

UV-tunable laser induced phototransformations of matrix isolated anethole.

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Streszczenie

A matrix isolation study of the infrared spectra and structure of anethole (1-methoxy-4-(1-propenyl)benzene) has been carried out, showing the presence of two *E* conformers (AE1, AE2) of the molecule in the as-deposited matrices. Irradiation using ultraviolet-tunable laser light at 308–307 nm induced conformationally selective phototransformations of these forms into two less stable *Z* conformers (AZ1, AZ2). The back reactions were also detected upon irradiation at 301 nm. On the whole, the obtained results allow for full assignment of the infrared spectra of all the four experimentally observed anethole isomers and showed that the narrowband UV-induced *E-Z* photoisomerization is an efficient and selective way to interconvert the two isomers of anethole into each other, with conformational discrimination. Photolysis of anethole was observed as well, with initial methoxyl O–C bond cleavage and formation of CH₃ and *p*-propenylphenoxy (AR) radicals, followed by radical recombination to form 2-methyl-4-propenyl-2,4-cyclohexadienone, which subsequently undergoes ring-opening generating several conformers of long-chain conjugated ketenes. Interpretation of the experimental observations was supported by density functional theory (B3LYP and B2PLYPD) calculations.

Adres publiczny

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