New photophysical properties of nitropyridine N-oxide derivative revealed by theoretical calculations, crystal structure and time-resolved spectroscopy

Autorzy

Anna Szemik-Hojniak

Irena Deperasińska

Katarzyna Ślepokura

Monika Gawłowska

Yuval Erez

Rok wydania

2026

Czasopismo

Journal of Molecular Structure

Numer woluminu

1367

Strony

146120/1-146120/17

DOI

10.1016/j.molstruc.2026.146120

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

In this paper, we present molecular dynamics results of 3-methylamino-4-nitropyridine N-oxide (3M4N) in n-propanol obtained using femtosecond fluorescence conversion and time-correlated single photon counting (TCSPC) techniques. Our main goal was to identify the photoinduced pathways of 3M4N caused by the ortho-substitution of its alkylamino group (-NHCH3) with respect to the nitro group as electron acceptor. Fluorescence up-conversion signals in n-propanol allowed the determination of an ultrafast (200 ∼ 300 fs) intersystem crossing (ISC) between the S_1^{FC} (ππ*) state and the upper (nπ*) triplet state (T_3).We believe that an efficient ultrafast ISC is strongly influenced by the torsion of the nitro group, isoenergetics of the S_1 state with the triplet (T_3), spin change that takes place simultaneously with the change of electronic configurations [S_1 (π - π*) → T_3 (n - π*)] and significant spin-orbit coupling of T_3 with the S_1 state [the value of Hso (S_1,T_3) is 6.94 cm^{-1}]. The time constants of the three minima found by TD DFT calculations on the potential energy surface are for the n-π* type S_1(NP) → S_0 transition (0.6 ps), the planar bright structure of the locally excited state S_1 (LE) (3.2 ps) of π -π* character, and the final dark form TICT (8.0 ps), formed from the S_1(LE) state.

Słowa kluczowe

Crystal structure, 4-nitropyridine N-Oxide derivatives, Fluorescence up-conversion dynamics, TD-DFT calculations, Ultrafast instersystem crossing

Adres publiczny

http://dx.doi.org/10.1016/j.molstruc.2026.146120

Strona internetowa wydawcy

http://www.elsevier.com