Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Emission enhancement of cationic tetraphenylethylene derivatives by encapsulation in cucurbit[10]uril host in water

Chang Liu,[a] Yong Wu,[a] Xie Han[a] and Simin Liu*[a,b]

[a] *The State Key Laboratory of Refractories and Metallurgy, School of Chemistry and Chemical Engineering, Wuhan University of Science and Technology, Wuhan 430081, China. E-mail: liusimin@wust.edu.cn*

[b] *Institute of Advanced Materials and Nanotechnology, Wuhan University of Science and Technology, Wuhan 430081, China*

Table of Contents Page

Experimental Section

CB[10] were prepared by the corresponding literature procedures.[1] Compound TPE derivatives (**1-5**) were synthesized using the previously reported methods.[2-6] All ^{1}H NMR, ^{13}C NMR, COSY spectra were collected on Agilent 600 MHz DD2. Mass spectrometry was performed using a Bruker Agilent 1290-micrOTOF Q II. UV/Vis were performed on a SHIMADZU UV-3600 instrument with 1 cm pathlength cells at 298 K. Fluorescence spectra were collected on a PerkinElmer LS-55 machine.

[1] X. Yang, Z. Zhao, X. Zhang and S. Liu, *Sci. China Chem.*, 2018, **61**, 787-791.

[2] S. Xu, X. Bai, J. Ma, M. Xu, G. Hu, T. D. James and L. Wang, *Anal. Chem.*, 2016, **88**, 7853-7857.

[3] Y. Wu, H. Hua and Q. Wang, *New J. Chem.*, 2018, **42**, 8320-8324.

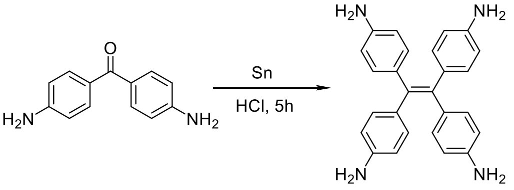
[4] H. Xie, F. Zeng, C. Yu and S. Wu, *Polym. Chem.*, 2013, **4**, 5416-5424.

[5] Y.-X. Zhu, Z.-W. Wei, M. Pan, H.-P. Wang, J.-Y. Zhang and C.-Y. Su, *Dalton Trans.*, 2016, **45**, 943-950.

[6] G.-J. Liu, S.-N. Tian, C.-Y. Li, G.-W. Xing and L. Zhou, *ACS Appl. Mater. Interfaces*, 2017, **9**, 28331-28338.

Synthesis

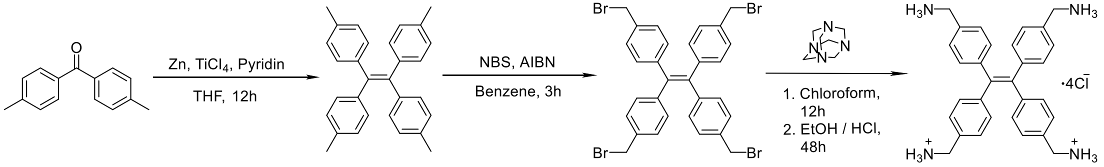
Preparation of 1



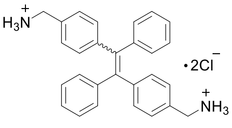
1

Compound **1** was prepared following published methods.[2]

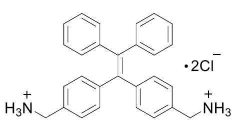
Preparation of 2, 4, 5



2



4



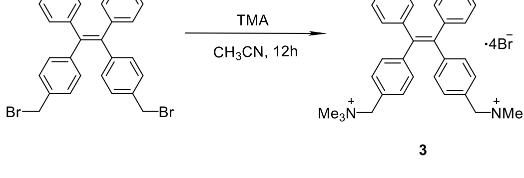
5

Compound **2**, **4** and **5** was prepared following published methods.[3-5]

Compound **4** (50% yield); ^{1}H NMR (600 MHz, DMSO-d_6) δ (TMS, ppm): 7.18-7.11 (m, 16H), 4.03 (s, 4H). ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 143.54, 143.34, 140.71, 132.64, 131.05, 128.81, 128.45, 127.20, 42.10. HRMS (ESI) (m/z) [M]$^+$ calcd: 392.54, Found: 392.2239.

