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 CH$_3$CN/water mixtures with different fractions of water ($f_w$).

![UV-vis spectra of 8, 11, 16, 17, 24 and 25 in CH$_3$CN/water mixtures with different fractions of water ($f_w$).](image)

*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 CH$_3$CN/water mixtures with different fractions of water ($f_w$).

2. Optimized structures based on DFT (B3LYP/6-31G*) calculations
3. Partial 1H NMR spectra of [2]rotaxanes 17a-b

Figure S3. $^1$H NMR spectra (600 MHz in CD$_3$CN at r.t.) of 17a (A); 16 (B) and 17b (C).

4. Photographs of 24 and 25 in CH$_3$CN/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 CH$_3$CN/water mixtures with different fractions of water ($f_w$) taken under UV illumination.

5. NMR and Mass spectra
MALDI-MS

MALDI-MS

600 MHz $^1$H NMR Spectrum in CDCl$_3$ at RT
100 MHz $^1$H NMR Spectrum in CD$_2$CN at RT
MALDI-MS

15

[structure image]

16

600 MHz $^1$H NMR Spectrum in CD$_2$CN at RT

[structure image]
MALDI-MS

16

\[ 100 \text{MHz } ^{13}\text{C} \text{ NMR Spectrum} \]

\[ \text{in CD}_{2}\text{CN at RT} \]
MALDI-MS

17a

2 PF₆⁻

17b

600 MHz ¹H NMR Spectrum in CD₃CN at RT