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Synthesis and characterization of new helically chiral heptacyclic systems

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Abstract- New helically chiral heptacyclic systems with cyano groups at selected positions have been synthesized in good yields, *via* a four-step sequence, from readily available materials. The optical properties of the target helicenes were investigated by UV-visible absorption and photoluminescence spectroscopy and an emission in the visible region was observed. The energy levels of these organic materials were determined by cyclic voltammetry and showed a relatively high electronic affinity, indicating that they may be good candidates for electron-injection holeblocking layer in organic light-emitting diodes.

Keywords: Helicenes, Heck coupling, Photocyclization, Optical properties, Visible emission.

Carbohelicenes, represent an intriguing class of polycyclic aromatic hydrocarbons (PAHs) and are composed of *ortho*-fused aromatic rings with a fully conjugated system and a non-planar topology.¹ They have attracted great interest owing to their unique structural features and widespread potential applications as chiral luminescent materials,^{2,3} or as building blocks for helical conjugated polymers.⁴ They are also considered useful for wave guides,⁵ non-linear optics,⁶ biomolecular recognition⁷ and asymmetric synthesis.⁸ Helicenes were shown to be effective in the development of materials with chiroptical properties which are useful for molecular-based electronic applications.⁹

For instance, heptahelicene is a particularly interesting [*n*]helicene containing one complete turn of the helix and high optical stability (racemization barrier 40.5 kcal mol⁻¹).¹⁰ Such heptacyclic structures have seen interest for their silver-binding interactions *via* the central cavity.¹¹ In addition, theoretical studies for alkali metal cations and transition metals have been established¹² and their deposition onto metal surfaces have also been investigated.¹³

Since Newman and Lednicer reported the first helicene in 1956,¹⁴ various methods for the synthesis of helicenes including successive silylenol ether coupling with benzoquinone,¹⁵

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