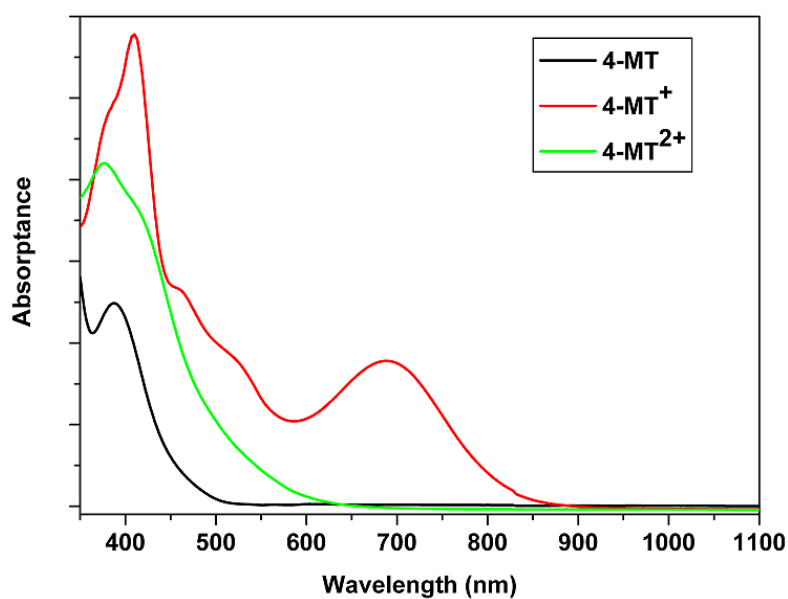


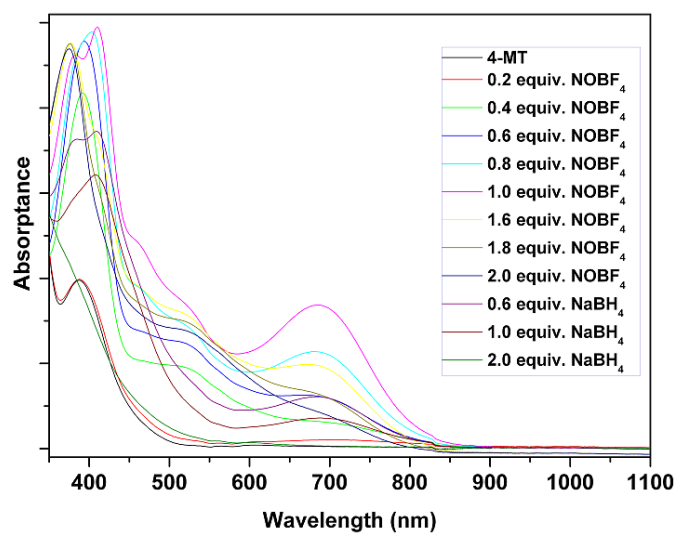
Supporting Information For

**New TTF derivatives: several molecular logic gates based on their  
switchable fluorescent emissions**

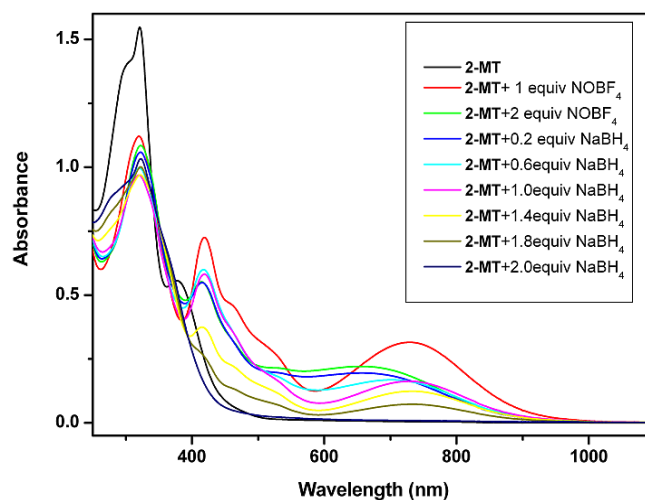
Chen-Jie Fang, Zhi Zhu, Wei Sun, Chun-Hu Xu, and Chun-Hua Yan\*



