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Title of the Thesis: Functionalization and π-Extension of the Planar Blatter Radical
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Abstract

Stable organic radicals have attracted tremendous attention as structural elements for the development of modern functional materials due to their outstanding performance in a variety of fields. Particularly attractive in this context are π-delocalized radicals based on the benzo[*e*][1,2,4]triazin-4-yl known as the Blatter radicals, which stand out for their exceptional stability, spin delocalization, low excitation energies, and interesting electrochemical and photophysical properties. Planar Blatter radicals can be obtained through planarization of the N(1) aryl substituent, which offers greater spin delocalization, change in packing of the solid state, and a new platform for the design of functional materials. The methods for increasing the stability of radicals and preparation of Blatter radicals and planar Blatter radicals and synthesis of their extended and substituted derivatives in previous works are described in the Introduction. The main goal of this Doctoral Thesis, is to conduct research on synthetic methods that will allow for the systematic and detailed characterization of a new type of paramagnetic nanographenes which is docked to the [1,2,4]triazinyl fragment for fundamental studies in the context of electronic and magnetic applications.

In the first part of the Thesis, synthesis of derivatives of π-expanded planar Blatter radicals as a new class of paramagnetic nanographenes, through two different methodologies and understand their structure-property relationships are presented. To assess the effect of π expansion on the electronic properties, the radicals were characterized using spectroscopic (UV−vis and electron paramagnetic resonance (EPR)) and electrochemical methods, and the results are described.

In the second part of this Thesis, preparative routes to five new functionalized derivatives of S-*peri*-annulated benzo[*e*][1,2,4]triazinyl, containing CO_2Me, CN, CF_3 and NO_2 groups at the C(10) or C(9) positions through TMS_3SiH-assisted cyclization of aryl iodides are discussed. The goal of this effort was to gain a better knowledge of the parameters that govern the crystal packing of benzo[*e*][1,2,4]triazinyl derivatives and their impact on magnetic interactions. Spectroscopic, structural, electrochemical, chemical properties and the investigation of the impact of chemical structure and morphology on these properties, are provided.