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# Observation of Photophysical Processes of a TIPS-Heptacene

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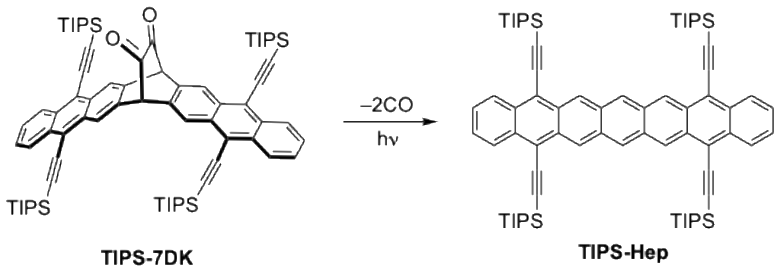
Abstract:

Linearly fused higher acenes, particularly those with more than five benzene rings, have attracted considerable attention for their potential in near-infrared (NIR) optoelectronics and organic semiconductors. Their unique optical and electronic properties, derived from extended π-conjugation and zigzag-edged structures, make them ideal model systems for exploring magnetism in carbon-based nanostructures. However, this structural motif leads to an exceptionally narrow HOMO–LUMO gap as the acene length increases, which significantly compromises their intrinsic stability.

Herein, we report the design, synthesis, and photophysical characterization of 5,9,14,18-tetrakis(triisopropylsilylethynyl)heptacene (**TIPS-Hep**). **TIPS-Hep** was prepared from the photo-precursor, **TIPS-7DK** via the in situ Strating–Zwanenburg reaction (Scheme 1). We achieved a significant breakthrough by successfully observing stable heptacene fluorescence in solution at room temperature—a long-standing challenge in the photophysics of higher acenes. In spin-coated thin films, **TIPS-Hep** exhibited accelerated and enhanced triplet state formation. Given the involvement of multiple excited species in femtosecond transient absorption spectroscopy (fs-TAS), various kinetic models were evaluated; a sequential singlet fission (SF) model was identified as the most accurate description of the process. These findings provide deeper insights into the photophysical dynamics of extended acenes and offer valuable guidelines for the development of next-generation organic electronic devices (Figure 1).




*Scheme 1. Strating–Zwanenburg reaction from **TIPS-7DK** to **TIPS-Hep**.*

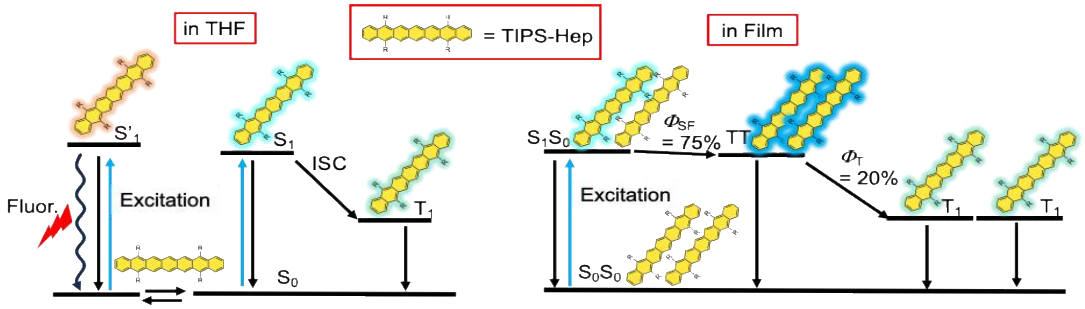



*Figure 1. Kinetic models of **TIPS-Hep** in THF (left) and in film (right).*

References:

[1] Shinjiro Suzuki, Hayato Sakai, Mitsuaki Yamauchi, Hironobu Hayashi, Yoshiyuki Mizuhata, Tatsuhisa Kato, Takashi Hirose,* Taku Hasobe,* and Hiroko Yamada*, *J. Am. Chem. Soc.* **2026**, *148*, 6000-6011.