Electronic Supplementary Information (ESI)
for

Organic & Biomolecular Chemistry

A specific chemodosimeter for fluoride anion based on a pyrene derivative with trimethylsilylethynyl groups

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I. Supplementary data

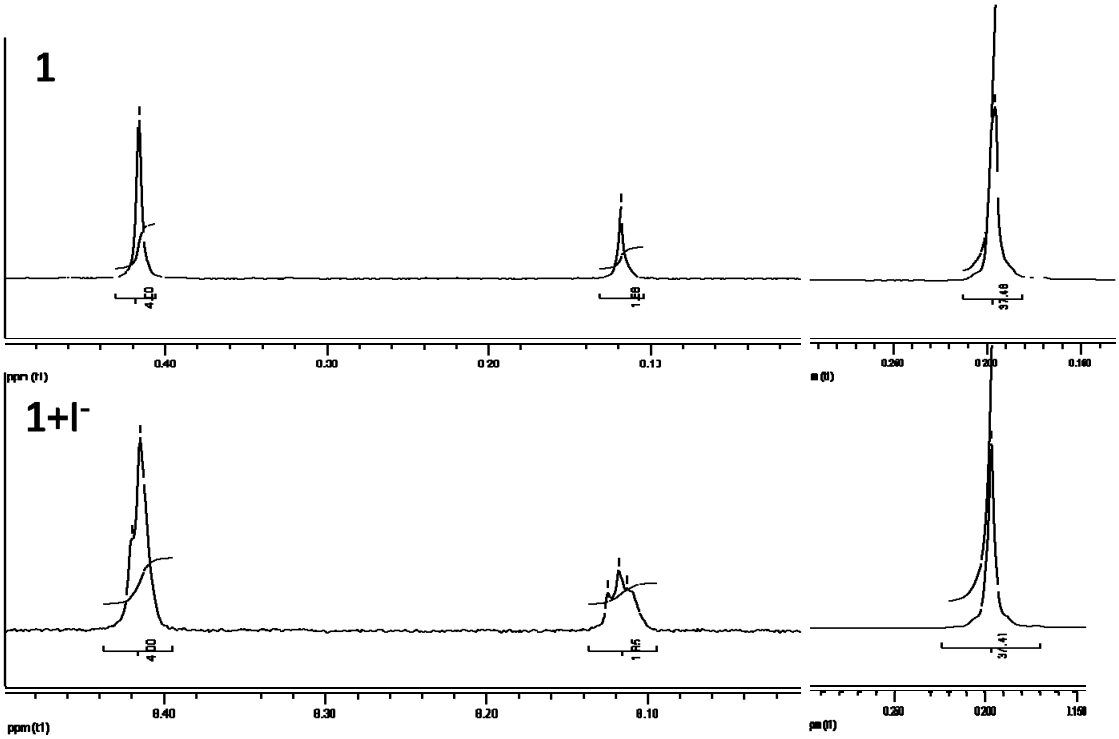

Fig S1. ^{1}HNMR spectrum of **1** and **1**+I^- in $CDCl_3$ contaning 10% DMSO-d_6.

Table S1. Selected TD-DFT results for **1** and **TEP**.

Dye	NO	λ[nm]	f[a]	Energy[eV]	Wave function[b]
1	$S_0 \rightarrow S_1$	468	1.0395	2.64	0.6345 | L←H>,
	$S_0 \rightarrow S_5$	323.7	1.0792	3.83	0.4841 | L+1←H>, 0.4021 | L←H-1 ….
TEP	$S_0 \rightarrow S_1$	409.7	0.7445	3.03	0.6382 | L←H>, -0.1229 | L+1←H-1>,
	$S_0 \rightarrow S_5$	299.8	0.6342	4.14	0.4465 | L+1←H>, -0.4394 | L←H-1 ….

[a] Oscillator strength.[b] The wave functions based on the eigenvectors predicted by TDDFT.

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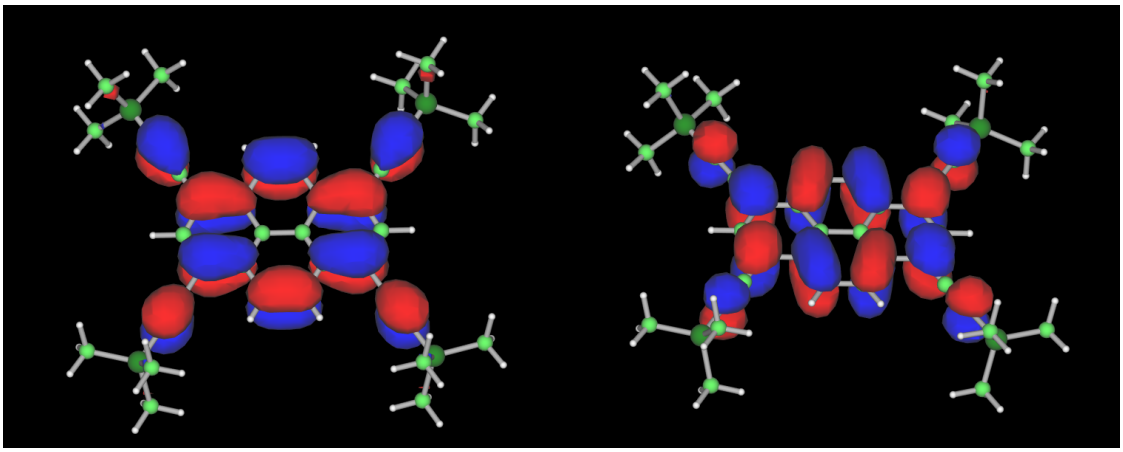

HOMO LUMO

Fig S2. Frontier MOs of **1** at an isosurface value of 0.02.

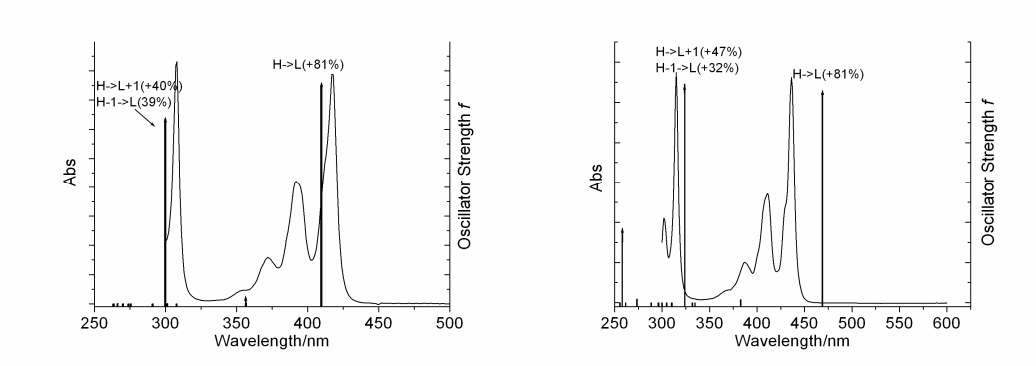

Fig S3. The experimental absorption spectrum in THF and the corresponding TD–DFT calculation