

Photoelectron spectroscopy investigations of pyrrolo[1,2-*a*][1,10]phenanthroline derivatives

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Abstract

Thin films of new pyrrolo[1,2-*a*][1,10]phenanthroline derivatives have been investigated by ultraviolet photoelectron spectroscopy, with a view of future applications in optoelectronic devices. The electronic band structure of investigated compounds (for electron energies ≤ 25 eV) is to a great extent determined by substituent (R = NO₂, Cl) induced transformations of molecular orbitals.

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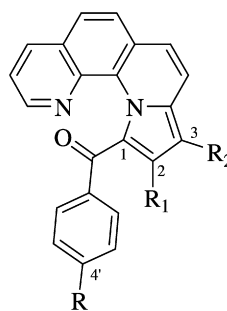
1. Introduction

Pyrrolo[1,2-*a*][1,10]phenanthroline derivatives are promising candidates for the technology of solid-state devices [1], in particular of organic light emitting diodes (OLEDs) [2]. These materials are very attractive for optoelectronic devices owing to their suitable ionization potential and electron affinity, favoring electron injection at the cathode [2,3]. Also, due to their specific chemical structures, there is ample opportunity to tune molecular orbitals by introducing donor or acceptor groups, getting emissive or electron transporting/hole blocking materials [4,5]. In order to improve the quality of such devices, great attention has to be paid not only to materials synthesis, but also to the study of their electronic structures, which is able to give a deep insight to understanding their behavior in organic electronic devices. In this study we investigate the valence electronic structure of two pyrrolo[1,2-*a*][1,10]phenanthroline derivatives, using the ultraviolet photoelectron spectroscopy (UPS).

2. Experimental

In Fig. 1 the chemical structure of pyrrolo[1,2-*a*][1,10]phenanthroline derivatives is illustrated. Their synthesis is described further.

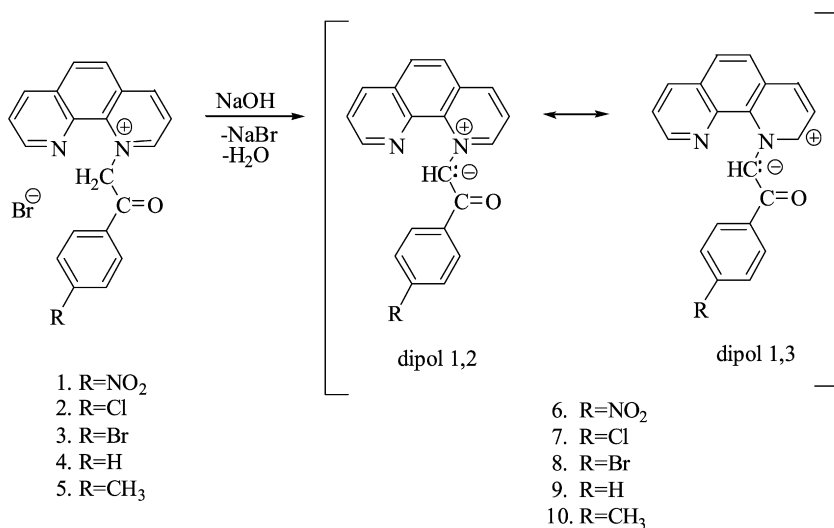
The non-stable monosubstituted heteroaromatic *N*-ylides obtained in situ by deprotonation of the corresponding cycloimmonium salts in the presence of base, are 1,3-dipoles which undergo cycloaddition with activated symmetrical or nonsym-



