Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Supplementary Information

Diarylethene-derived probe for colorimetric detection of CN^- and highly selective fluorescent recognition of I^-

Xugang Tang, Hongliang Liu*, Shouzhi Pu*

Jiangxi Key Laboratory of Organic Chemistry, Jiangxi Science and Technology Normal University, Nanchang 330013, PR China

***Corresponding author:** E-mail address: liuhongliang@163.com (H. Liu), pushouzhi@tsinghua.org.cn (S. Pu); Tel./ Fax: +86-791-83831996.

Fig. S1 Changes in the absorption of **1O** induced by the addition of 9 eq. various anions in tetrahydrofuran (2.0×10^{-5} mol L^{-1}): (A) absorption spectral changes, (B) photographs of the color changes in solution, (C) absorption intensity at 474 nm changes.

Fig. S2 Change in absorbance at 474 nm with different CN^- concentration.

Fig. S3 Partial ^1H NMR (400 MHz) spectra of **1O** and **1O** + CN^-.

Fig. S4 MS spectrum of **1O** + CN^-.

Fig. S5 Change in absorbance at 297 nm with different I^- concentration.

Fig. S6 The calibration curve absorbance of **1O** as a function of I^- concentration.

Fig. S7 Detection limit of **1O** to I^-.

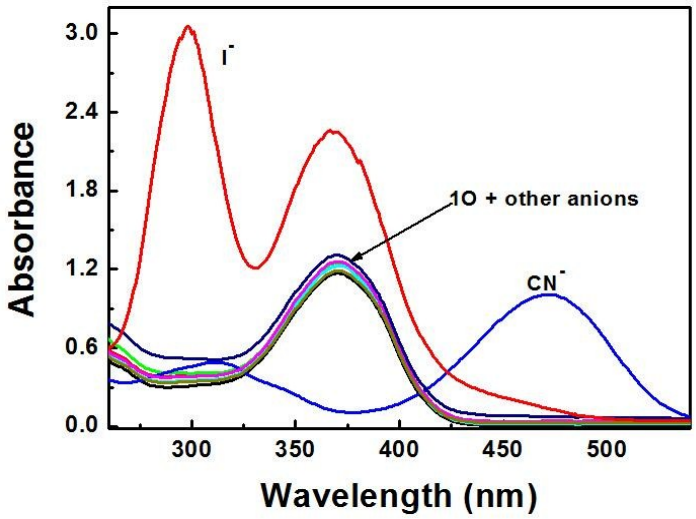
Fig. S8 Competitive tests for the absorption intensity of **1O** at 297 nm to various anions in tetrahydrofuran (2.0×10^{-5} mol L^{-1}). The black bars represent the absorption intensity induced by the addition of various anions. The red bars represent the absorption intensity of anion-contained solution followed by the addition of I^-, the $(A-A_0) / A_0$ ratio of **1O** at 297 nm in the presence of various ions (9.0 equiv.) and subsequent additional I^- (9.0 equiv.).

Fig. S9 Change in fluorescence intensity at 474 nm with different I^- concentration.

Fig. S10 Competitive tests for fluorescence intensity of **1O** at 480 nm in the presence of various anions (15.0 eq.) and subsequent additional I^- (9.0 eq.). The red bars represent the fluorescence intensity of **1O** induced by the addition of anions. The black bars represent the fluorescence intensity of ion-contained solution followed by the addition of I^-.

Fig. S11 Partial ^1H NMR (400 MHz) spectra of **1O** + I^-.

