Supporting Information for the following manuscript:

# A highly selective fluorescence turn-on detection of cyanide based on the aggregation of the tetraphenylethylene molecule induced by chemical reaction

Xianhong Huang, Xingui Gu, Guanxin Zhang, \* Deqing Zhang\*

Beijing National Laboratory for Molecular Sciences, Organic Solids Laboratory,

Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

E-mail: dqzhang@iccas.ac.cn

## **Table of Contents**

1. General information for synthesis and characterization	<b>S1</b>
2. Variation of Absorption spectra of compound 1 in the prensence of CN <sup>-</sup>	S2
3. Variation of the relative fluorescence intensity at 466 nm of 1 (20.0 $\mu$ M) in the prese	ence of
metal ions	<b>S2</b>
4. The DLS data of 1 in the absence and presence of CN <sup>-</sup>	<b>S</b> 3
5. <sup>1</sup> H NMR spectral change of 1 in CD <sub>3</sub> OD and D <sub>2</sub> O upon addition of CN <sup>-</sup>	S3-
S4	
5. Photos of the filter papers containing spots of 1 under UV light upon addition of dif	ferent
amounts of CN <sup>-</sup>	<b>S4</b>

6. <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra of compound 1 S5-S6

#### 1. Materials and characterization techniques

All the chemicals obtained from commercial sources were analytical pure and used without further purification. Stock solutions of all anions (all in the form of sodium salts) were prepared with pure water. The pure water was purified with a Millipore filtration system. The toxic sodium cyanide was used with caution!

<sup>1</sup>H NMR and <sup>13</sup>C NMR were collected on Bruker Avance 400-MHz spectrometer. Mass spectra were recorded on an APEXII- electrospray ionization (ESI) instrument. Fluorescence spectra and UV/Vis absorption spectra were recorded on a Hitachi F-4500 spectrophotometer and Jasco V-570 at 25 °C . Fluorescence confocal laser scanning images were recorded with an Olympus FV1000-IX81. Dynamic light scattering (DLS) experiments were carried out with Malvern Instrument (Nano Series).



Scheme S1 Synthetic approach to compound 1

Synthesis of compound 1. A mixture of compound 2 (0.20 g, 0.66 mmol), compound 3 (0.24 g, 0.66 mmol) and NaOH (0.01 g, 0.27 mmol) in ethanol (20 mL) were refluxed for 6.0 hours under argon. After cooling to room temperature, the solvent was evaporated under reduced pressure. The residue was dissolved in CH<sub>2</sub>Cl<sub>2</sub> and the organic phase was washed with water for three times. The organic layer was dried over anhydrous MgSO<sub>4</sub>, filtered and evaporated. The residue was subjected to column chromatography with CH<sub>2</sub>Cl<sub>2</sub>/CH<sub>3</sub>OH (v/v, 200/1) as eluant. Compound 1 was obtained as red solid (0.3 g, 0.47 mmol) in 70% yield. <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD):  $\delta$  8.33 (1H, d *J*=16 Hz), 7.83–7.81 (4H, m), 7.66–7.64 (2H, m), 7.57 (1H, d, *J*=16 Hz), 7.22 (2H, d, *J*=8 Hz), 7.17–7.02 (m, 15H), 4.15 (s, 3H), 1.84 (s, 6H). <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD) :  $\delta$  189.12, 182.08, 154.00, 150.68, 142.90, 142.82, 141.53. 131.39, 131.30, 128.08, 128.00, 127.75, 115.14, 112.38, 52.57, 37.30, 26.91, MS (ESI, positive): 516

(M<sup>+</sup>). Elemental analysis: calcd. for C<sub>39</sub>H<sub>34</sub>IN ·0.1 CH<sub>2</sub>Cl<sub>2</sub>, C, 72.02; H, 5.29; N, 2.15; Found:
C, 71.84; H, 5.27; N, 2.17.



## 2. Variation of the absorption spectrum of compound 1 after addition of CN

Figure S1 (A) Absorption spectra of the aqueous solution of **1** (20.0  $\mu$ M) in the presence of different amounts of CN<sup>-</sup> (from 0 to 18  $\mu$ M); inset shows photos of the aqueous solution of **1** (20.0  $\mu$ M) in the absence (A) or presence (B) of CN<sup>-</sup> (20.0  $\mu$ M) under daylight; (B) The plot of (1- A/A<sub>0</sub>) at 436 nm *vs.* the concentration of CN<sup>-</sup>; inset shows the linear relation for concentration of CN<sup>-</sup> in the range of 0-8.5  $\mu$ M.

