

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

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Supporting Information for

**Tetraphenylethene Modified [n]Rotaxanes: Synthesis,
Characterization and Aggregation-Induced Emission Behaviors**

Guoxing Liu,[†] Di Wu,[†] Jinhua Liang, Xie Han, Sheng Hua Liu, Jun Yin*

Key Laboratory of Pesticide and Chemical Biology, Ministry of Education, College of Chemistry, Central

China Normal University, Wuhan 430079, P. R. China.

E-mail: yinj@mail.ccnu.edu.cn

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1. UV-vis spectra of 8, 11, 16, 17, 24 and 25 in CH₃CN/water mixtures with different fractions of water (f_w).

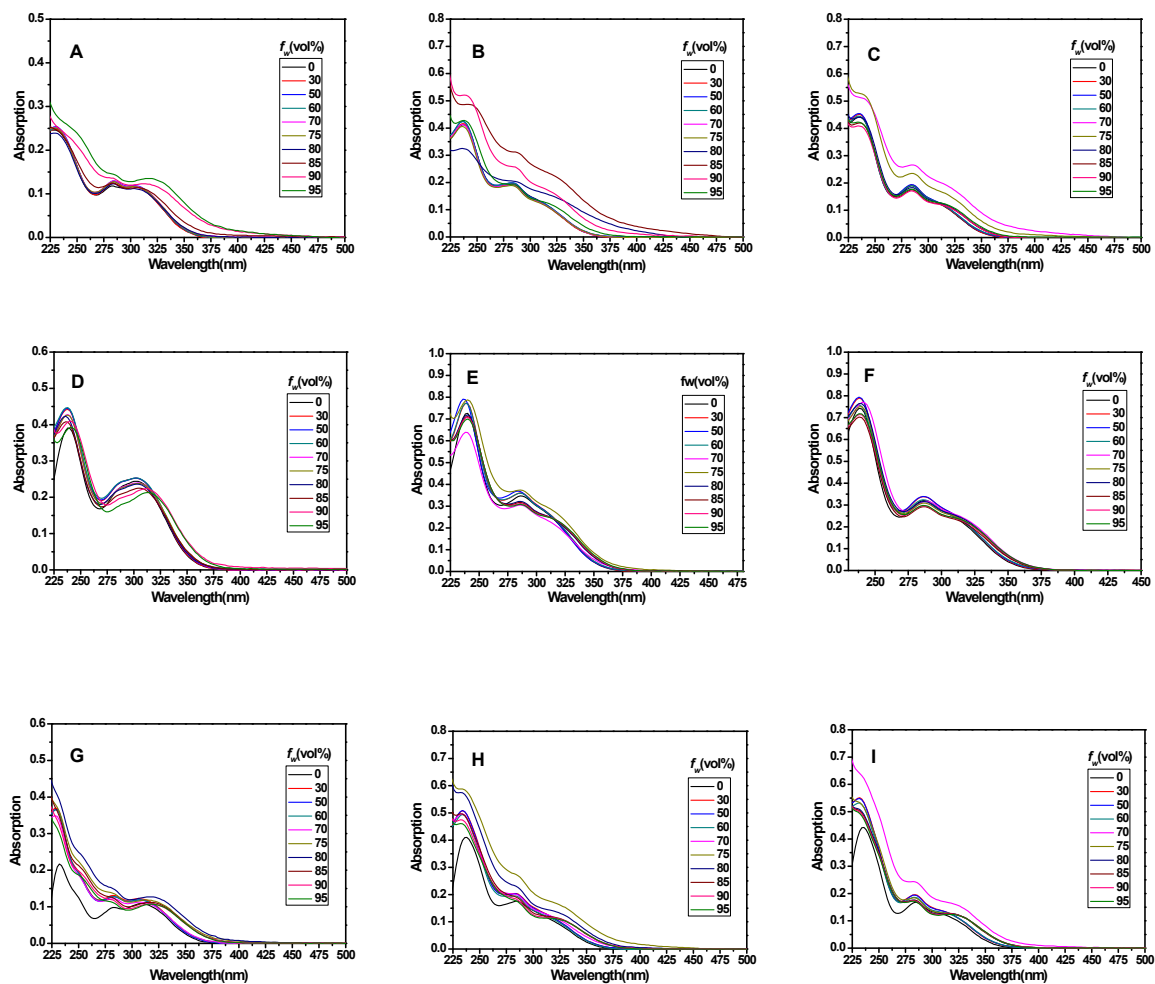


Figure S1. UV-vis spectra of 8(A), 11a(B), 11b(C), 16(D), 17a(E), 17b(F), 24(G), 25a(H) and 25b(I) in CH₃CN/water mixtures with different fractions of water (f_w).

2. Optimized structures based on DFT (B3LYP/6-31G*) calculations

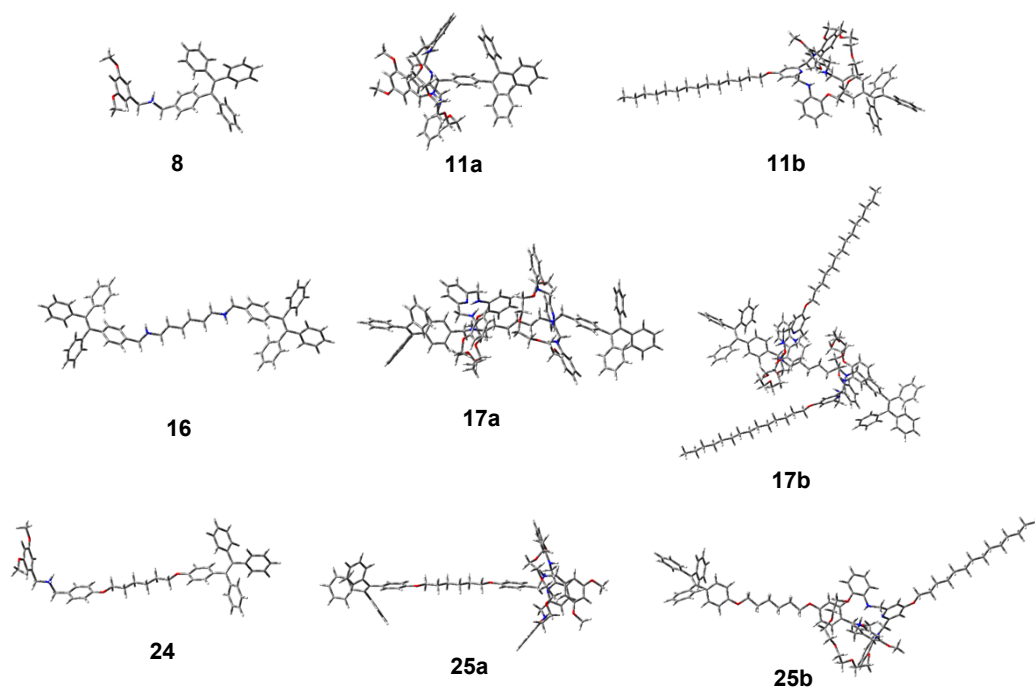


Figure S2. Optimized structures based on DFT (B3LYP/6-31G*) calculations. **8**, **11a-b**, **16**, **17a-b**, **24** and **25a-b**.

