

The hydroperoxy radical as a hydrogen bond acceptor. HOO–HCl complexes—*ab initio* study.

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Streszczenie

Protonacceptor properties of the HOO radical were investigated previously by means of *ab initio* as well as topological Atoms in Molecules (AIM) and Electron Localization Function (ELF) methods. It was pointed out that in the radical there are three nonequivalent positions most susceptible to protonation, and on this basis three structures of possible hydrogen bonded complexes were proposed. Results reported in the present article concern all possible 1:1 complexes formed by HCl and HOO molecules, and fully confirm suppositions given on the basis of the above-mentioned investigations. There are three various complexes referring to the local minima, and the transition structure predicted by topological methods has been found as well. The cyclic structure appeared to be the most stable one, which confirms conclusions given in the experimental article. Apart from structure optimization, harmonic as well as anharmonic spectra of the complexes have been simulated. Anharmonicity of H–Cl stretching vibration was of special interest, as the frequency of this vibration characterizes the Cl–H · · · O hydrogen bond in these complexes. To obtain values of these frequencies the one-dimensional Hamiltonian has been diagonalized numerically. The potential for this Hamiltonian has been taken from a set of single-point scanning of the part of the Potential Energy Surface (PES) connected with this vibration. The potential calculated on the MP2 level leads to the result close to the experimental value, whereas the B3LYP method is inappropriate for the purpose of PES investigation of these complexes

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