

Carboxylic group and its tetrazolyl isostere in one molecule. Matrix isolation FTIR and DFT studies on thermal decomposition and photochemistry of (tetrazol-5-yl)acetic acid.

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Streszczenie

The title compound (tetrazol-5-yl)acetic acid (TA) is an interesting molecule that contains both a carboxylic group and its isostere tetrazolyl group. Out of nine theoretically predicted stable structures of TA, three appeared to be present in solid argon. Thermal decomposition of the species aided by water molecules was studied in detail both experimentally using FTIR matrix isolation technique and theoretically at the B3LYP/6-311++G(2d,2p) level. Experimentally, it was found that the decarboxylation process appeared at the presence of water traces in the system. Theoretically, it was shown that the energy barrier of the water assisted process was lower by ca. 30 kJ mol⁻¹ comparing to the process without water participation. The UV photolysis of the TA/Ar system was studied using both broad-band and narrow-band sources. The main photoproducts appeared to be carbodiimidylacetic acid and (1*H*-diaziren-3-yl)acetic acid. The progress of the reactions induced was followed by FTIR spectroscopy, whereas interpretation of the results was supported by quantum chemical calculations (DFT, TD-DFT).

Adres publiczny

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<https://www.acs.org/content/acs/en.html>