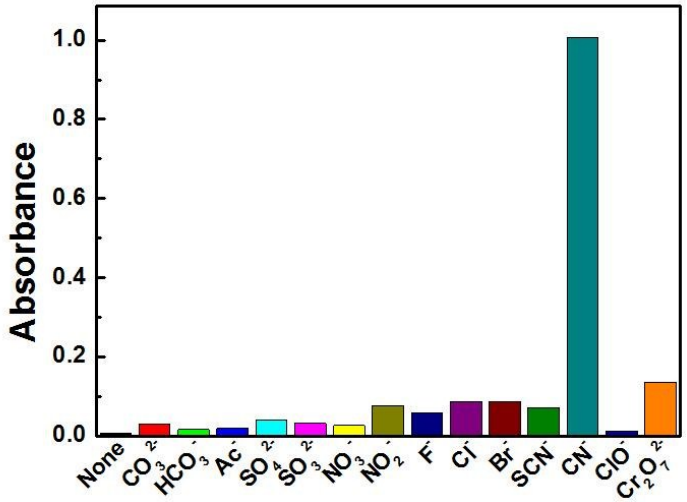
Fig. S12 MS spectrum of **1O** + I^-.


Absorbance
Wavelength (nm)
I-
1O + other anions
CN-
3.0
2.4
1.8
1.2
0.6
0.0
300
350
400
450
500

(A)


None
I-
CO3 2-
HCO3-
CH3COO-
SO4 2-
SO3 2-
NO3-
NO2-
F-
Cl-
Br-
SCN-
CN-
ClO-
Cr2O7 2-

(B)


Absorbance
1.0
0.8
0.6
0.4
0.2
0.0
None
CO3 2-
HCO3-
Ac-
SO4 2-
SO3 2-
NO3-
NO2-
F-
Cl-
Br-
SCN-
CN-
ClO-
Cr2O7 2-

(C)

Fig. S1

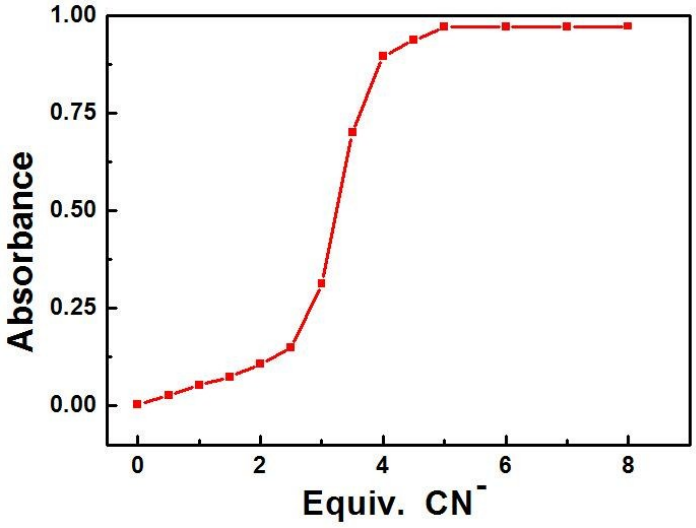


Fig. S2

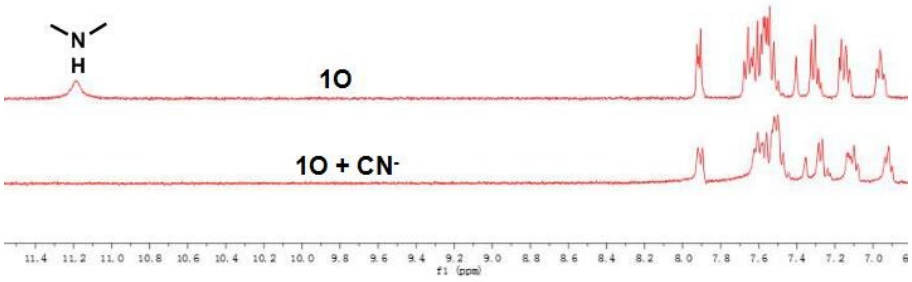

N
H
1O
1O + CN-
11.4 11.2 11.0 10.8 10.6 10.4 10.2 10.0 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)