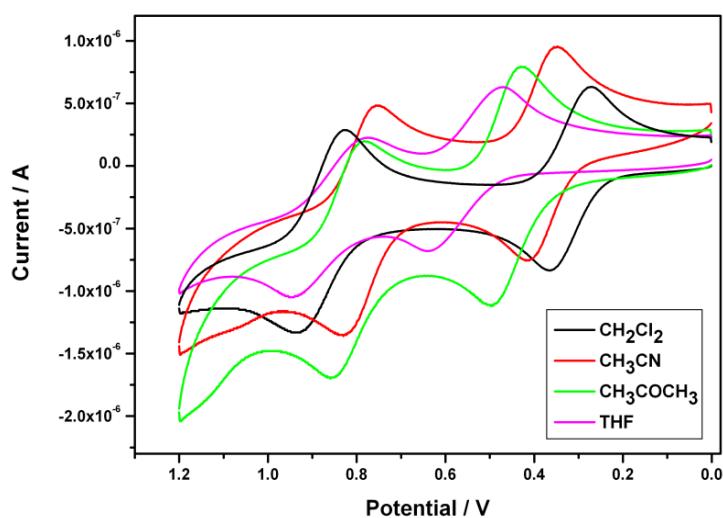
**Fig. S1.** Absorption of 0.1 mM neutral, cationic and dicationic 4-MT in CH<sub>2</sub>Cl<sub>2</sub>) upon the addition of NOBF<sub>4</sub> in acetonitrile.



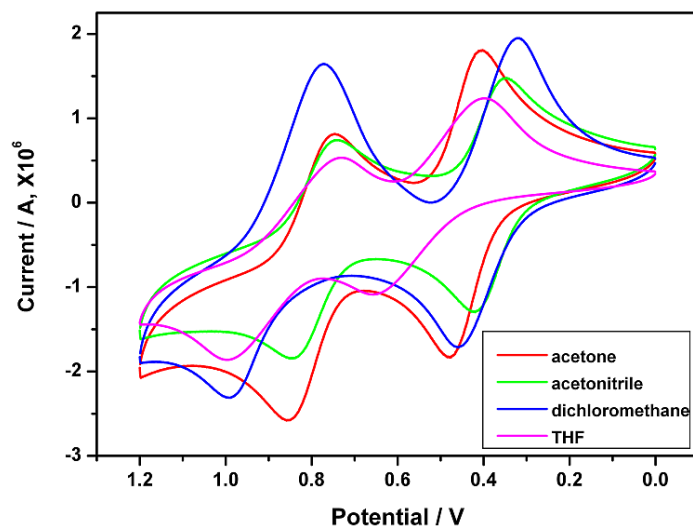
**Fig. S2.** The evolution of absorption spectra of 0.1 mM 4-MT upon addition of NOBF<sub>4</sub> and NaBH<sub>4</sub>.



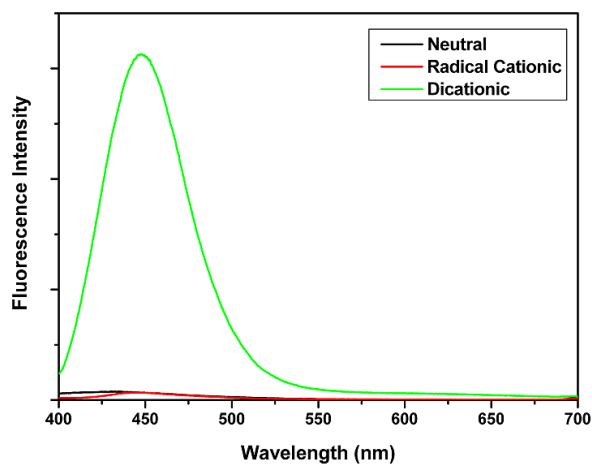
**Fig. S3.** The evolution of absorption spectra of  $5.0 \times 10^{-5}$  M 2-MT upon addition of NOBF<sub>4</sub> and NaBH<sub>4</sub>.



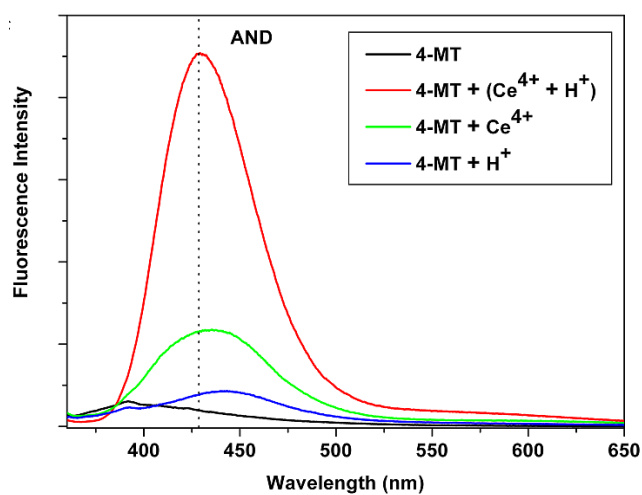
**Fig. S4.** Cyclic voltammograms of  $1 \times 10^{-4}$  2-MT in different solvents with  $1 \times 10^{-2}$  Bu<sub>4</sub>NPF<sub>6</sub> as supporting electrolyte at a scan rate of 100 mV/s with a Pt disk used as working electrode, a Pt wire as the counter electrode, and a Ag/AgCl electrode as the reference electrode.



