

Crystal structure, spectroscopic and DFT studies on *E* and *Z* isomers of ethyl 2-(2,3-dioxo-2,3-dihydro-1*H*-indol-1-yl)-3-phenyl-2-propenoate.

Autorzy

Ali Ramazani
Masooma Sheikh
Hamideh Ahankar
Morteza Rouhani
Sang Woo Joo
Katarzyna Ślepokura
Tadeusz Lis

Rok wydania

2017

Czasopismo

Journal of Chemical
Crystallography

Numer woluminu

47

Strony

198-207

DOI

10.1007/s10870-017-0697-8

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The crystal structures of two compounds, ethyl- (E)-2-(2,3-dioxo-2,3-dihydro-1*H*-indol-1-yl)-3-phenyl-2-propenoate and ethyl-(Z)-2-(2,3-dioxo-2,3-dihydro-1*H*-indol-1-yl)-3-phenyl-2-propenoate were determined from single-crystal X-ray diffraction and characterized by FT-IR, ¹H NMR and ¹³C NMR spectroscopy. The quantum theoretical calculations for two structures were performed by density functional theory (DFT/B3LYP/6-311+G*). From the optimized structure, geometric parameters were obtained and experimental measurements were compared with the calculated data. Frontier molecular orbitals, total density of states, molecular electrostatic potential, molecular properties, thermodynamic parameters and NBO analysis for *E* and *Z* isomers were investigated by theoretical calculations.

Słowa kluczowe

crystal structures, density functional theory, NBO analysis

Adres publiczny

<http://dx.doi.org/10.1007/s10870-017-0697-8>

Strona internetowa wydawcy

<http://link.springer.com>

Plik został wygenerowany dnia 2026-10-06 19:12:35

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