

The examination of the hydroperoxy radical and its closed-shell "analogues" by means of topological methods of quantum chemistry: AIM and ELF.

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Streszczenie

This paper analyses the properties of the HOO radical as well as the HOF and the HOOH molecule by means of topological methods. The data describing the O–O and the O–F bonds are not typical for covalent bonds. These bonds should be classified as “covalent depleted”. The places were found in the analysed molecules which could be susceptible to protonation. In particular, in the HOO molecule there are three non-equivalent positions susceptible to the protonation. The results prompted certain conclusions concerning the geometrical parameters of protonated molecules, which are important for the future investigations of hydrogen bonded complexes between these molecules and proton-donors.

Słowa kluczowe

Peroxy radical, ELF, AIM, Molecular bonding, Lone pairs

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