1,2,3-TRIETHOXYCARBONYL-4H-CYCLOPENTA[b]-QUINOXALINE

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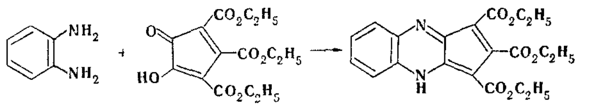
We have found that the condensation of 3,4,5-triethoxycarbonyl-2-hydroxycyclopentadienone [1] with o-phenylenediamine in methanol at 60°C leads to the formation of 1,2,3-triethoxycarbonyl-4H-cyclopenta[b]quinoxaline (I), a new π-electronic analog of azulene. Yield 80%. Red crystalline substance sparingly soluble in organic solvents, mp 217°C (decomp.). Found, %: C 62.5; H 5.2; N 7.2. $C_{20}H_{20}N_2O_6$. Calculated, %: C 62.5; H 5.2; N 7.3. Like the 4H-cyclopentaquinolines [2], compound (I) is characterized by a broad absorption band of low intensity in the visible region (λ_{max} 500 nm, log ε 3.4) and intense absorption in the UV region (λ_{max} 370, 280 nm; log ε 4.3, 5.0).



I

Unlike pyridines [3] and cyclopentaquinolines unsubstituted on the nitrogen atom [4], substance (I) exists predominantly in the form of the 4H, and not the 1H, tautomer (absorption band at 3270 cm^{-1} characteristic for an intramolecular NH hydrogen bond). In the PMR spectrum (in pyridine) the signals of the protons of the ethoxycarbonyl groups in positions 1 and 3 are equivalent, which apparently shows a rapid exchange of protons between the nitrogen atoms. Compound (I) forms a stable yellow sodium salt, and a strongly acid solution which has a blue color (protonation at N_9).

LITERATURE CITED

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