Fig. S3

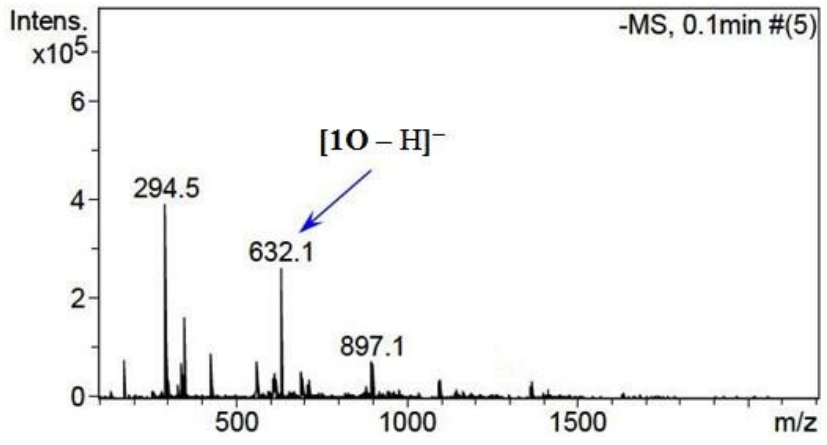

Intens.
x10^5
-MS, 0.1min #(5)
6
4
2
0
[1O – H]⁻
294.5
632.1
897.1
500
1000
1500
m/z

Fig. S4

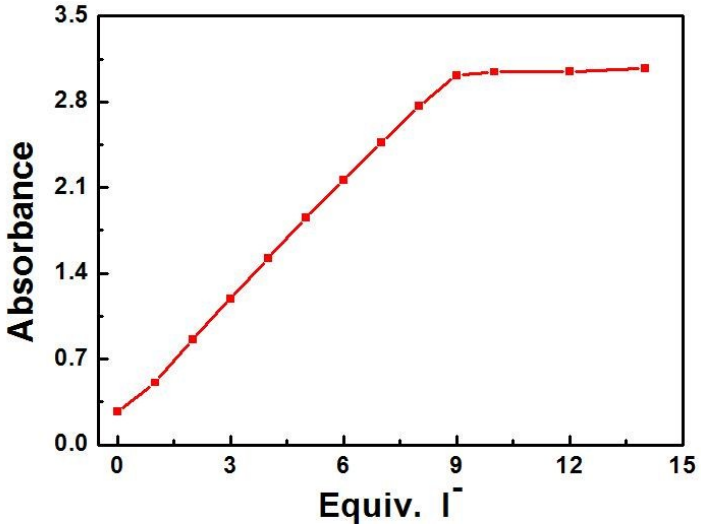


Fig. S5

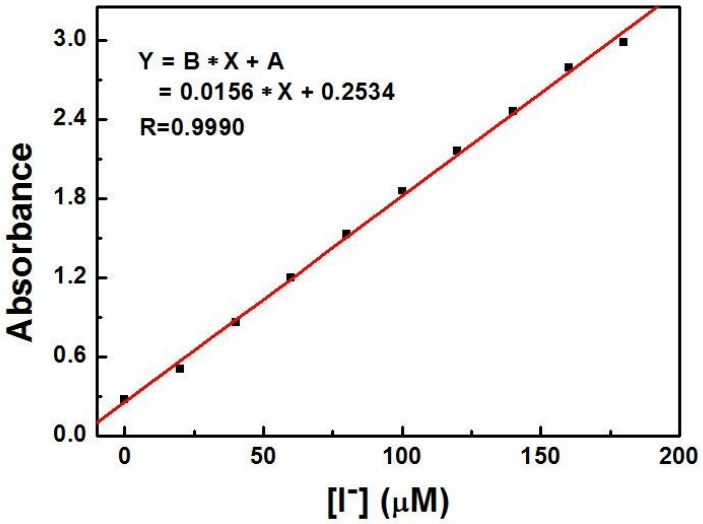

Y = B * X + A
= 0.0156 * X + 0.2534
R=0.9990
Absorbance
[I⁻] (μM)
0.0
0.6
1.2
1.8
2.4
3.0
0
50
100
150
200