Compound **5** (40% yield); ^{1}H NMR (600 MHz, D_2O) δ (TMS, ppm): 7.17-7.11 (m, 16H), 4.04 (s, 4H). ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 143.61, 143.28, 142.88, 132.73, 131.44, 131.05, 130.87, 128.85, 128.35, 127.14, 42.23. HRMS (ESI) (m/z) [M]$^+$ calcd: 392.54, Found: 392.16.

Preparation of 3



3

1,1,2,2-tetrakiss(4-(bromomethyl)phennyl)ethane (0.2g, 0.28 mmol) was dissolved in acetonitrile. Then 33% trimethylamine alcoholic (0.47 mL, 2 mmol) solution was added to the mixture, and the contents were stirred at rt for 12 h. Both organic solvent and the excess trimethylamine were evaporated from the crude product mixture under reduced pressure followed by addition of diethyl ether. After stirring at rt for another 2 h, the mixture was filtered and the white solid was rinsed with diethyl ether (160 mg, 60%).[6] ^{1}H NMR (600 MHz, DMSO-d_6) δ (TMS, ppm): 7.19 (d, J = 6 Hz, 8H), 6.94 (d, J = 6 Hz, 8H), 4.34 (s, 8H), 2.81 (s, 36H). ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 144.32, 141.27, 132.84, 131.52, 127.61, 67.43, 52.07. HRMS (ESI) (m/z) [M-2Br$^-$]$^{2+}$ calcd: 390.485, Found: 390.1577.

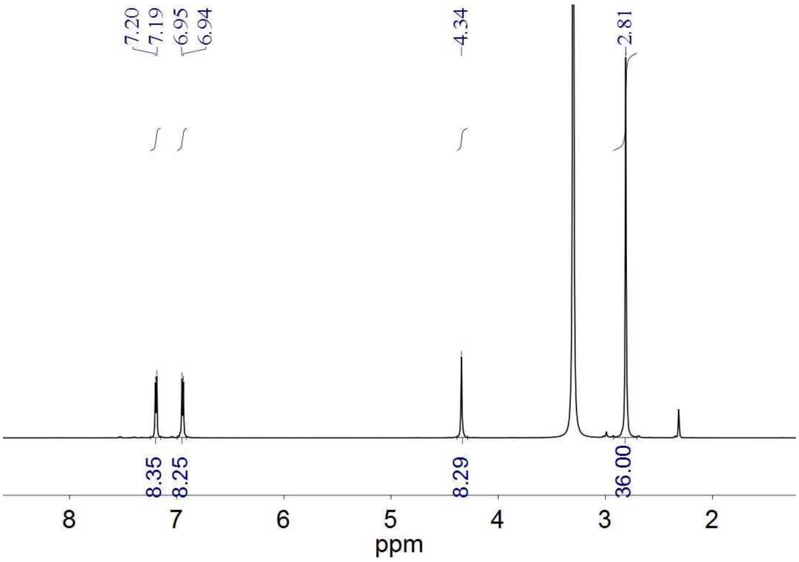


Fig. S1 ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of **3**.

