

Functionalization at Nonperipheral Positions of Triazatruxene: Modular Construction of 1, 6, 11-Triarylated-Triazatruxenes for Potentially Organic Electronics and Optoelectronics

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Abstract

Functionalization from nonperipheral positions of triazatruxene is representing a challenge. Triarylation of the nonperipheral positions (1, 6, and 11) in triazatruxene scaffold has been achieved for the first time via two approaches. The transformations involve arylation/cyclotrimerization and cyclotrimerization/arylation sequences. POCl₃-mediated direct cyclotrimerization of oxindoles containing electron-deficient substituents on the aryl group at the C7-position resulted in the formation of 2-chloroindoles, whereas oxindoles containing electron-donating substituents gave the triazatruxenes. Furthermore, desired triazatruxenes were achieved through cyclotrimerization of 7-bromooxindole followed by coupling with arylboronic acids. NMR structural analysis exhibited that two of the suitably substituted oxindole and triazatruxene may have atropisomerism at room temperature. As a representative triazatruxene scaffold, the optoelectronic properties of 9a have also been studied via ultraviolet–visible (UV–vis) absorption spectra and fluorescence spectra of 9a thin films. Also, density functional theory calculation was realized to get knowledge about frontier molecular orbitals. In the light of the information obtained, an organic light-emitting diode (OLED) device utilizing 9a as an emissive layer was applied to obtain white emission. In brief, this study provides the first examples of the synthesis of triazatruxenes bearing aryl substituents at the nonperipheral positions as candidate compounds for organic electronics, optoelectronics, and material chemistry.

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Biography

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