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Indoloindolizines: The Complete Story of a Polycyclic Aromatic Scaffold from Theoretical Design to Organic Field-Effect Transistor Applications

The development of stable and tunable polycyclic aromatic compounds (PACs) is crucial for the advancement of organic optoelectronics. Conventional PACs, such as acenes, often suffer from poor stability due to photooxidation and oligomerization, which are linked to their frontier molecular orbital energy levels. To address these limitations, we designed and synthesized a new class of π-expanded indoloindolizines by merging indole and indolizine moieties into a single polycyclic framework. We developed a scalable synthetic protocol to produce a wide range of π-expanded derivatives. The structural, electronic, and optical properties of these compounds were extensively characterized. We achieved precise modulation of the electronic structure by controlling the aromaticity of specific rings. Benzannulation at targeted positions allowed fine-tuning of the HOMO–LUMO gap, leading to distinct shifts in the optoelectronic properties. Single-crystal X-ray diffraction confirmed their molecular structures, while theoretical calculations provided insights into the observed experimental trends. These indoloindolizines exhibit vivid colors and fluorescence across the visible spectrum and enhanced stability against photooxidation. Reactivity studies demonstrated high regioselectivity in electrophilic substitutions, highlighting the indole-like behavior of these compounds and opening avenues for further functionalization. To showcase the practical utility of our design rules, we fabricated organic field-effect transistors (OFETs) using the newly developed indoloindolizines, which revealed remarkable performance with ambipolar charge transport properties. Overall, our work establishes indoloindolizines as a promising platform for the development of stable, tunable organic materials for optoelectronic applications. Through rational molecular design, we have provided a new pathway for molecular innovation in organic electronics.

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