

Structure and photochemistry of the methanol complexes with methylglyoxal and diacetyl: FTIR matrix isolation and theoretical study.

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Streszczenie

The FTIR spectra of the argon matrices doped with methanol and methylglyoxal or diacetyl have been studied. The matrices were irradiated with the output of medium pressure mercury lamp. The spectra analysis indicate the presence of hydrogen bonded complexes between methanol and α -dicarbonyl in solid argon. The structures of the complexes are established by the ab initio MP2/6-311++G(2d,2p) calculations. Methylglyoxal in solid argon subjected to $\lambda \geq 395$ nm radiation photodissociates mostly into carbon monoxide and methane but when it is exposed to the full output of mercury lamp acetaldehyde and carbon monoxide are the main photodissociation products. Irradiation of the methylglyoxal–methanol complex leads to its photo-conversion into the methylhydroxyketene–methanol complex.

Słowa kluczowe

Matrix isolation, Infrared spectra, Photochemistry, Hydrogen bond, Methylglyoxal, Diacetyl

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