Buchwald-Hartwig Reaction to Synthesize Luminescent Liquid Crystals

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Exciton migration and processability are important concepts in the emerging technologies of molecular electronics and optoelectronic devices, including photovoltaic cells and organic light-emitting diodes (OLEDs)1. The first one is important to optimizing the energies of excited states and energy transfer processes, the second one is important to evaluate how this materials will be applied in the devices. Bipolar molecules, which can accept and transport both holes and electrons, are attractive candidates for optoelectronic studies because the same molecule has both parts of P-N junction; and liquid crystals are widely used because of their physical properties as self-assembling and fluidity.

Heteroaromatic rings play an important role in the field of OEM awarding interesting electronic behaviour and polarity to the molecules, in former works2 were found that isoxazoles can induce mesogenic behaviour and can behave like a \( \pi \)-acceptor, and triarylamines are a widely known \( \pi \)-donator group used in OEMs. In this work were synthesized a group of isoxazoles/arylamines using the Buchwald–Hartwig (B-H) reaction in order to obtain bipolar molecules with liquid crystalline properties (figure below).

\\[ \text{Buchwald-Hartwig reaction between 3,5-isoxazoles and dissubstituted amines.} \]

The B-H reaction between previously synthesized isoxazoles and secondary amines showed medium to good yields; the compounds 6a-6d didn’t show mesomorphic behaviour neither fluorescence, compounds 6e-6h showed liquid crystalline behaviour and fluorescence, whereas branched alkyl chain in compounds 6i-6k prevent the liquid crystalline behaviour, but improve solubility of materials.

Absorption and emission spectra of compound 6k.

A complete photophysical analysis of all compounds is in progress. As a representative example 6k shows Strokes shift of 228 nm, equivalent to HOMO-LUMO gap of 2.98 eV, the quantum yield is 1.76 % (C_{18}H_{8} was used as standard). Despite of low quantum yield of 6k to be used as OLEDs it can be act as molecular filter in photovoltaic device.

References:

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