



Effects of xenon insertion into hydrogen bromide. Comparison of the electronic structure of the $\text{HBr}\cdots\text{CO}_2$ and $\text{HXeBr}\cdots\text{CO}_2$ complexes using quantum chemical topology methods: electron localization function, atoms in molecules and symmetry adapted perturbation theory.

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Streszczenie

Quantum chemistry methods have been applied to study the influence of the Xe atom inserted into the hydrogen–bromine bond ($\text{HBr} \rightarrow \text{HXeBr}$), particularly on the nature of atomic interactions in the $\text{HBr}\cdots\text{CO}_2$ and $\text{HXeBr}\cdots\text{CO}_2$ complexes. Detailed analysis of the nature of chemical bonds has been carried out using topological analysis of the electron localization function, while topological analysis of electron density was used to gain insight into the nature of weak nonbonding interactions. Symmetry-adapted perturbation theory within the orbital approach was applied for greater understanding of the physical contributions to the total interaction energy.

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