Supporting Information

Sensitive and fast fluorescence-based indirect sensing of TATP

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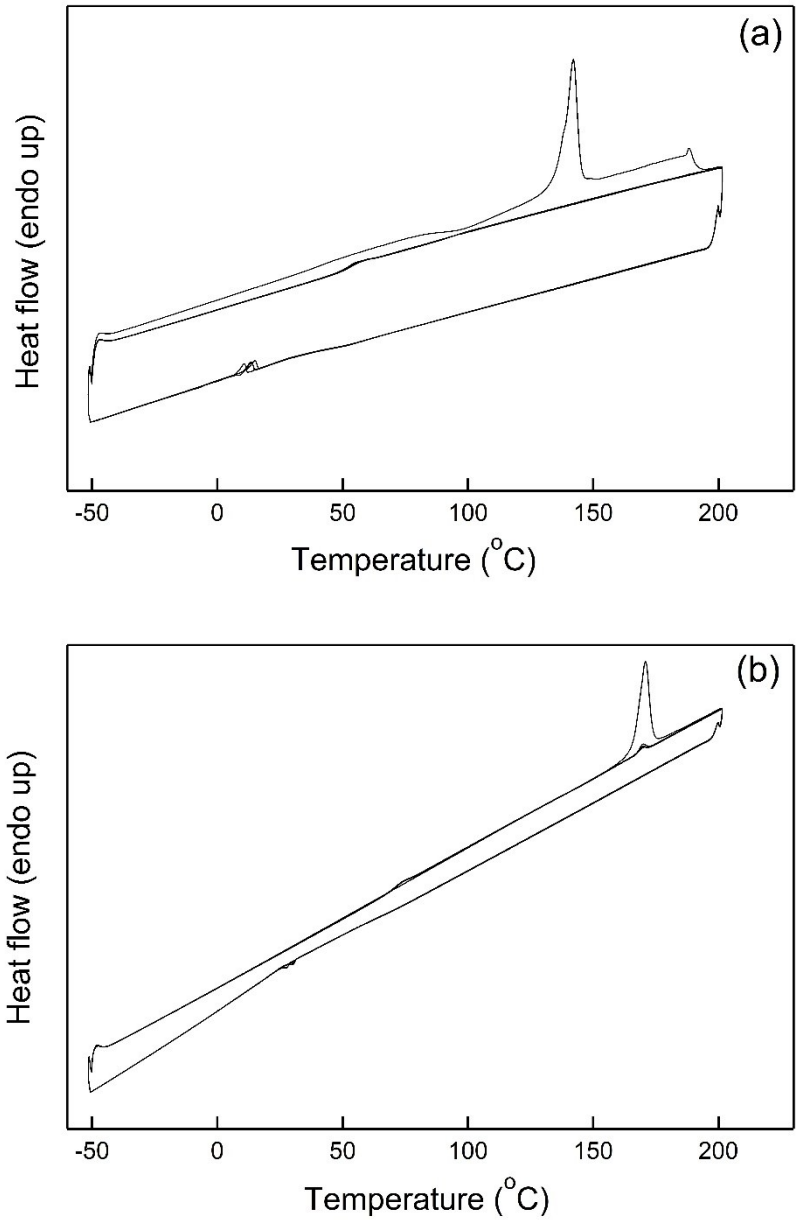


Figure S1 Differential scanning calorimetry (DSC) analysis of (a) **1** and (b) **2**. (4 scans; scan rate 50 °C/min).

