

## ABSTRACT

The thesis entitled “*Synthesis and Optoelectronic Properties of 5,6-Fused Conjugated Carbocycles*” is divided into four chapters.

**Chapter 1** provides a concise overview of the 5,6-fused carbocycles and their applications in pharmaceutical and material sciences. The chapter delves into the investigation of indenones, benzofulvenes, and pentalenes, demonstrating their synthesis via various routes and exploring the optoelectronic properties of these molecules. The following chapters address the research gap regarding their synthetic versatility and photophysical and electrochemical properties.

[*Eur. J. Org. Chem*, **2024**, Submitted].

**Chapter 2** of the thesis focuses on the synthesis of indenones via an *in situ* triflation/tandem cross-coupling of indan-1,3-dione. The methodology was extended further to synthesize an array of benzofulvenes from unconjugated indenones. A total synthesis of a neolignan natural product and a formal synthesis of Indatraline were demonstrated using this methodology. Here, indan-1,3-dione with alternating electrophilic and nucleophilic sites has been introduced as a common synthon to achieve indenones and benzofulvenes. UV-Vis spectroscopy and DFT studies were performed to investigate the photophysical characteristics and the FMO energy gaps. [*Adv. Synth. Catal.*, **2024**, 10.1002/adsc.202400529].

**Chapter 3** is divided into two parts:

**Chapter 3A** focuses on the Heck/Sonogashira coupling cascade of *gem*-dibromo olefins. However, various attempts to achieve the cascade coupling proved inefficient due to the inert nature of the Heck intermediate (2-bromobenzofulvene) to further undergo Sonagashira coupling. The unsuccessful attempt to coupling bromobenzofulvene has been taken as a challenge and addressed in the next part of the chapter.

**Chapter 3B** is dedicated to the studies on the synthesis and optoelectronic properties of *bis*-benzofulvenes from bromobenzofulvenes via a Ni-mediated pathway. The optoelectronic properties were investigated using UV-Vis spectroscopy and cyclic voltammetry. The experimental values correlated well with the results from the DFT studies.

[*Org. Lett.*, **2023**, 3941–3945 ]

**Chapter 4** is devoted to the synthesis of unsymmetrical dibenzopentalenes via a Suzuki coupling/carbopalladation cascade involving *gem*-dibromo olefins and 1,2-diboronic esters. The methodology was extended to synthesize monoarenopentalenes. Photophysical, CV, and DFT studies were used to study their optoelectronic properties.

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Overall, the thesis addresses the long-standing challenges in the synthesis and provides valuable insights into the optoelectronic properties of 5,6-fused conjugated carbocycles.

**Keywords:** *Indenones, Benzofulvenes, Pentalenes, Cascade coupling reactions, Optoelectronic properties*