

Synthesis and Optical Properties of Diazadibenzo[*hi*,*st*]ovalene Derivatives

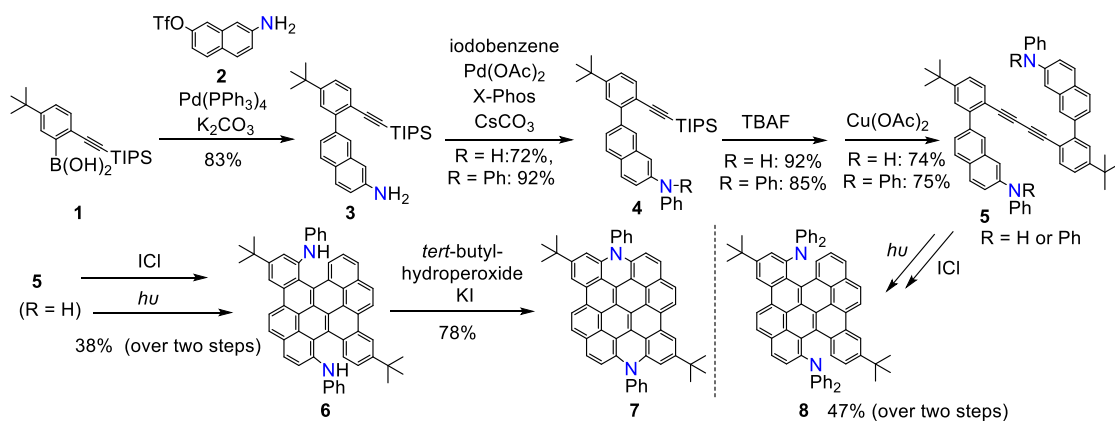
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A substantial array of graphene molecules, namely large polycyclic aromatic hydrocarbons (PAHs), has been synthesized, demonstrating diverse optoelectronic characteristics. Nevertheless, their prospective utilization in photonic applications has largely remained underexplored.¹ Dibenzo[*hi*,*st*]ovalene (DBOV) derivatives display remarkable photo-physical characteristics, such as intense fluorescence, high photo-stability, and intrinsic fluorescence blinking, making them promising for super-resolution fluorescence imaging.² Moreover, diaza-DBOV showed fluorescence sensitive to pH and metal ions, which is still rare for fluorescent probes with blinking properties.² The primary limitation of diaza-DBOV was its poor solubility. In this study, the incorporation of a phenyl ring at the nitrogen atoms was considered to address this solubility issue, simultaneously leading to electronic rich variants of diaza-DBOV.

Here, we present a synthesis of a diphenyl derivative of diaza-DBOV **7** in nine steps in a total yield of 9% (Scheme 1). Nitrogen-incorporated zigzag edges were formed via oxidative cyclization of phenylamino groups. We also obtained diphenylamino-substituted PAH **8**, as a tetraphenyl analog of diaza-DBOV, in eight steps in a total yield of 17% (Scheme 1). The optical properties of **7** and **8**, including its pH and solvent-polarity dependence were studied by UV-vis absorption and fluorescence spectroscopy and other spectroscopic methods.

Scheme 1. Synthesis of N-DBOV derivative **7** and **8**



1) G. M. Paternò, Goudappagouda, Q. Chen, G. Lanzani, F. Scotognella, A. Narita, *Adv. Optical Mater.* **2021**, 9, 2100508. 2) E. Jin, Q. Yang, C.-W. Ju, Q. Chen, K. Landfester, M. Bonn, K. Müllen, X. Liu, A. Narita, *J. Am. Chem. Soc.* **2021**, 143, 10403–10412.