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Short Note

8-[2-(1*H*-indol-3-yl)vinyl]-10,10-dimethyl-10*H*-pyrido[1,2-*a*] indolium Perchlorate

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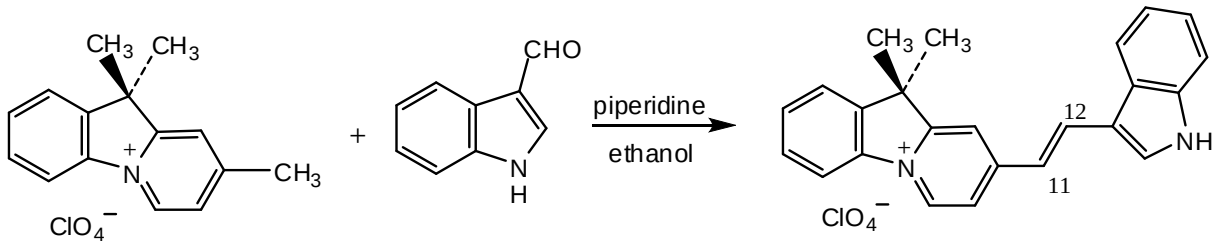
Abstract: A novel compound, 8-[2-(1*H*-indol-3-yl)vinyl)]-10,10-dimethyl-10*H*-pyrido[1,2-*a*]indolium perchlorate, was synthesized by the condensation of 8,10,10-trimethyl-10*H*- pyrido[1,2-*a*]indolium perchlorate and indole-3-carbaldehyde in the presence of piperidine. The structure of the target compound was characterized by IR, ^{1}H NMR and elemental analysis, and its UV-visible absorption and emission spectra were also determined.

Keywords: 10*H*-pyrido[1,2-*a*]indolium perchlorate; indole-3-carbaldehyde; condensation

The substituted 10*H*-pyrido[1,2-*a*]indolium perchlorates can be used as photosensitive dyes, fluorescent whiteners and organic light-guide sensitizers [1,2]. Many of this kind of compounds have been synthesized, such as methyl, phenyl, styryl or furyl-substituted 10*H*-pyrido[1,2-*a*]indolium perchlorates [3-6]. In order to study the relationship between the structure and absorption maximum (λ_{max}), the crystal structures of some compounds in this series were determined [7,8], and found that the introduction of a conjugation group in the 8-position significantly increases the λ_{max}. To obtain a compound with a larger λ_{max}, herein, we introduced 2-(1*H*-indol-3-ly)vinyl (a group making up a conjugated system with the 10*H*-pyrido[1,2-*a*]indole moiety) onto 8-position and synthesized the target compound.



Experimental

A mixture of 8,10,10-trimethyl-10*H*-pyrido[1,2-*a*]indolium perchlorate (0.62 g, 0.002 mol), indole-3-carbaldehyde (0.29 g, 0.002 mol) and piperidine (6 drops) in ethanol (15 mL) was refluxed for 3 h with stirring to give a brown precipitate. The solid was filtered off and recrystallized from methanol/ acetonitrile to yield the target compound as orange crystals.

Yield: 70%; Melting point: 271–273 ℃.

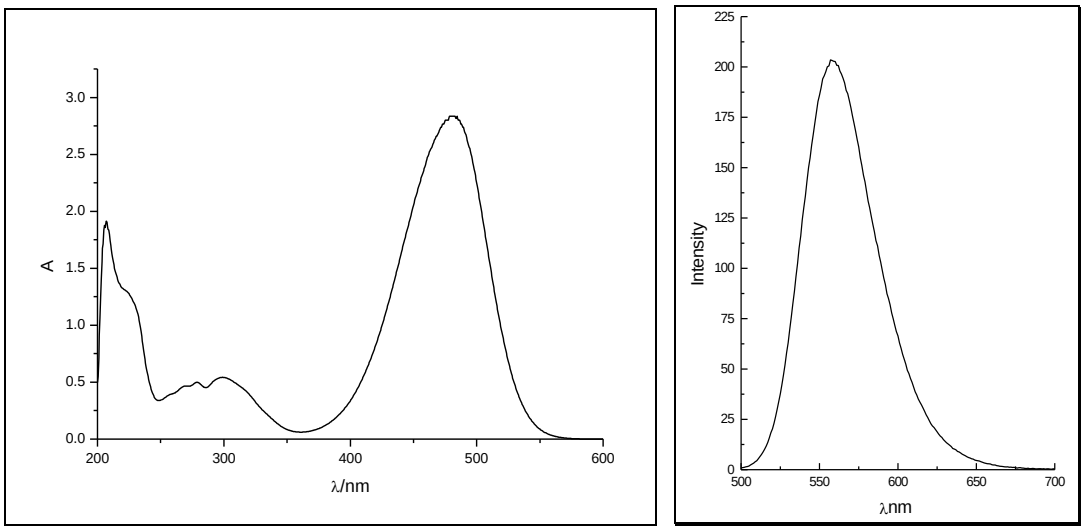
IR (KBr) ν cm^{-1}: 3310 (N-H), 1600 (C=N^{+}), 1365{C(CH$_3$)$_2$}, (1090, 623 (ClO$_4^-$), 965 {H-C=C-H (*E*)}.

UV-Vis (EtOH): λ_{max} = 480.5 nm; ε = 4.68 ×10^4 cm^2•mol $^{-1}$.

^{1}H NMR (400 MHz, DMSO-d_6) δ ppm: 11.99 (s, 1H, N-H), 9.52 (d, 1H, J = 6.8 Hz, 6-H), 8.59 (s, 1H, 9-H), 8.39 (d, 1H, J = 16.1 Hz, 12-H), 8.29 (d, 1H, J = 7.4 Hz, 7-H), 8.00 (s, 1H, pyrrole-C-H), 7.42 (d, 1H, J = 16.1 Hz, 11-H), 7.27-8.22 (m, 8H, Ph-H), 1.72 (s, 6H, 2×CH$_3$).

Elemental analysis: Calcd for $C_{24}H_{21}ClN_2O_4$ C, 65.98%, H, 4.84%, N, 6.41%. Found: C, 65.75%, H, 4.93%, N, 6.75%.

Figure 1. UV-Visible absorption (left) and emission spectrum (right) of the target compound.



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