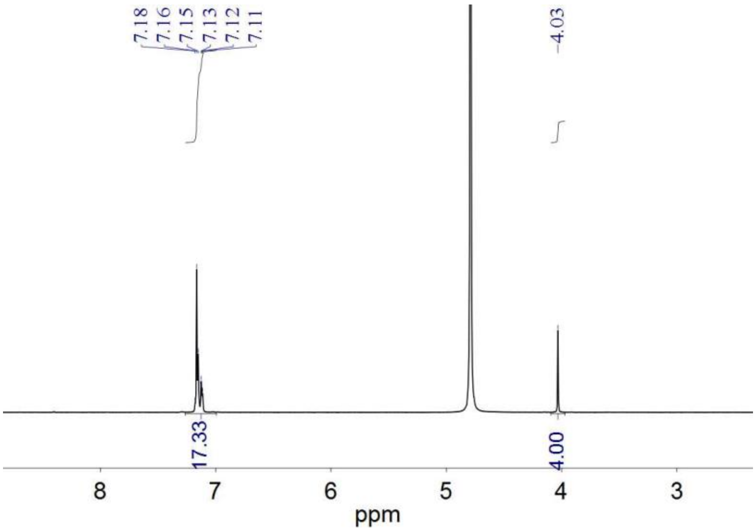


Fig. S2 ^{1}H NMR spectrum (600 MHz, D_2O) of **4**.

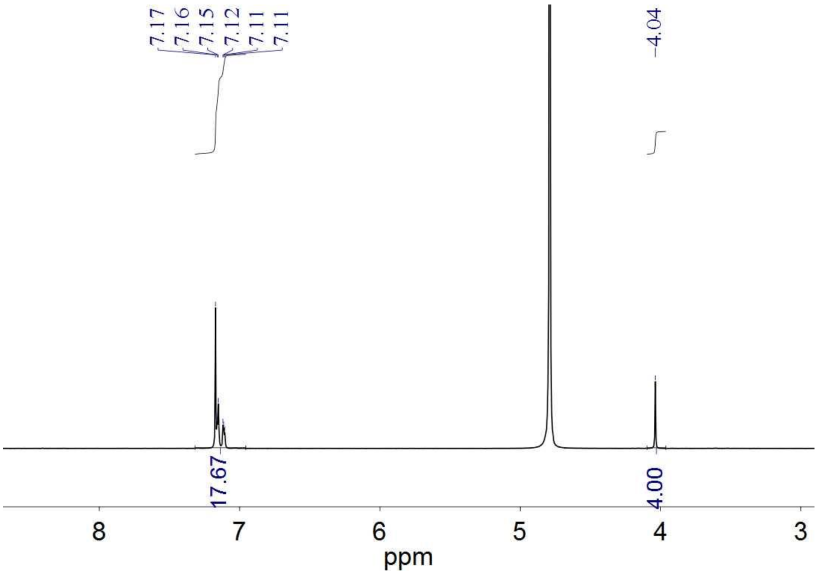


Fig. S3 ^{1}H NMR spectrum (600 MHz, D_2O) of **5**.

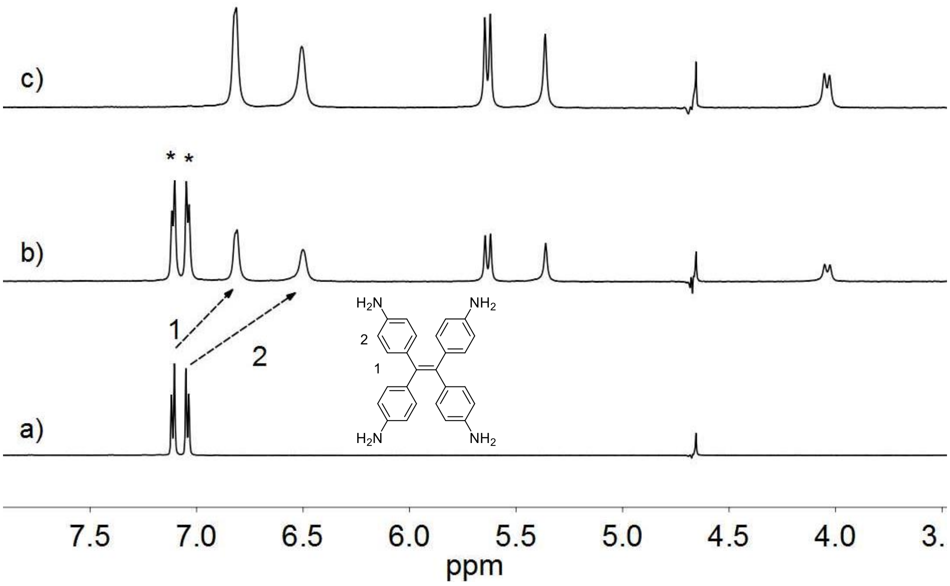


Fig. S4 ^{1}H NMR spectra (600 MHz, 0.01M DCl in D_2O) of: a) free **1** (1.0 mM); b) 2:1 mixture of **1** and CB[10]; c) **1** with excess CB[10] (resonances of free **1** are marked with *).