**Fig. S5.** Cyclic voltammograms of  $1 \times 10^{-4}$  M 4-MT in different solvents with  $1 \times 10^{-2}$  M  $\text{Bu}_4\text{NPF}_6$  as supporting electrolyte at a scan rate of 100 mV/s with a Pt disk used as working electrode, a Pt wire as the counter electrode, and a Ag/AgCl electrode as the reference electrode.



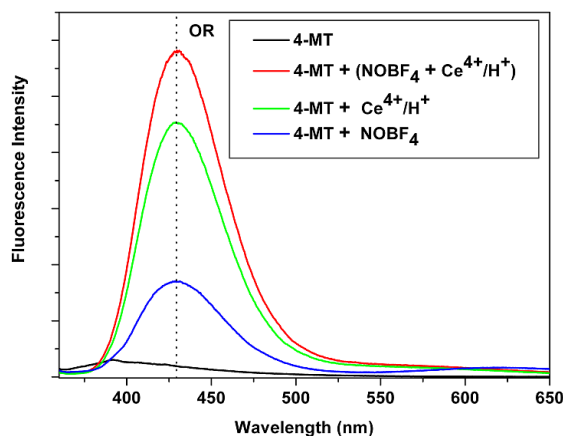
**Fig. S6.** The fluorescence spectra of neutral, cationic and dicationic 4-MT in  $\text{CH}_2\text{Cl}_2$ .



The truth table for AND gate for 4-MT

Ce <sup>4+</sup>	H <sup>+</sup>	PL
0	0	0 (0.04)
1	0	0 (0.26)
0	1	0 (0.09)
1	1	1 (1.00)

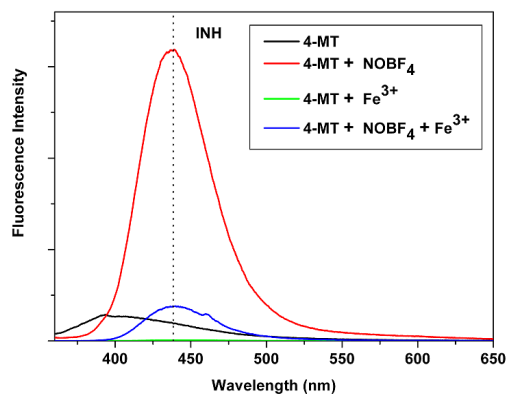
**Fig. S7.** Fluorescence spectra of 4-MT ( $1.0 \times 10^{-5}$  M) in  $\text{CH}_2\text{Cl}_2$  under different input conditions ( $2.0 \times 10^{-5}$  M  $(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$  and  $6.5 \times 10^{-5}$  M  $\text{CF}_3\text{COOH}$  in acetonitrile) and the truth table for AND logic gate. The normalized fluorescence intensities (PL) are shown in the brackets.



The truth table for OR gate for 4-MT

$\text{Ce}^{4+} + \text{H}^+$	$\text{NOBF}_4$	PL
0	0	0 (0.03)
1	0	1 (0.78)
0	1	1 (0.29)
1	1	1 (1.00)

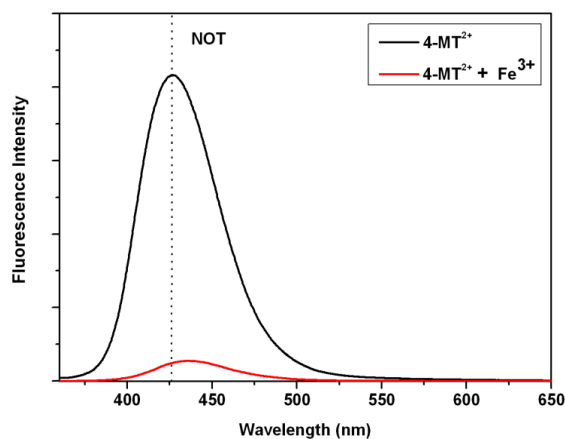
**Fig. S8.** Fluorescence emission spectra for 4-MT ( $1.0 \times 10^{-5}$  M) in  $\text{CH}_2\text{Cl}_2$  under different input conditions ( $2.0 \times 10^{-5}$  M  $(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$ ,  $6.5 \times 10^{-5}$  M  $\text{CF}_3\text{COOH}$  and  $7.5 \times 10^{-5}$  M  $\text{NOBF}_4$  in acetonitrile) and the truth table for OR logic gate. The normalized fluorescence intensities (PL) are shown in the brackets.



