

Influence of number and substitution position of phenyl rings on the aggregation-induced emission feature of multi-phenyl substituted benzenes

Lingzhi Li (21229048)^a, Jing Zhi Sun^a, Anjun Qin^{*a}, and Ben Zhong Tang ^{*a,b}

^a MOE Key Laboratory of Macromolecular Synthesis and Functionalization, Department of Polymer Science and Engineering, Zhejiang University, Hangzhou 310027, China

^b Department of Chemistry, The Hong Kong University of Science & Technology, Clear Water Bay, Kowloon, Hong Kong, China

INTRODUCTION

Aggregation-induced emission (AIE) is of both academic and practical. Among the reported AIE-active luminogens, lots of them are tetraphenylethene (TPE) derivatives. While there still remains arguments on the mechanism of TPE because of its containing

double bond, which is also not stable for OLED applications. Here, we developed a series of multi-phenyl substituted benzenes. Interestingly, with different number and position of substituted phenyl rings on the benzene cores, some of them are AIE-active or feature the aggregation-enhanced emission. It is anticipated that such AIE-active luminogens are very stable and could find wide applications in diverse areas including light-emitting devices, chemosensors and bioprobes.

RESULTS AND DISCUSSION



Photophysical property

I/1₀

425

vol%

В



Scheme 1. Structures of multi-phenyl substituted benzenes.

Crystal structure



Wavelength(nm)

Water fraction(%)

40

20

- 135-TPB

60

m-terpheny

80

100

Figure 1. (A) Photoluminescence (PL) spectra of *m*-terphenyl in THF/water mixtures with different water fractions; $\lambda_{ex} = 248$ nm, [*m*-terphenyl] = 10 μ M. (B) Changes in the PL intensity of *m*-terphenyl and 1,3,5-TPB in THF/water mixtures with different water fractions.



water fractions; λ_{ex} = 275 nm, [TPB] = 10 µM. (B) Changes in the fluorescence intensity of 1,2,4-TPB, TPB, PPB and HPB in THF/water mixtures with different water fractions.

Figure 3. Molecular structures and torsion angles (left) and representative intermolecular C-H...π interactions with indicative distance (right) of 1,3,5-TPB and 1,2,4-TPB, respectively.

CONCLUSIONS

An unambiguous structure-property relationship of multiphenyl substituted benzenes was established. The number and position of substituted phenyl rings on the benzene cores play crucial roles in determining their photophysical properties. More phenyl rings attached to the central benzene cores will induce more pronounced AIE effect, which provide an ideal platform to investigate the mechanism of AIE.

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