

Cryogenic fluorescence and absorption spectroscopy studies on monomeric and dimeric species of 2-butylamino-6-methyl-4-nitropyridine *N*-oxide.

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Streszczenie

2-Butylamino-6-methyl-4-nitropyridine-*N*-oxide (2B6M) belongs to a group of compounds that can undergo not only excited-state intra-, but also intermolecular proton transfer. The latter of course requires the presence of dimeric species. Previously, we have shown that for 2B6M in aprotic non-polar solvents in the liquid state such dimers play no role. Under these conditions, only one single monomeric species exists, exhibiting anomalous fluorescence behavior, i.e. proton transfer not only starting from the lowest excited electronic singlet state, but also from higher excited states. However, we also noted that under frozen, crystalline matrix conditions more species show up in the spectra.

In order to study this multi-species system in more detail, we present absorption and fluorescence experiments on 2B6M, recorded in *n*-octane at various temperatures between 293 and 5 K. High-resolution spectra are included, not only in fluorescence but also in absorption. We demonstrate that under cryogenic conditions three species can be discerned, two of these providing high-resolution spectra with their main 0–0 lines around 452 and 465 nm, respectively. A detailed vibrational analysis of their emission spectra is included. The third species gives broad-banded spectra, in absorption extending to about 520 nm with its long-wavelength maximum around 460 nm, in emission with a maximum around 535 nm. We tentatively assign the three species to a monomer, a H-bonded dimer and a strongly interacting (π – π -stacked) dimer, respectively. We conclude from the excitation spectra that (anomalous) intramolecular proton transfer at higher excited states is still operative under cryogenic conditions. Indications for excited-state intermolecular proton transfer in the stacked dimeric species were not found.

Słowa kluczowe

Excited-state proton transfer, Shpol'skii spectroscopy,
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