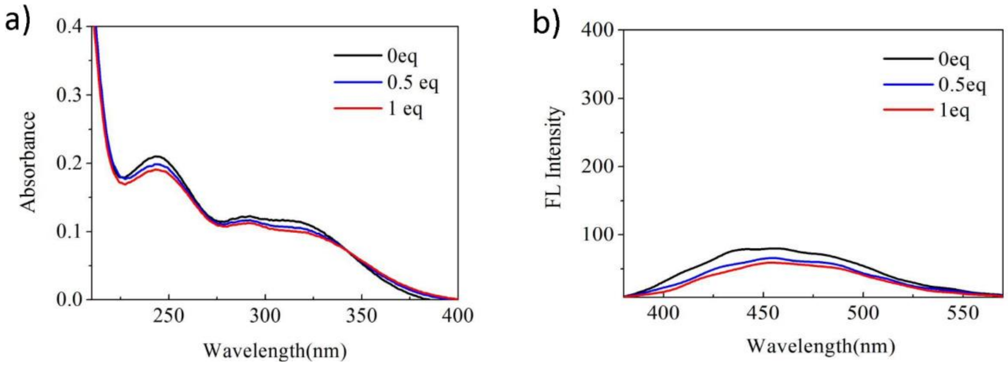


Fig. S5 UV/vis spectra (a) and fluorescence spectra (b) of **1** with addition of CB[10] ([**1**] = 10 μM. λ_{ex} = 300 nm, slit = 5 × 5 nm).

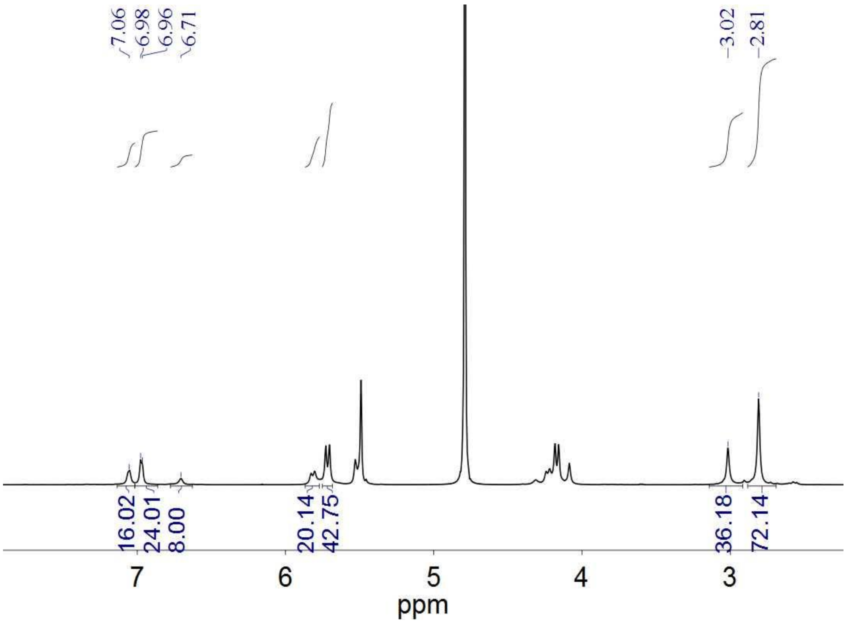


Fig. S6 ^{1}H NMR spectra (600 MHz, D_2O, 298K) of CB[10]•**3** (1.0 mM).

