

Structural and FTIR spectroscopic studies of matrix-isolated 3-thio-1,2,4-triazole complexes with dinitrogen. First experimental evidence for the UV-induced formation of thiol...N₂ complexes

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Complexes of 3-thio-1,2,4-triazole (ST) with N₂ were studied theoretically by the B3LYP-D3 method and experimentally by FTIR spectroscopy combined with the matrix isolation technique and UV laser irradiation. The computational results show that ST interacts specifically with dinitrogen in several different ways. For the 1:1 complexes of the most abundant ST thione tautomer, three stable minima have been located on the potential energy surface. The two most stable structures, containing both the N-H...N hydrogen bond and the S...N van der Waals contact, were detected experimentally in the argon matrix after deposition. Interestingly, it was found that laser irradiation at $\lambda = 270$ nm, apart from generating the thiol tautomer of ST, also leads to the formation of its corresponding complexes, characterized by N-H...N hydrogen bonds. What is more, it appeared that the efficiency of hydrogen atom transfer in ST complexed with N₂ is lower than in the monomeric form.

Słowa kluczowe

Azole, Thione, Hydrogen bond, Van der Waals interactions, Phototautomerization, DFT

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