

Ultrafast excited-state dynamics of a cyano-substituted "Proton sponge".

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Rok wydania

2015

Czasopismo

Journal of Physical Chemistry
A

Numer woluminu

119

Strony

11233-11240

DOI

10.1021/acs.jpca.5b06631

Kolekcja

Naukowa

Język

Angielski

Streszczenie

The dynamics of a substituted proton sponge—the 1,8-bis(dimethylamino)-4-cyanonaphthalene (DMAN-CN) molecule—was investigated after excitation in the S_1 state. Experimental and theoretical information are reported. The former includes absorption, fluorescence, and time-resolved transient absorption spectra, which were recorded in solution. Real-time dynamics measurements were also performed on gas-phase isolated DMAN-CN. TD DFT/6-31G(d,p) level and CIS/6-31G(d,p) excited-state calculations complement these results. This has allowed revisiting the energy transfer process between a locally excited (LE) and a charge transfer (CT) state, which is often invoked with this kind of molecule.

Adres publiczny

<http://dx.doi.org/10.1021/acs.jpca.5b06631>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>

Artykuł

Plik został wygenerowany dnia 2026-08-23 04:39:14

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/Ycy41t9>.