Abstract

Heterocyclic molecular systems play a key role in developing advanced materials for today's technologies. Such systems, characterised by cyclic structures, containing at least one heteroatom, express unique electronic and optical properties. This dissertation explores the synthesis, spectroscopic analysis, and potential applications of two classes of nitrogen-containing heterocyclic aromatic compounds with different electronic states of the nitrogen heteroatom: N^+ – electron-deficient cationic acridinium salts – and N^0 – electron-releasing carbazole derivatives. Both groups of compounds were studied in this work to gain a comprehensive understanding of luminescence phenomena, including photochemical and photophysical processes responsible for light emission, which may have practical applications in modern luminescence analytics and optoelectronics.

This work aimed to investigate the mechanisms of light emission in such selected molecular systems with potential applications in modern technologies, such as chemiluminescence-based analysis and organic light-emitting diodes (OLEDs). Specifically, the study focused on the photophysical and photochemical behaviour of organic molecules in their excited states. From a photochemical perspective, the emphasis was placed on enhancing the rate and efficiency of oxidation reactions that serve as sources of chemiluminescence. From the standpoint of photophysics, the research explored the mechanism of thermally activated delayed fluorescence (TADF), rates of radiative deactivation and spin-forbidden transitions, along with the influence of various parameters on such processes.

The **first part** of this work is dedicated to the study of acridine-based molecular systems. In this thesis, acridinum salts are employed as chemiluminescent indicators; a detailed background is provided in Thematic Area I, while this section focuses on the specific assays and validation results.

Part Ia focuses on developing a new luminometric method for quantifying biological sulphur nucleophiles. The study utilises 9-cyano-10-methylacridinium salts as a core component in this method. Biological sulphur nucleophiles, including N-acetyl-L-cysteine (NAC), glutathione (GSH), D-penicillamine (DPA), and acetylthiocholine chloride (ATC), play vital roles in various biochemical processes, including detoxification, cellular signalling, and enzymatic reactions. Accurate quantification of these nucleophiles is critical for understanding their biological functions and potential therapeutic roles. This subpart details the synthesis of the acridinium salts, the development of luminometric assays with their participation, and the analytical validation of the method, offering an original approach to detect and quantify these essential molecules.

Part Ib investigates the role of aromatic acridinium thioesters as chemiluminescent indicators for biological antioxidants. Antioxidants such as dithiothreitol (DTT), glutathione (GT), quercetin (QR), cysteine (CYS), and methionine (MET) play critical roles in protecting cells from oxidative damage by neutralising free radicals and reactive oxygen species. These compounds play a crucial role in maintaining cellular homeostasis and

preventing diseases associated with oxidative stress, including cancer, neurodegenerative disorders, and cardiovascular diseases. Accurate and sensitive detection of these antioxidants is vital for research and clinical diagnostics. A complete description can be found in the research, and the results are presented in publication **P2**.

The **second part** of the dissertation focuses on mechanistic studies of heterocyclic compounds exhibiting TADF, a phenomenon that enhances the efficiency of OLEDs by utilising the total energy of electrical excitation. OLED technology represents a significant advancement in display and lighting technologies, offering high efficiency, flexibility, and superior colour quality. This thesis describes the spectroscopic studies and theoretical calculations of the developed initially TMCz-BO TADF compound. This compound was reported as a promising deep blue emitter, a colour that is particularly challenging to achieve high efficiency in OLED technology. The deep blue emission is crucial for high displays and energy-efficient lighting. This study characterises the photophysical properties of this molecular system and proposes a mechanism for the TADF process, mentioned above, which can be helpful in designing future TADF materials. The paper **P3** provides an in-depth account of the study and presents its results in detail.