Intramolecular excited state proton transfer in Mannich base - 3,5,6-trimethyl-2(*N,N'*-diethylaminomethyl) phenol.

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Rok wydania

1993

Czasopismo

Journal of Photochemistry and Photobiology A-Chemistry

Numer woluminu

72

Strony

123-132

DOI

10.1016/1010-6030(93)85019-5

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Steady state fluorescence spectra of 3,5,6-trimethyl-2(*N,N'*-diethylaminomethyl) phenol (**I**) in various solvents at room temperature and in *n*-propanol solution at low temperature were investigated. Dual fluorescence was only observed in polar solvents. It was attributed to the existence of two tautomeric forms in the excited state: the molecular and ionic forms of the intramolecular hydrogen bond of **I**. Ground state semiempirical structure optimization was performed within the GRINDOL, MNDO, MINDO/3, AM1 and PM3 techniques. Only AM1 and PM3 gave a reasonable geometry of the hydrogen-bonded chelate ring. For these geometries calculation of the electronic excited states by the GRINDOL-CI method confirmed the ^1L_b, state as the lowest emitting state in the hydrogen-bonded form of **I**. The existence of single and double fluorescence in non-polar and polar solvents respectively was correctly reproduced by the GRINDOL-CI procedure.

Adres publiczny

https://doi.org/10.1016/1010-6030(93)85019-5

Strona internetowa wydawcy

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