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Novel Amidine Derivatives of Benzanthrone: Effect of Bromine Atom on the Spectral Parameters

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Abstract

Several new substituted amidine derivatives of benzanthrone were synthesized by condensation reaction from 2-bromo-3-aminobenzo[de]anthracen-7-one and appropriate aromatic or aliphatic amides. The novel benzanthrone derivatives were characterized by TLC analysis, NMR, IR, MS, UV/Vis, and fluorescence spectroscopy. The obtained derivatives have yellow or orange fluorescence in organic solvents. The solvent effect on photophysical behaviors of these dyes was investigated, and the results showed that the introduction of a bromine atom causes a blue-shift of the absorption and emission bands and decrease in the fluorescent quantum yield in comparison with unbromated analogues. The difference in the excited state and the ground state dipole moments was estimated by using the variation of Stokes shift and by semiempirical molecular calculations. The crystal structure and packing of four novel dyes has been revealed by the X-ray single crystal structure analysis.

Keywords: benzanthrone dyes; fluorescence; solvatofluochromism; dipole moment; crystal structure

1. Introduction

Aromatic systems with strong electron-donor and acceptor substituent groups often exhibit environmentally sensitive luminescence properties due to internal charge-transfer processes in the excited state. Luminophores with such a D-A structure attract great scientific and practical interest because they can serve as photoactive materials in molecular electronics [1].

Benzo[a]anthracene-7-one derivatives are polyaromatic hydrophobic substances with useful photophysical properties. These compounds have been intensively studied because of the possibility of a wide variety of applications involving colouration of polymeric materials [2,3], as laser active media [4,5], host emitters in organic light-emitting devices [6], fluorescent probes in biology [7,8], liquid crystal displays [9,10] and ion probes [11].

Recently, we have published the design, synthesis, characterization and properties of new benzanthrone dyes, which appeared to be particularly interesting because they lead to perspective luminescent materials. In previous works, a series of benzanthrone amines and amidines were prepared [12-14]. These solvatofluochromic substances have a large extinction coefficient and a significant Stokes shift.

In recent years, phosphorescent organic substances (with a lifetime of excited state 0.1-10 ms) with a perspective for producing highly effective emitting materials [15,16] have attracted researchers. It is known that phosphorescence is observed for organic compounds containing sufficiently heavy elements, metal complexes or bromine/iodine atoms [17]. The high luminescence intensity of such materials appears due to the total emission from singlet and triplet levels.

In connection with these knowledges and in continuation of our interest toward the synthesis of new emissive nitrogen-containing benzanthrone derivatives, a series of novel benzanthrone dyes which contain bromine atom at 2-position and substituted amidino group at 3-position of benzanthrone core scaffold were synthesized and investigated. The thermal and spectral properties, fluorescent

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