On three-electron bonds and hydrogen bonds in the open-shell complexes. $[H_2X_2]^+$ for X= F, Cl and Br.

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Streszczenie

The $[H_2X_2]^+$ (X = Cl, Br) formula could refer to two possible stable structures, namely, the hydrogen-bonded complex and the three-electron-bonded one. In contrary to the results published by other authors, we claim that for the F-type structures the hydrogen-bonded form is the only possible one and the $[HFFH]^+$ complex is an artifact as its wave function is unstable. For all analyzed molecules, the IR anharmonic spectra have been simulated, which enabled a deeper analysis of other authors' published results of IR low-temperature matrix experiments. Topological atoms in molecules and electron localization function investigations have revealed that the nature of the bond in three-electron-bonded structures is similar to the covalent-depleted one in F_2 or HOO molecules, but the effect of removing electrons from the bond area is stronger.

Słowa kluczowe

Chemical structure, Noncovalent interactions, Electron density, Chemical calculations, molecules

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