

Conformational properties and photochemistry of new allyl tetrazoles; matrix isolation FTIR and computational approach.

Autorzy

Magdalena Pagacz-
Kostrzewa

Małgorzata Mucha

Marek Weselski

Maria Wierzejewska

Rok wydania

2013

Czasopismo

Journal of Photochemistry
and Photobiology A-
Chemistry

Numer woluminu

251

Strony

118-127

DOI

10.1016/j.jphotochem.2012.10.023

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The photochemistry and molecular structure of 1-allyltetrazole (1-ALT) and 2-allyltetrazole (2-ALT) were studied in argon matrices by infrared spectroscopy and B3LYP/6-311++G(2d,2p) calculations. Both allyltetrazoles were found to possess three stable conformers (1-ALT1, 1-ALT2, 1-ALT3 and 2-ALT1, 2-ALT2, 2-ALT3) differing in the orientation of the allyl group relative to the ring. Matrix isolation technique together with the annealing experiments allowed for detection of all 1-ALT and 2-ALT conformers. A conformational cooling phenomenon was observed for the 1-ALT3 → 1-ALT1 process in agreement with the predicted low energy barrier of 4.84 kJ mol⁻¹ for this reaction. The broad-band UV irradiation of 1-ALT/Ar and 2-ALT/Ar matrices led to the same photoproducts. The main product N-allylcarbodiimide (P1) and two minor photoproducts allylcyanamide (P2) and C-allylnitrilimine (P3) are formed through the tetrazole ring cleavage and N2 elimination. None of these molecules have been described before.

Słowa kluczowe

allylcarbodiimide colling, DFT, Conformational cooling,
allylcyanamide

Adres publiczny

<http://dx.doi.org/10.1016/j.jphotochem.2012.10.023>

Strona internetowa wydawcy

<http://www.elsevier.com>