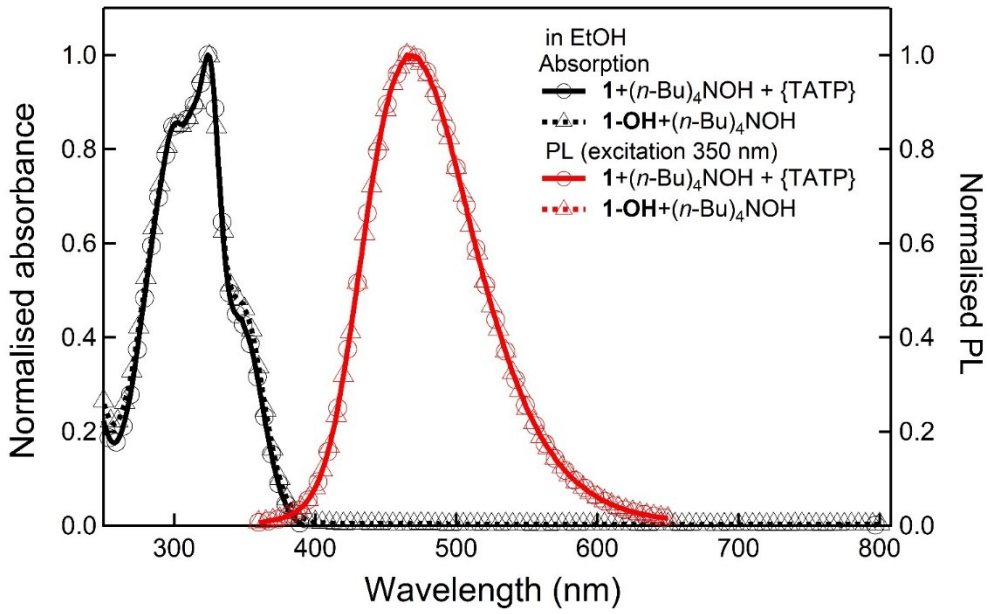


Figure S2 UV-vis absorption and photoluminescence spectra of boronate ester **1** in ethanol after exposure to {TATP} in comparison with the corresponding phenoxide. **1**+(n-Bu)$_4$NOH+{TATP}: **1** (1.4×10^{-5} M) and (n-Bu)$_4$NOH (9.4×10^{-5}) in ethanol was exposed to {TATP} (derived from 16 ppm TATP) for 5 min; **1-OH**+(n-Bu)$_4$NOH: **1-OH** (2.0×10^{-5} M) and (n-Bu)$_4$NOH (9.4×10^{-5}) in ethanol.

