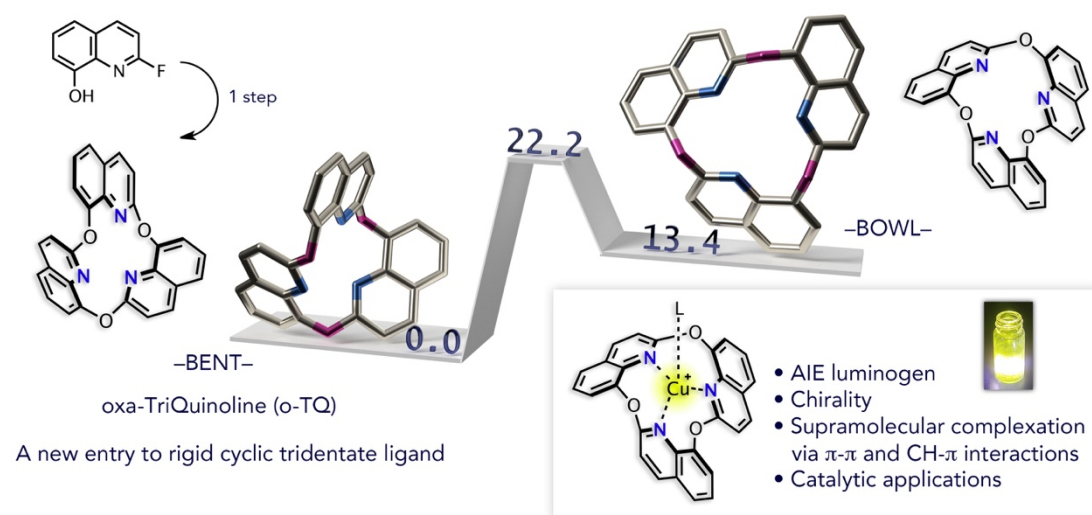


Design and Synthesis of Oxygen-Embedded TriQuinoline and its Strategic Applications

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Recently, a head-to-tail type quinoline trimer featuring an atomic size void space, TriQuinoline (TQ), was uncovered as a pseudo-planar material exhibiting unusual physicochemical properties.¹ We designed a new non-flat quinoline trimer oxa-TriQuinoline (o-TQ) comprising of three quinoline units concatenated at 2,8-positions with three oxygen atoms. o-TQ was synthesized from a known compound, 2-fluoroquinolin-8-ol, by conventional S_NAr reaction in a single step. While X-ray crystallography and DFT calculation revealed that o-TQ preferred a bended structure, complexation with Cu(I) cation in a tridentate fashion furnished a conformationally fixed bowl-shape o-TQ/Cu(I) complex. This complex exhibited aggregation-induced emission (AIE) properties and strongly emissive ($\lambda_{\text{max}} = 592 \text{ nm}$, $\Phi = 0.21$) in the solid state. Conformational restriction endowed the complex with chirality and the thus obtained π -bowl displayed supramolecular complexation with non-flat aromatics of specific curvature *via* both π - π and CH- π interactions. ¹H/¹³C NMR and CSI-MS provided experimental evidence for the complexation of o-TQ/Cu(I) with corannulene, sumanene, a fullerene derivative as well as [12]CPP, which were also supported by DFT calculations.



1) S. Adachi, M. Shibasaki, N. Kumagai, *Nat. Commun.* **2019**; *10*, 3820.