

Structure and photochemistry of nitrous acid-methanethiol complexes in solid argon.

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Streszczenie

The products formed in the CH₃SH/HONO/Ar matrices after their deposition and after irradiation with $\lambda > 345$ nm have been studied by FTIR spectroscopy and DFT/B3LYP/aug-cc-pVTZ method. The spectra recorded directly after matrix deposition indicated formation of the CH₃SH...HONO complexes stabilized by the OH...S bond. The irradiation of the matrices produced CH₃SNO...H₂O complexes. In more concentrated matrices the CH₃SSCH₃, (NO)₂, and N₂O photoproducts were also detected. The presence of both dopants: CH₃SH and HONO was essential in the formation of (NO)₂ and N₂O in the studied systems. The reactions leading to photoproducts are proposed. The structures of the complexes present in the studied matrices, CH₃SH...HONO and CH₃SNO...H₂O, are discussed on the basis of comparison of their theoretical spectra with the experimental ones.

Słowa kluczowe

Hydrogen bond, molecular complexes, photochemistry, Matrix isolation, theoretical calculations, methanethiol

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