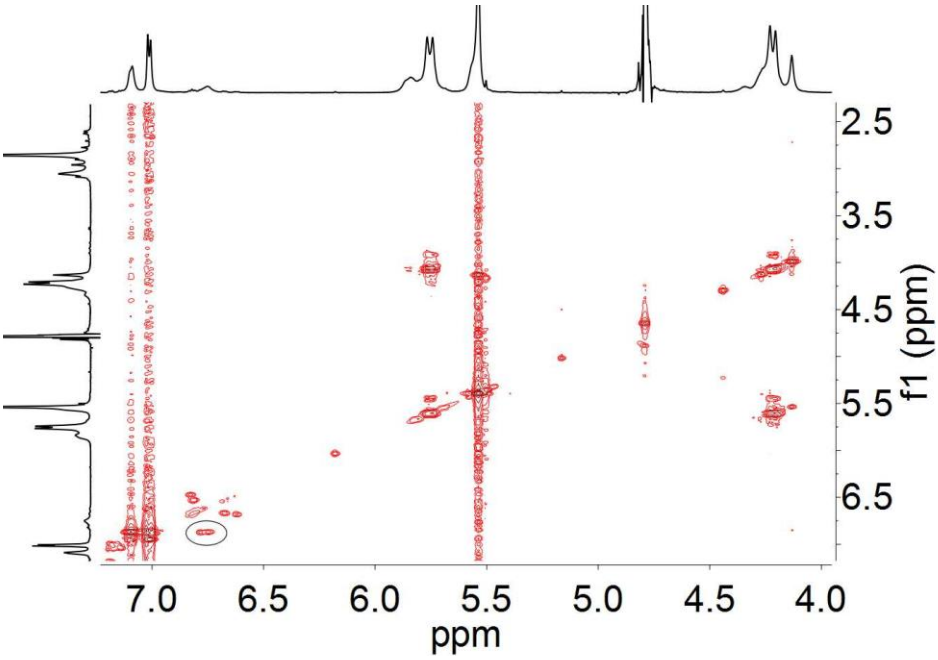


Fig. S7 COSY NMR spectrum (600 MHz, D_2O, 298K) of CB[10]•**3**.

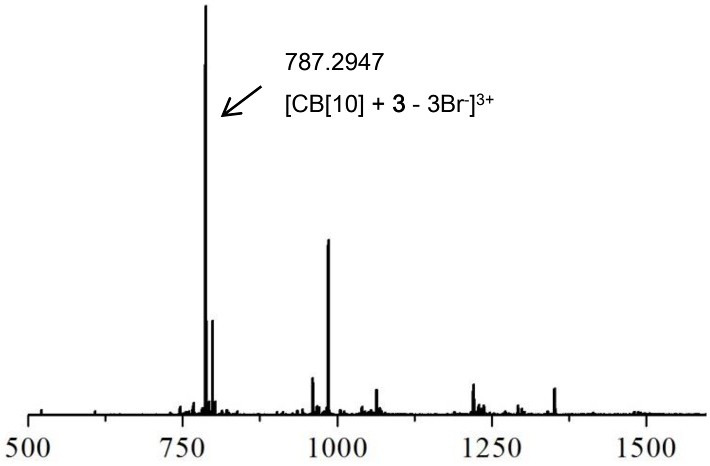


Fig. S8 ESI-MS spectrum of CB[10]•**3**.

