Journal of Molecular Structure 1157 (2018) 119–126

Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: http://www.elsevier.com/locate/molstruc

One pot synthesis, X-ray crystal structure of 2-(2′-hydroxyphenyl) oxazolo[4,5-b]pyridine derivatives and studies of their optical properties

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ARTICLE INFO

Article history:
Received 31 August 2017
Accepted 16 December 2017
Available online 18 December 2017

Keywords:
Oxazolopyridines
Photophysical properties
Organic semiconductors
Phenylboronic acid
Fluorescence quantum yield
TDDFT

ABSTRACT

A series of five 2-(2-hydroxyphenyl)oxazolo [4,5-b]pyridines (HPOP) (**3a-e**), where four are novel, were synthesized by a mild, one pot, phenylboronic acid-NaCN catalyzed reaction. Spectroscopic characterization and photophysical properties of these compounds are reported. Absorption and excitation spectra of the compounds were dependent on the substituents in the phenyl ring. Fluorescence quantum yields (0.009–0.538) were associated with the donor strength and the position of the substituents. Also, DFT analysis allowed us to determine the contribution of diethylamino and methoxy moieties to the π-system, which is in agreement with the experimental data analyzed in solution and by cyclic voltammetry. The results obtained in the solid state by single-crystal X-ray diffraction experiments indicate that, the quasi-planarity envisioned for the explored compounds is present, supporting the hypothesis that both the H-bonding of a hydroxyl group to the C=N moiety and a donor groups such as diethylamino and methoxy **moieties** favor an electronic communication. Due to the facile synthesis and their photophysical properties, the novel HPOP **3a-e** have potential application as organic semiconductors.
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1. Introduction

Oxazolo compounds containing different substituents, such as oxazolo [4,5-b]pyridine and benzoxazole derivatives, have received considerable attention because of their biological activities [1], such as anticancer [2], and Alzheimer's disease [3]. Additionally, their remarkable optical properties [4] have made them useful as laser dyes [5] and fluorescent molecular tags [6]. Recently, we reported an exceptionally mild, one pot, phenylboronic acid catalyzed synthesis of 2-arylbenzoxazoles from salicylaldehydes and 2-aminophenol in the presence of potassium cyanide [7].

Oxazolopyridines exhibit excited-state intramolecular proton transfer (ESIPT) which has been extensively studied theoretically and experimentally because of their intrinsic four energy level photocycle process [8]. Some of these compounds have wide application as lasers, probes, sensor and molecular devices [9].

Hence, an efficient and rapid preparation of novel functional organic molecules with specific photophysical and electrochemical properties remains an important goal and challenge for researchers both in organic chemistry and materials science. In this work we describe a mild, *one pot*, phenylboronic acid catalyzed synthesis of such 2-(2-hydroxyphenyl)oxazolo [4,5-b]pyridines (HPOP) directly from salicylaldehydes and 2-amino-3-hydroxypyridine in the presence of sodium cyanide.

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https://doi.org/10.1016/j.molstruc.2017.12.059
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