3. Partial ^1H NMR spectra of [2]rotaxanes **17a-b**

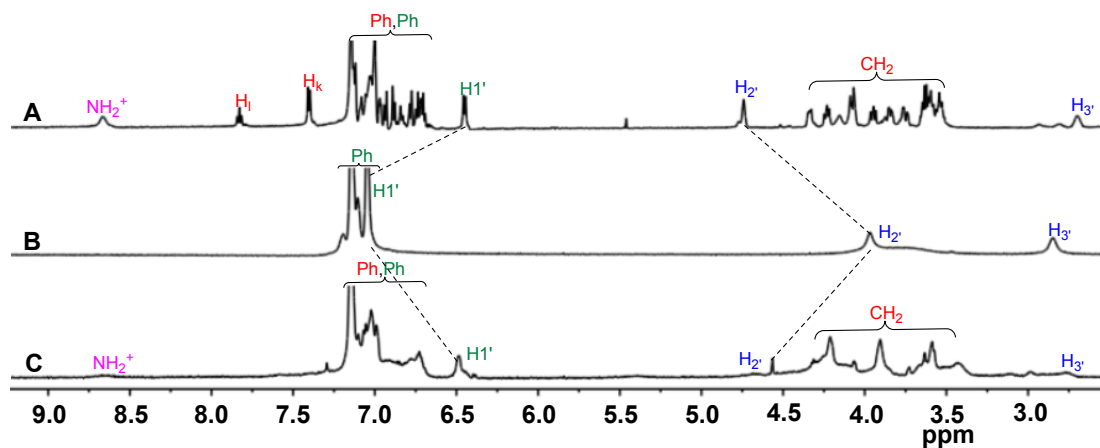


Figure S3. ^1H NMR spectra (600 MHz in CD_3CN at r.t.) of **17a** (A); **16** (B) and **17b** (C).

4. Photographs of **24** and **25** in CH_3CN /water mixtures with different fractions of water (f_w) taken under UV illumination.

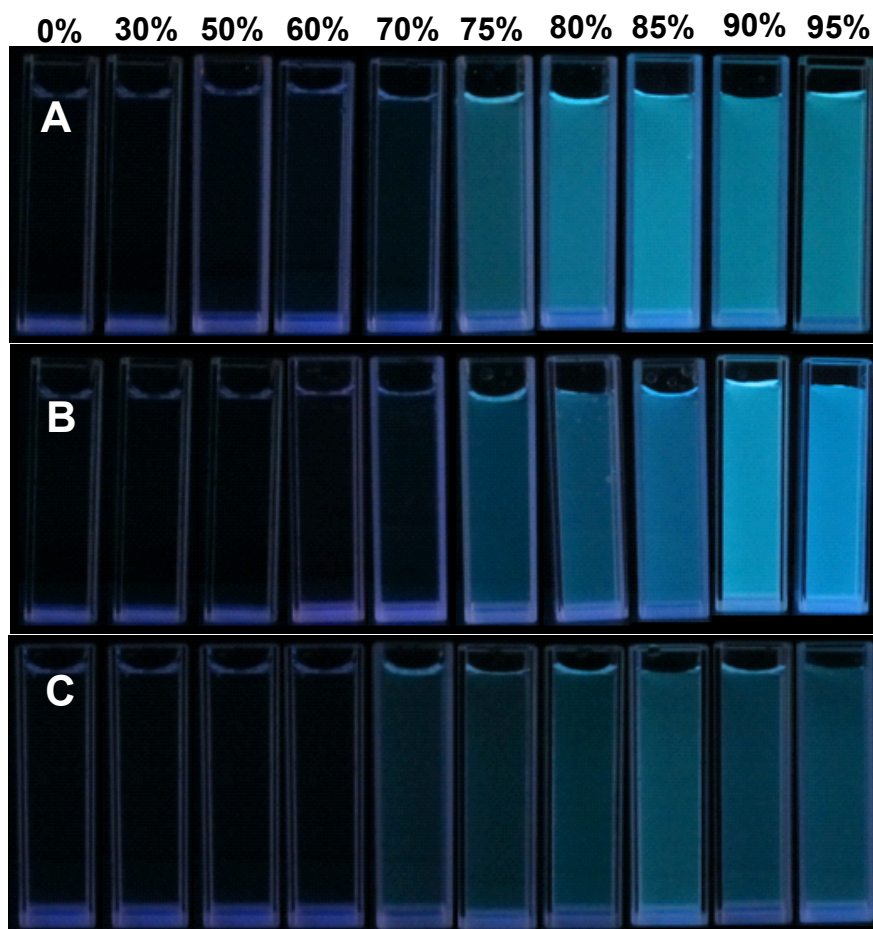


Figure S4. Photographs of **24(A)**, **25a(B)** and **25b(C)** in $\text{CH}_3\text{CN}/\text{water}$ mixtures with different fractions of water (f_w) taken under UV illumination.

5. NMR and Mass spectra

