Title: Synthesis and study of stable radical derivates from the carbazole

heterocycle

Student: Daniel Valero Moreno

Date: June 2017

Supervisor/s: Dra. Dolors Velasco Castrillo

Departament de Química Inorgànica I Orgànica (secció Q. Orgànica)

Organic materials in molecular electronics present many advantages over inorganic semiconductors, such as the possibility of manufacturing light, flexible and large-surface devices with a low associated production cost. This project has focused on a specific group of radical derivatives from the carbazole heterocycle. These derivatives have a great interest due their optical and redox properties. They show relatively intense luminescence and reversible oxidation processes to stable radical cations, making them good hole carriers. Thus, they are suitable as photoconductors and charge transporting materials. Therefore, in the present work we have taken advantage from the properties afforded from the combination of the carbazole unit and the tris(2,4,6-trichlorophenyl)methyl radical (TTM radical). The resulting system shows great stability, reversible reduction and oxidation processes, and paramagnetic behaviour.

On the basis of these considerations, the main aim of the present work has been the production and further characterization of the radical derivatives from the carbazole-TTM adduct, which incorporate different halogen atoms on the carbazole core. These compounds have been synthesized through the direct coupling between the corresponding carbazole derivative and the TTM radical followed by an oxidation to obtain the radical desired. All compounds prepared have been characterized by ¹H NMR, ¹³C NMR and infrared (IR) spectroscopies, and mass spectrometry.

The radical character of the different carbazole-TTM radical derivatives have been studied by means of magnetic susceptibility measurements and electron paramagnetic resonance (EPR) spectroscopy.

Finally, their optical and electrochemical properties were also analysed by means of UV-visible and fluorescence spectroscopies, and cyclic voltammetry, respectively.

Keywords: Carbazole heterocycle, TTM radical, photoconductors, charge transport, organic materials, organic synthesis.