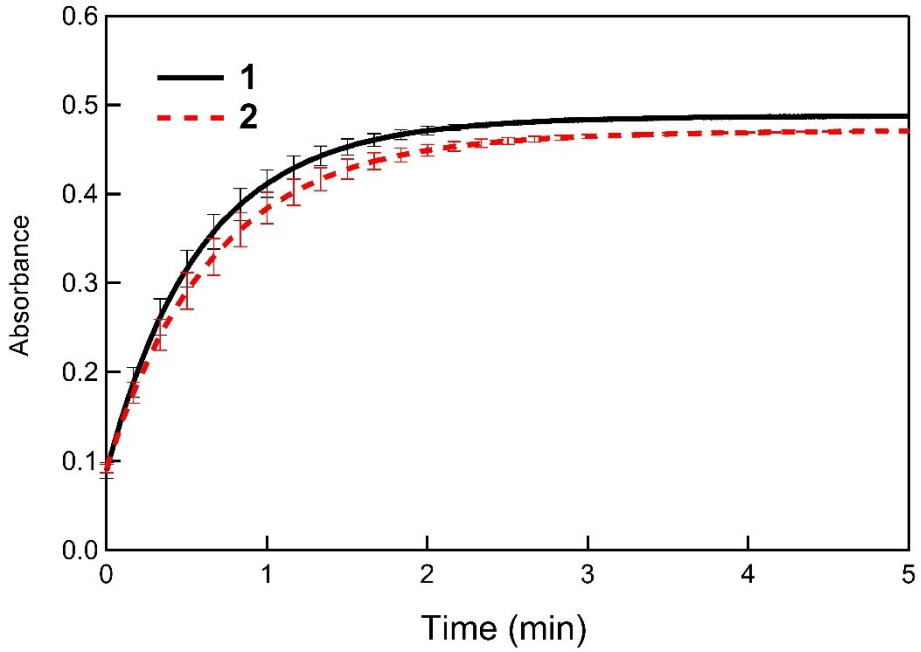


Figure S3 UV-visible absorption kinetics for the conversion of boronate esters (**1** or **2**) to phenoxides (**1-O**$^-$ at 349 nm or **2-O**$^-$ at 362 nm) by reaction with H_2O_2. The measurements were undertaken by adding aqueous H_2O_2 (2.5×10^{-4} M) to a solution of **1** (2.0×10^{-5} M) or **2** (1.6×10^{-5} M) and (n-Bu)$_4$NOH (1.3×10^{-3} M) in ethanol. The half-life ($t_{1/2}$) was estimated from fitting an exponential function to be 15 and 18 s for **1** and **2**, respectively. The errors represent the deviation of the average of three measurements.

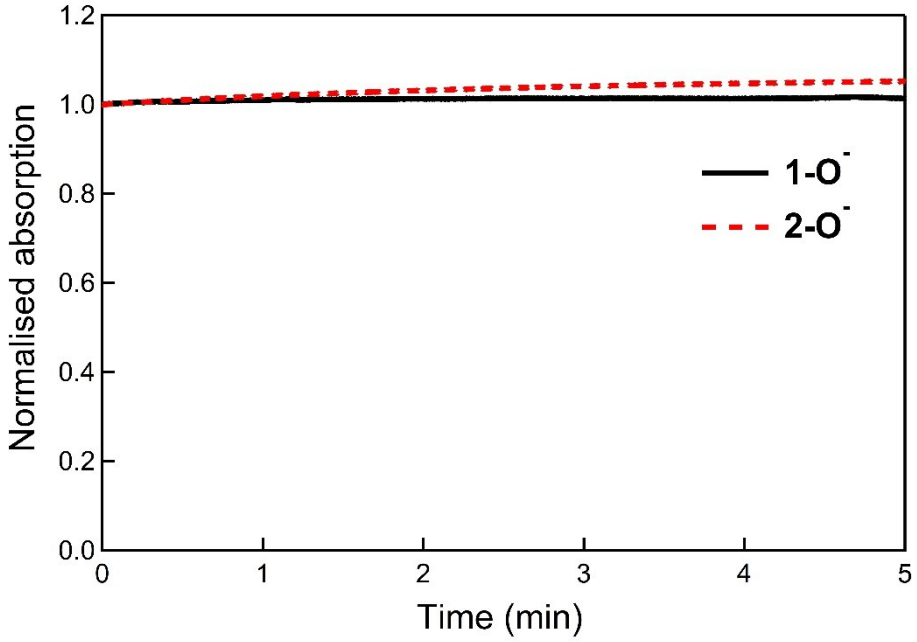
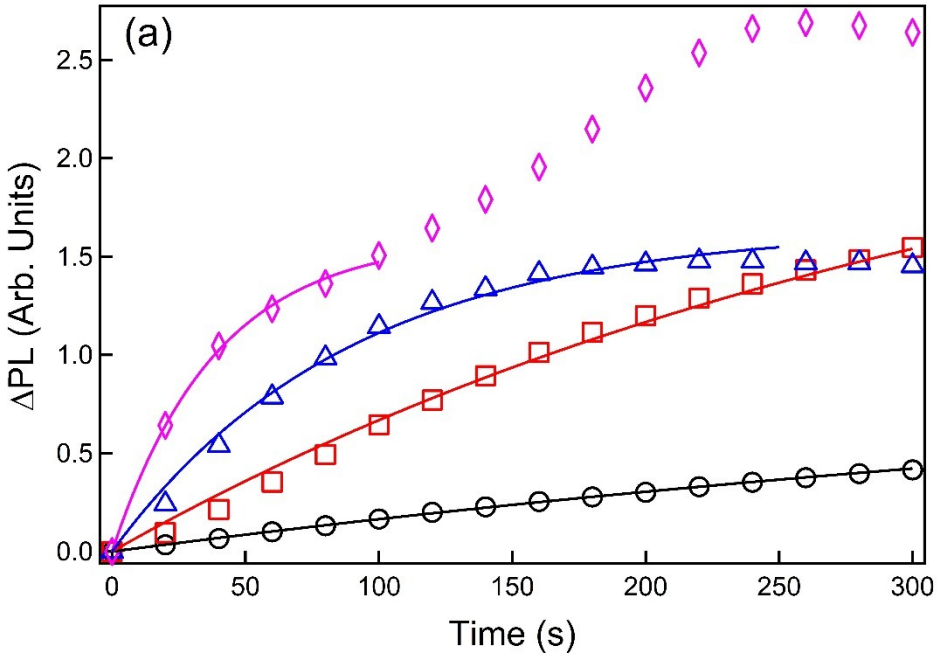