The truth table for INHIBIT gate for 4-MT

$\text{Fe}^{3+}$	$\text{NOBF}_4$	PL
0	0	0(0.06)
1	0	0 (0.00)
0	1	1(1.00)
1	1	0(0.12)

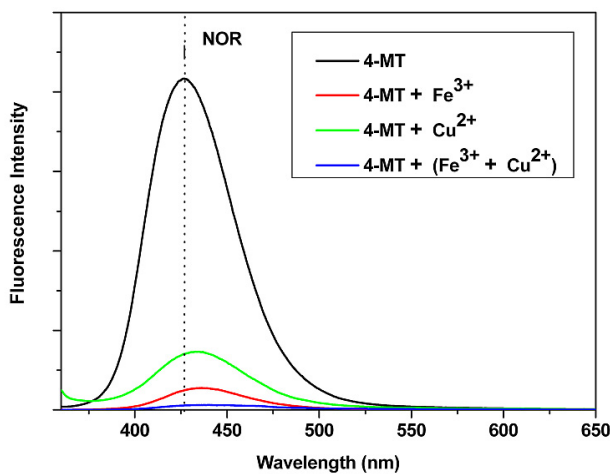
**Fig. S9.** Fluorescence emission spectra for 4-MT ( $1.0 \times 10^{-5}$  M) in  $\text{CH}_2\text{Cl}_2$  under different input conditions ( $1.5 \times 10^{-4}$  M  $\text{NOBF}_4$  and  $4.0 \times 10^{-4}$  M  $\text{FeCl}_3$  in acetonitrile) and the truth table for INHIBIT logic gate. The normalized fluorescence intensities (PL) are shown in the brackets.



The truth table for NOT gate for 4-MT

$\text{Fe}^{3+}$	PL
0	1(1.00)
1	0(0.06)

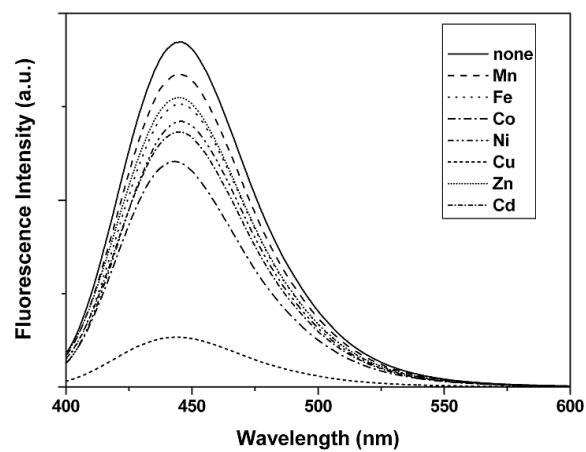
**Fig. S10.** Fluorescence emission spectra for  $4\text{-MT}^{2+}$  ( $1.0 \times 10^{-5}$  M) in  $\text{CH}_2\text{Cl}_2$  under input of  $4.0 \times 10^{-4}$  M  $\text{FeCl}_3$ , in acetonitrile and the truth table for NOT logic gate. The normalized fluorescence intensities (PL) are shown in the brackets.



The truth table for NOR gate for 4-MT

$\text{Cu}^{2+}$	$\text{Fe}^{3+}$	PL
0	0	1 (1.00)
1	0	0 (0.17)
0	1	0 (0.06)
1	1	0 (0.00)

**Fig. S11.** Fluorescence emission spectra for  $4\text{-MT}^{2+}$  ( $1.0 \times 10^{-5}$  M) in  $\text{CH}_2\text{Cl}_2$  under different input conditions ( $4.0 \times 10^{-4}$  M  $\text{FeCl}_3$  and  $1.6 \times 10^{-3}$  M  $\text{CuCl}_2$  in acetonitrile) and the truth table for NOR logic gate. The normalized fluorescence intensities (PL) are shown in the brackets.



**Fig. S12.** Fluorescent spectra of 2-MT<sup>2+</sup> ( $5.0 \times 10^{-5}$  M) in CH<sub>2</sub>Cl<sub>2</sub> in the presence of various metal ions ( $1.0 \times 10^{-3}$  M, in acetonitrile)