3. Variation of the relative fluorescence intensity at 466 nm of 1 (20.0  $\mu$ M) in the presence of metal ions



**Figure S2.** Variation of the relative fluorescence intensity at 466 nm of **1** (20.0  $\mu$ M) in the presence of CN<sup>-</sup> (20.0  $\mu$ M) and metal ions (Cu<sup>2+</sup> (Cu(ClO<sub>4</sub>)<sub>2</sub>) /Zn<sup>2</sup> (Zn(ClO<sub>4</sub>)<sub>2</sub>)/ Ca<sup>2+</sup> (Ca(ClO<sub>4</sub>)<sub>2</sub>)/ Fe<sup>2+</sup>(Fe(ClO<sub>4</sub>)<sub>2</sub>)/ Ni<sup>2+</sup>(Ni(ClO<sub>4</sub>)<sub>2</sub>)/ Mn<sup>2+</sup> (Mn(ClO<sub>4</sub>)<sub>2</sub>) /Pb<sup>2+</sup> (Pb(ClO<sub>4</sub>)<sub>2</sub>) /Cd<sup>2+</sup>(Cd(ClO<sub>4</sub>)<sub>2</sub>) /Hg<sup>2+</sup>

 $(Hg(ClO_4)_2)$  /Nd<sup>2+</sup> (Nd(ClO\_4)\_2) /Ag<sup>+</sup> (AgClO\_4)/), respectively; the concentration of each metal ion except CN<sup>-</sup> was 200  $\mu$ M; all solutions were prepared in aqueous solution and excitation wavelength was 330 nm.

4. The DLS data of 1 in the absence and presence of CN<sup>-</sup>



Figure S3 DLS profiles for 1 (20  $\mu$ M) in H<sub>2</sub>O before (black) and after the addition of 2.0 equiv of CN<sup>-</sup> (red).



# 5. <sup>1</sup>H NMR spectral variation for 1 upon addition of CN<sup>-</sup>

**Figure S4** <sup>1</sup>H NMR spectra of **1** in CD<sub>3</sub>OD before (A) and after addition of 2.0 equiv of CN (B).



**Figure S5** (*left*) Photos of the solution of **1** (1.0 mM) in the mixture of DMSO-d<sub>6</sub> and D<sub>2</sub>O (v/v, 1/1) in the absence (A) or presence (B) of CN<sup>-</sup> (2.0 eq.) under daylight; (*right*) Photos of the solution of **1** (1.0 mM) in the mixture of DMSO-d<sub>6</sub> and D<sub>2</sub>O (v/v, 1/1) in the absence (C) or presence (D) of CN<sup>-</sup> (2.0 eq.) under UV light (365 nm).



**Figure S6** <sup>1</sup>H NMR spectra of **1** in the mixture of DMSO-d<sub>6</sub> and D<sub>2</sub>O (v/v, 1/1) before and after addition of CN<sup>-</sup>; the spectra were recorded under the same conditions.

6. Photos of the filter papers containing spots of 1 under UV light upon addition of different

amounts of CN



Figure S7 Photos of the filter papers containing spots of **1** under UV light (365 nm) before (upper) and after (bottom) exposure to different amounts of CN<sup>-</sup>: A (0.001 M, 2.0  $\mu$ L), B (0.002 M, 2.0  $\mu$ L), C (0.004 M, 2.0  $\mu$ L). D (0.006 M, 2.0  $\mu$ L), E (0.008 M, 2.0  $\mu$ L), F (0.01 M, 2.0  $\mu$ L), G (0.025 M, 2.0  $\mu$ L), H (0.05 M, 2.0  $\mu$ L) and I (0.1 M, 2.0  $\mu$ L); after aqueous solution of **1** (1.0 mM, 2.0  $\mu$ L) was dropped on the neutral filter paper and dried, an orange spot (the diameter is about 0.1 cm) with red-emission under UV light (365 nm) was formed, and each spot was individually stained with 2.0  $\mu$ L aqueous solution of CN<sup>-</sup> of different concentrations.



**Figure S8.** The <sup>1</sup>H NMR spectrum of  $\mathbf{1}$  in CD<sub>3</sub>OD.



**Figure S9.** The  ${}^{13}$ C NMR spectrum of **1** in CD<sub>3</sub>OD.