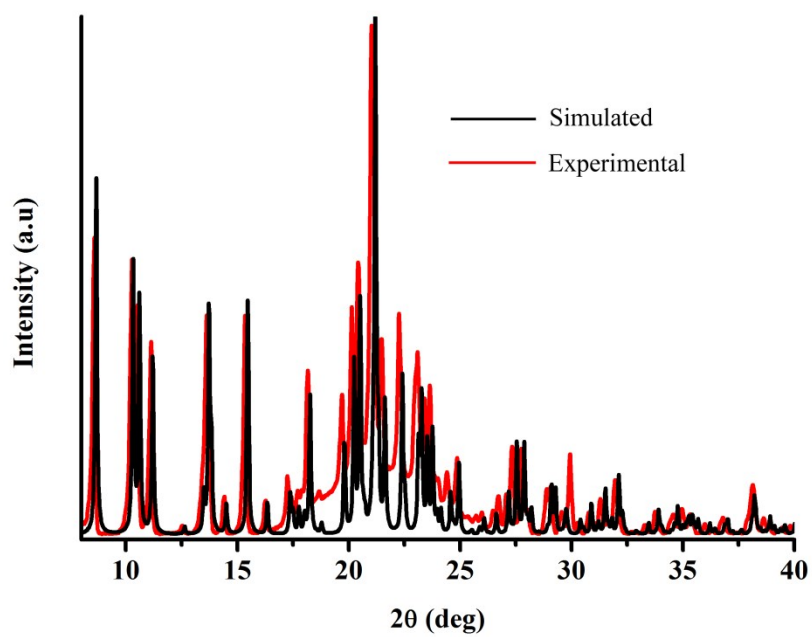


Fig. S6. PXRD pattern of TPPFY-1

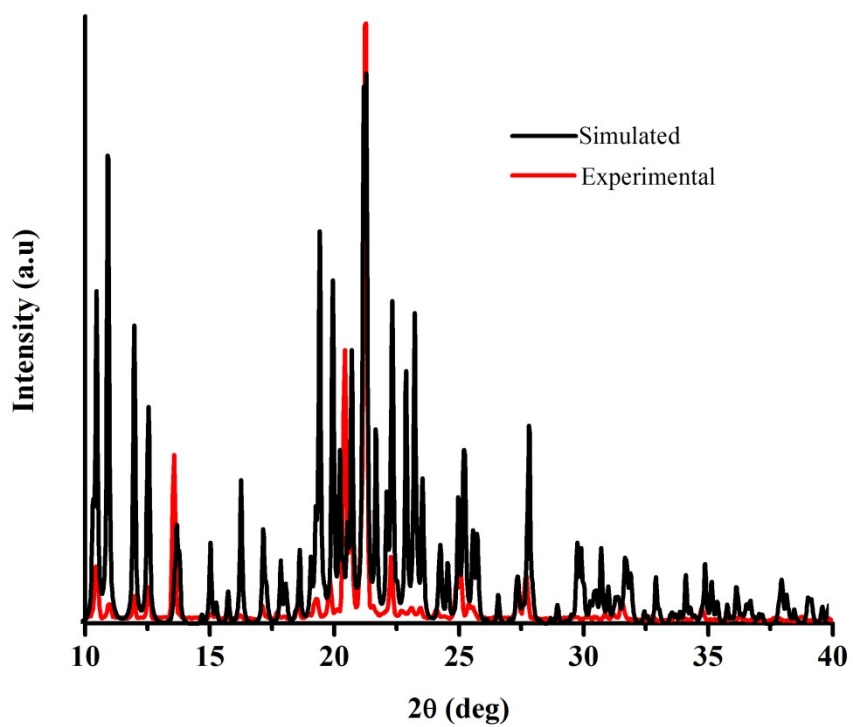


Fig. S7. PXRd pattern of TPPFY-2.