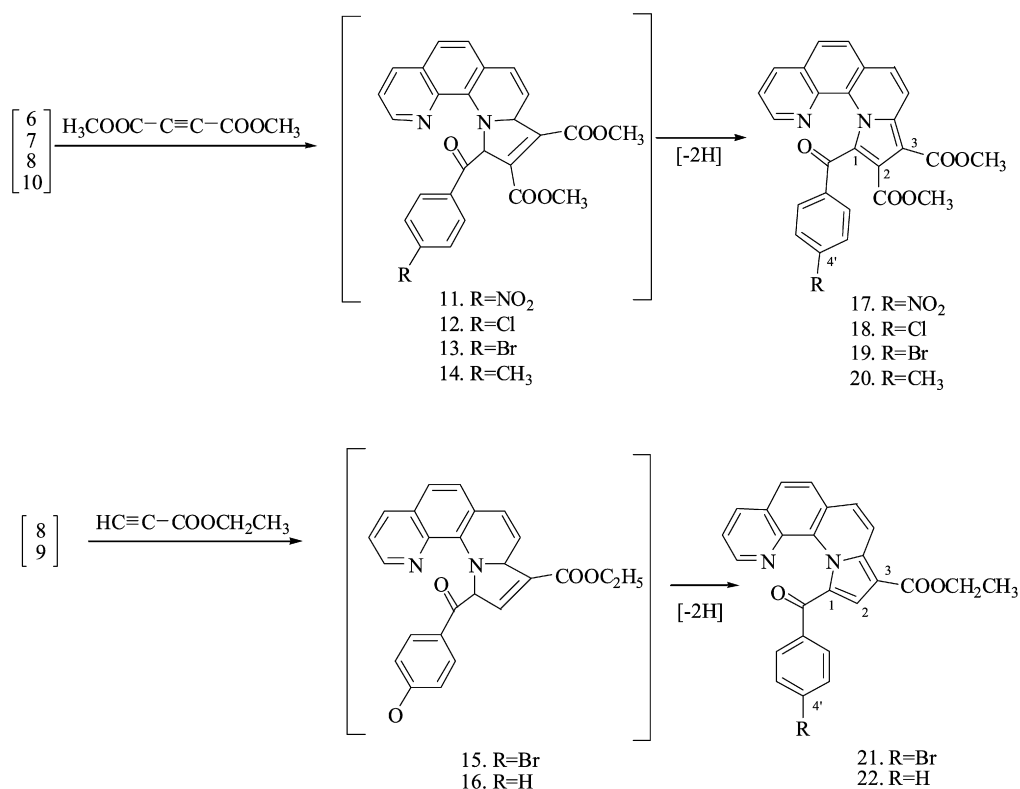
- RA1: R= NO₂, R₁=R₂= COOCH₃
- RA2: R= Cl, R₁=R₂= COOCH₃
- RA3: R= Br, R₁=R₂= COOCH₃
- RA4: R= CH₃, R₁=R₂= COOCH₃
- RA5: R=Br, R₁= H, R₂= COOC₂H₅
- RA6: R=R₁= H, R₂= COOC₂H₅

Fig. 1. Chemical structures of investigated compounds.

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Scheme 1.



Scheme 2.

metrical olefins and alkynes resulting in the formation of a fused five-member nitrogen heterocycle [6–9]. We performed some reactions of 1,10-phenanthroline-ylides with dimethyl acetylenedicarboxylate (DMAD) and ethyl propiolate to yield novel pyrrolo[1,2-*a*][1,10]phenanthroline derivatives [10].

Initially, for obtaining 1,10-phenanthroline salts 1–5, reaction of 1,10-phenanthroline with reactive halide derivatives was considered [11]. Reaction between the salts 1–6 suspended in different mixtures of organic solvents and an aqueous solution of 0.2 N of sodium hydroxide (NaOH) gave in situ 1,10-phenanthroline-ylides 6–10 (Scheme 1), which

on stereoselective 3 + 2 dipolar cycloaddition with dimethyl acetylenedicarboxylate or ethyl propiolate furnished the following compounds: (1-(4'-R-benzoyl)-2,3-dimethoxycarbonyl-pyrrolo[1,2-*a*][1,10]phenanthroline) 17–20 and (1-(4'-R-benzoyl)-3-ethoxycarbonyl-pyrrolo[1,2-*a*][1,10]phenanthroline) 21 and 22, respectively (Scheme 2).

As it is shown in Scheme 2, the cycloaddition reaction firstly generated non-isolating intermediate cycloadducts of types 11–16, which due to the tendency of stabilization suffered an oxidative dehydrogenation process, because the reactions were carried out in ambient conditions.

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