Figure S4 Normalised absorption of **1-O**$^-$ and **2-O**$^-$ solutions under illumination at 349 nm and 362 nm in the spectrometer, respectively for 5 min after generation with H_2O_2 as per Figure S3.



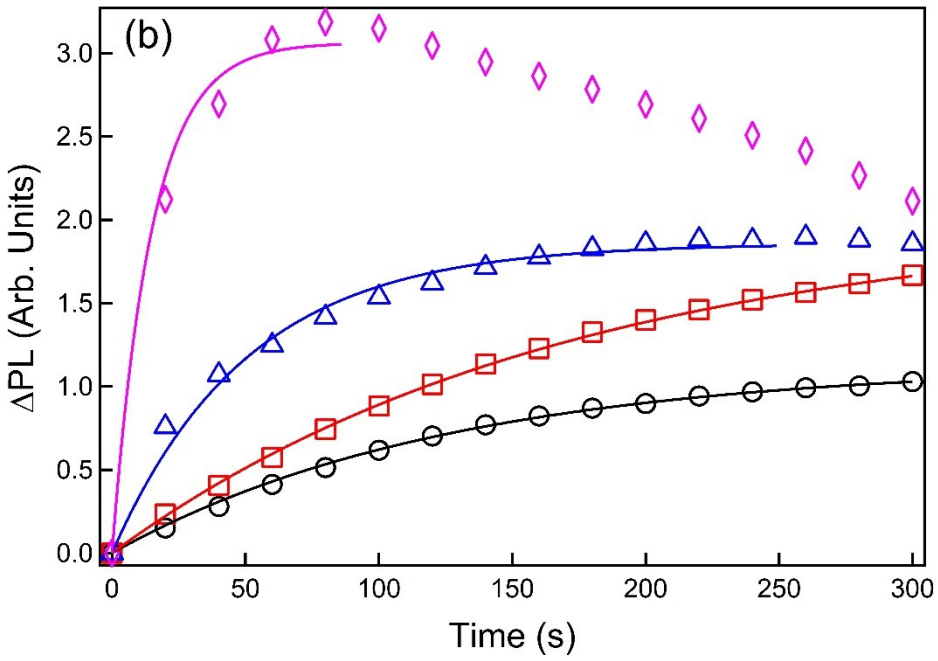


Figure S5 Representative PL kinetics at various TATP vapour concentrations (○: 0.3 ppm; □: 0.9 ppm; △: 1.7 ppm; ◊: 5.3 ppm) and fitted curves (solid lines) using the first-order reaction equation, $\Delta PL=K(1-e^{-kt})$ (ΔPL = the increase of fluorescence intensity, K = constant, and *k* is a constant related to the overall reaction rate).[1] The films were fabricated by drop-casting a solution of the boronate ester sensing material (a) **1**, or (b) **2** containing $(n\text{-Bu})_4NOH$ (6 equiv). The data used for the fits was chosen to minimize the effect of photodegradation on the determination of the rate constants. Despite the competing reactions of phenoxide generation and subsequent photodegradation we find that the PL kinetics curves can be fitted with a first-order reaction equation, $\Delta PL=K(1-e^{-kt})$.[1]

References

1 M. Xu, J.-M. Han, Y. Zhang, X. Yang and L. Zang, *Chem. Commun.*, 2013, **49**, 11779-11781.