Fig. S6

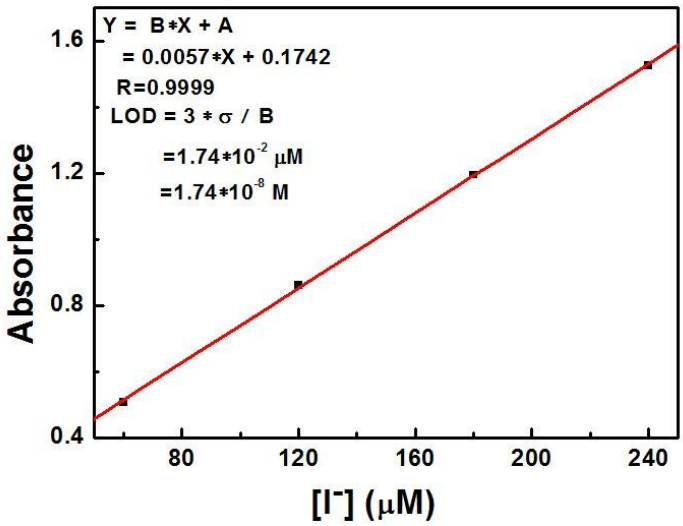

Y = B*X + A
= 0.0057*X + 0.1742
R=0.9999
LOD = 3 * σ / B
=1.74*10-2 μM
=1.74*10-8 M
Absorbance
1.6
1.2
0.8
0.4
80
120
160
200
240
[I-] (μM)

Fig. S7

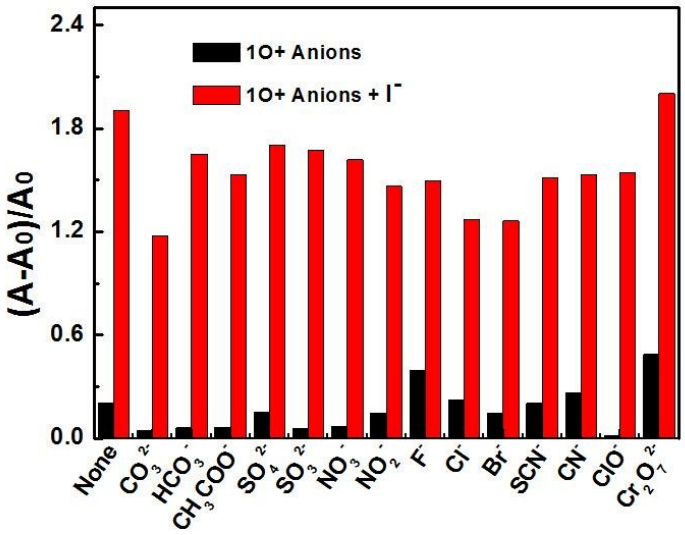

2.4
1.8
1.2
0.6
0.0
(A-A0)/A0
1O+ Anions
1O+ Anions + I-
None
CO3 2-
HCO3 -
CH3COO -
SO4 2-
SO3 2-
NO3 -
NO2 -
F-
Cl-
Br-
SCN-
CN-
ClO-
Cr2O7 2-

