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

allylcarbodimide 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