Are hydrogen bonds to sulfur and oxygen different? Theoretical study of dimethylsulfide and dimethylether complexes with nitric acid.

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Ab initio and DFT calculations have been performed on the $(CH_3)_2S–HNO_3$ and $(CH_3)_2O–HNO_3$ systems. The results are discussed and compared for these complexes considering both structural and energetic consequences of the hydrogen bonding. Vibrational parameters are also presented and compared to the available experimental data.

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