

Theoretical study of hydrogen bonded complexes of dimethyl disulfide or dimethyl peroxide with nitric acid.

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Streszczenie

Ab initio and DFT calculations performed on the title systems revealed two types of structures for both DMDS–HNO₃ and DMDO–HNO₃ complexes. In both structures two hydrogen bonds are formed between the OH group interacting with one of sulfur (or oxygen) atoms and methyl CH group being a proton donor to one of the oxygen atoms of the NO₂ group of nitric acid. Depending on the location of the interacting methyl group with respect to the S or O acceptor of the main O–H···S(O) bond, the seven or eight-membered ring structures are formed. For all the structures, the most pronounced changes in geometric parameters upon interaction are observed for the proton donor molecule. The calculated binding energies are between –20.86 and –29.95 kJ/mol at MP2 and between –17.52 and –27.47 kJ/mol at B3LYP using the 6-311++G(2d,2p) basis set. The complexes involving disulfide are slightly weaker by ca. 6.7–8.6 kJ/mol than the corresponding peroxide complexes. The performed NBO analysis reveals that the charge transferred to σ*(OH) orbital of the nitric acid molecule comes mainly from the high p-character lone pair orbital of sulfur or oxygen atom being the hydrogen bond acceptor site in the disulfide or peroxide molecule.

Słowa kluczowe

Hydrogen bonded complexes, Dimethyl disulfide, Dimethyl peroxide, Nitric acid

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