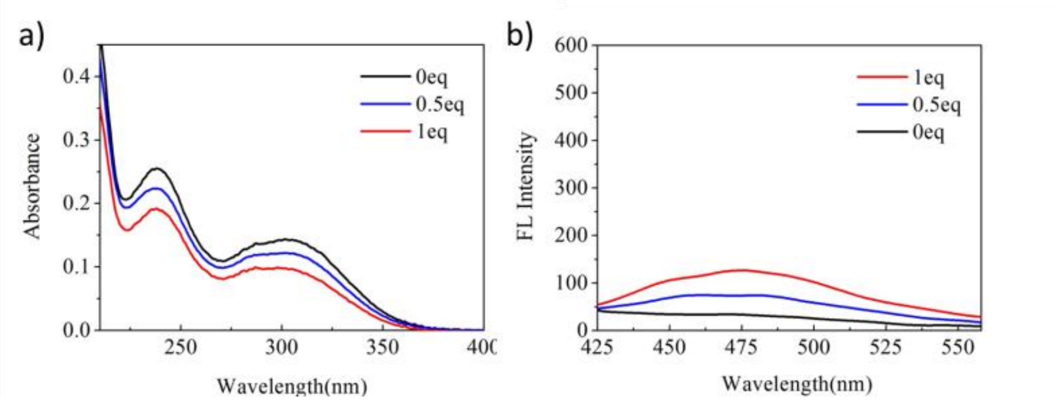


Fig. S9 UV/vis spectra (a) and fluorescence spectra (b) of **4** with addition of CB[10] (0, 0.5 eq, 1.0 eq) ([**4**] = 10 μM, λ_{ex} = 350 nm, slit = 5 × 5 nm).

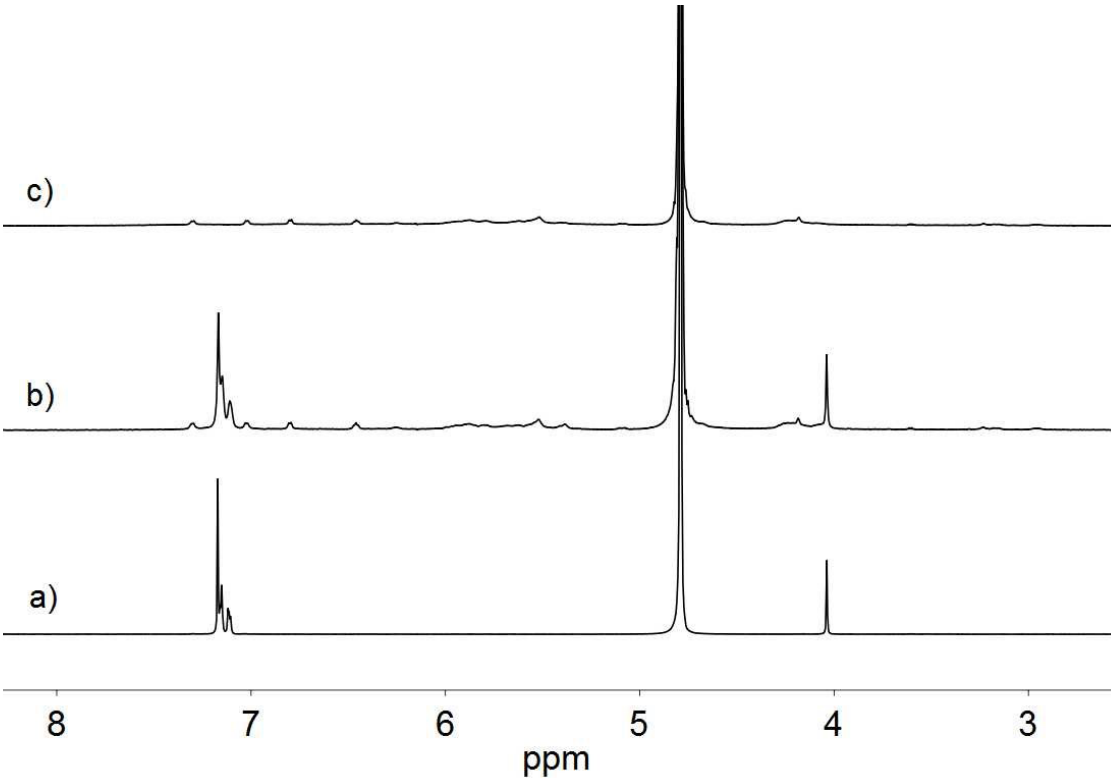


Fig. S10 ^{1}H NMR spectra (600 MHz, D_2O) of: a) free **5** (1.0 mM); b) **5** with 0.5 equiv. of CB[10]; c) **5** with 1 equiv. of CB[10].