Fig. S8

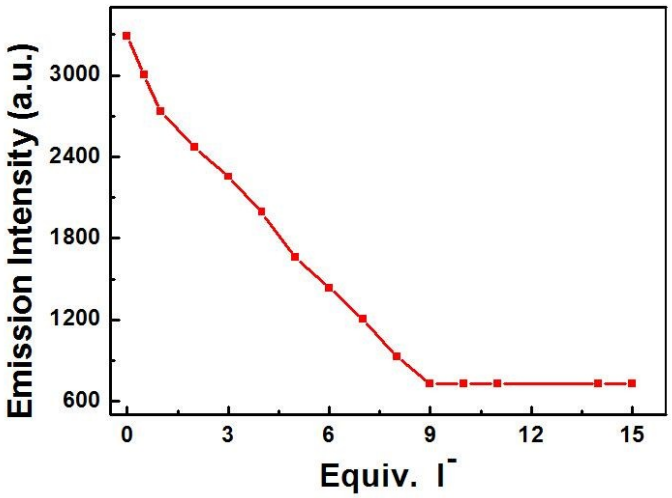

Emission Intensity (a.u.)
3000
2400
1800
1200
600
0
3
6
9
12
15
Equiv. I-

Fig. S9

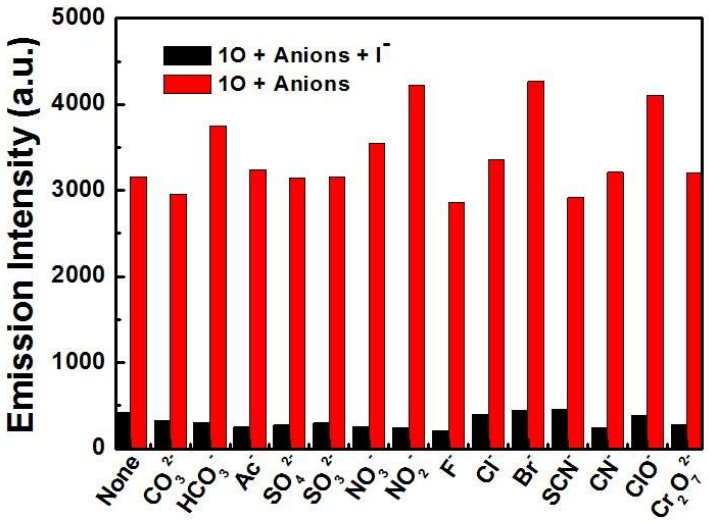

Emission Intensity (a.u.)
5000
4000
3000
2000
1000
0
1O + Anions + I-
1O + Anions
None
CO3 2-
HCO3 -
Ac-
SO4 2-
SO3 2-
NO3 -
NO2 -
F-
Cl-
Br-
SCN-
CN-
ClO-
Cr2O7 2-

Fig. S10

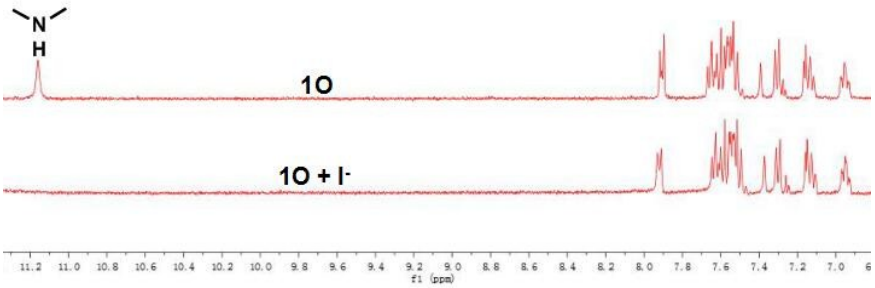

N
H
1O
1O + I-
11.2 11.0 10.8 10.6 10.4 10.2 10.0 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6
f1 (ppm)

Fig. S11

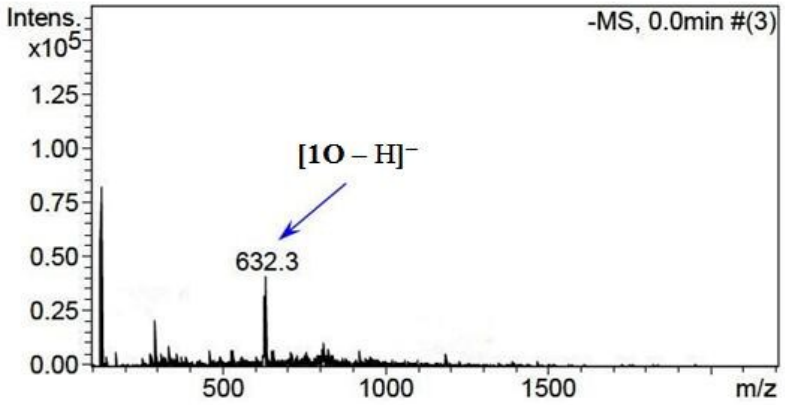

Intens.
x10^5
1.25
1.00
0.75
0.50
0.25
0.00
-MS, 0.0min #(3)
[1O – H]⁻
632.3
500
1000
1500
m/z

Fig. S12