

Crystal structure, spectroscopic, and theoretical studies of 2-methylamino-6-methyl-4-nitropyridine N-oxide.

Autorzy

Łukasz Wiśniewski
Agnieszka Urbanowicz
Lucjan Jerzykiewicz
A. Makarewicz
Irena Deperasińska
G. Van der Zwan
N. Haraszkiewicz
Aniela Puszek
Anna Szemik-Hojniak

Rok wydania

2009

Czasopismo

Journal of Molecular
Structure

Numer woluminu

920

Strony

45-51

DOI

10.1016/j.molstruc.2008.10.029

Kolekcja

Naukowa

Język

Angielski

Streszczenie

The structure and electronic spectra of 2-methylamino-6-methyl-4-nitropyridine N-oxide (2M6M) were investigated. The X-ray structure of 2M6M molecule shows that it crystallizes in the monoclinic system of the $P2_1/n$ space group and forms internally hydrogen-bonded $[\text{NH}\cdots\text{O} = 2.563(3) \text{ \AA}]$ monomers linked by the same type of intermolecular $[2.799(3) \text{ \AA}]$ hydrogen bonds in linear oligomers. Due to weak intermolecular $\text{CH}\cdots\text{O}$ interactions such oligomers are arranged along the z-axis into a helical-shaped zigzag. The results of quantum chemical DFT/B3LYP/6-31G(d, p) calculations reproduce the absorption spectrum of 2M6M well. The 2M6M molecule shows complex photophysical and photochemical behavior. It exhibits dual fluorescence (with emission maxima at 476 and 536 nm) and decays bi-exponentially (with lifetimes of 2.13 and 0.1 ns). The temperature dependence of the fluorescence intensity in the two bands has a slope of 1450 cm^{-1} in the temperature ranges of 200–300 K. These effects are interpreted in terms of excited state intramolecular proton transfer (ESIPT) and creation of tautomeric form of 2M6M. Below 200 K we see the appearance of an emission which can be attributed to a dimeric form.

Słowa kluczowe

Alkylamino-4-nitro pyridine N-oxides, X-ray structure, Excited state intramolecular proton transfer, DFT calculations

Adres publiczny

<https://doi.org/10.1016/j.molstruc.2008.10.029>

Strona internetowa wydawcy

<http://www.elsevier.com>

Artykuł

Plik został wygenerowany dnia 2026-10-05 01:24:35

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/qGjpP3F>.